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Existing Substances Program

Canadian Environmental Protection Act, 1999 – CEPA 1999



Canadian Environmental Protection Act, 1999

Draft Ecological Screening Assessment Report on
4,6-dinitro-o-cresol (DNOC)

July 2006

Canada

4,6-Dinitro-*o*-cresol (DNOC)

CAS No. 534-52-1

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that meet the categorization criteria set out in the Act and Regulations to determine, in an expeditious manner, whether substances present or may present a risk to the environment or to human health. Based on the results of a screening assessment, the Ministers can propose taking no further action with respect to the substance, adding the substance to the Priority Substances List (PSL) for further assessment or recommending that the substance be added to the List of Toxic Substances in Schedule 1 and, where applicable, the implementation of virtual elimination.

A screening assessment involves an evaluation of a substance to determine whether the substance is “toxic” or capable of becoming “toxic” as defined in CEPA 1999. This ecological screening assessment examines various supporting information and develops conclusions based on a weight of evidence approach as specified under Section 76.1 of CEPA 1999. The screening assessment report does not present an exhaustive review of all available data; rather, it presents the most critical studies and lines of evidence supporting the conclusions. One line of evidence includes consideration of risk quotients to identify potential for ecological effects. However, other concerns that affect current or potential risk, such as persistence, bioaccumulation, chemical transformation and trends in ambient concentrations, are also considered.

4,6-Dinitro-*o*-cresol (DNOC) was included in a pilot project of 123 substances for screening assessment under CEPA 1999, on the basis of its anticipated high potential for human exposure. DNOC is also considered to be persistent and inherently toxic to aquatic organisms.

Data relevant to the ecological screening assessment of DNOC were identified in original literature, review documents and commercial and government databases. Searches were conducted of the open literature, conference proceedings and the Internet for relevant information. Data obtained as of August 2004 were considered in this document. Original studies that form the basis for determining whether the substance is “toxic” under CEPA 1999 have been critically evaluated by Environment Canada. The data from key toxicity studies were evaluated using Robust Study Summary forms similar to those recommended by the Organisation for Economic Co-operation and Development for the evaluation of studies for the Screening Information Data Sets of high production volume substances (OECD, 2003).

This ecological screening assessment report and associated unpublished supporting working documentation were written by Environment Canada evaluators under the lead of Barbara Elliott. The substance matter in this report has been subjected to a science review by

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individuals having relevant technical expertise, including Pierrette Blanchard (Meteorological Service of Canada, Environment Canada), Mark McMaster (National Water Research Institute, Environment Canada) and Suzanne Lesage (National Water Research Institute, Environment Canada).

The conclusions of the ecological and human health screening assessment reports were approved by the joint Environment Canada/Health Canada CEPA Management Committee. The supporting working documentation for the ecological assessment is available upon request by e-mail from existing.substances.existantes@ec.gc.ca. The supporting working documentation for the human health assessment is available upon request by e-mail from ExSD@hc-sc.gc.ca. Information on ecological and human health screening assessments under CEPA 1999 may be linked from the CEPA Registry at <http://www.ec.gc.ca/ceparegistry>.

The critical information and considerations upon which the assessment is based are summarized below.

Properties of DNOC

DNOC (CAS No. 534-52-1) is a yellow crystalline solid at ambient temperature (U.S. EPA, 1986a). It is also referred to as 2,4-dinitro-6-methylphenol; phenol, 2-methyl-4,6-dinitro-; 3,5-dinitro-2-hydroxytoluene; 4,6-dinitro-2-methylphenol; 6-methyl-2,4-dinitrophenol; Antinonin; Antinonnin; Arborol; Degrassan; Dekrysil; Detal; Dillex; and Kreozan.

Physical and chemical properties of DNOC, both measured and predicted, are presented in Table 1.

Table 1: Physical and chemical properties of DNOC

	Measured		Predicted	
	Value	References ¹	Value	Model
Molecular formula	C ₇ H ₆ N ₂ O ₅	1		
Molecular mass	198.1348	1		
Melting point (°C)	86.6	2	121.23	EPIWIN (v. 3.11)
	85.8	3	87.0	ASTER
Boiling point (°C)	378	2	344.23	EPIWIN (v. 3.11)
	220	3	401.38	MMP (v. 1.44)
			364	ASTER
Density (g/cm ³)	1.58 at 20°C	4	2.147 931	MMP (v. 1.40)
Vapour pressure (Pa)	4.31 × 10 ⁻² at 20°C	4	7.3 × 10 ⁻⁴	EPIWIN (v. 3.10)
	1.40 × 10 ⁻² at 25°C	4	7.4 × 10 ⁻⁸	MMP (v. 1.44)
	4.79 × 10 ⁻² at 35°C	5	1.4 × 10 ⁻⁴	ASTER
	1.6 × 10 ⁻² at 25°C	6		
Henry's law constant (Pa·m ³ /mol)	1.4 × 10 ⁻¹ at 25°C	4	3.09 × 10 ⁻³	EPIWIN (v. 3.11) Bond method
			4.94 × 10 ⁻⁶	EPIWIN (v. 3.11) Group method
			6.49 × 10 ⁻⁵	EPIWIN (v. 3.11) EPI method
			4.3 × 10 ⁻² at 20°C	SRC CHEMFATE Database

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	Measured		Predicted	
	Value	References ¹	Value	Model
Octanol/water partition coefficient (log K _{ow})	2.564	4	2.27	EPIWIN (v. 3.11)
	2.12 (neutral species)	7	1.91	PALLAS (v. 4.0)
	1.78 at pH 4	8	2.130	ClogP (v. 3.3)
	0.087 at pH 7	8	1.61	Hansch (MMP v. 1.44)
	1.32 at pH 10	8	2.1366	Ghose (MMP v. 1.44)
			2.29	ASTER
			1.809	TOPKAT (v. 6.1)
Water solubility (mg/L)	1000 at 15°C	1	691.9	EPIWIN (v. 3.11)
	198 at 20°C	7	467.3	EPIWIN (v. 3.11)
	21.3 at pH 4	8	48 875.4	MMP (v. 1.44)
	694 at pH 7	8		
	3300 at pH10	8		
	100 000 (DNOC Na salt)	9		
Other solubilities (g/g)	4.3/100 (ethanol)	6		
	100/100 (acetone)	6		
	37/100 (benzene)	6		
Organic carbon/water partition coefficient (log K _{oc})	2.35–2.77	5	2.779	EPIWIN (v. 3.11)
	2.564	4	2.58	ASTER
	1.3 (DNOC Na salt)	9		
Solid/water distribution ratio (K _d)	<5 (loam soil with organic matter of 0.8–3%)	10		
	1.93	11		
pKa	4.4	4	4.32	PALLAS (v. 4.0)
	4.31	2		
Air/water partition coefficient (K _{aw})	3.0 × 10 ⁻⁵ at 25°C	12		

¹ References:

1. ChemFinder
2. SRC PhyProp Database
3. Verschueren, 2001
4. HSDB
5. ATSDR, 1995
6. IPCS, 2000
7. Schwarzenbach *et al.*, 1988
8. UNEP/FAO, 2002
9. Vogue *et al.*, 1994
10. U.S. EPA, 1989
11. Jafvert, 1990
12. Schwarzenbach *et al.*, 2003

Scope of Assessment

Owing to the chemical nature of DNOC, it readily forms water-soluble sodium, potassium and ammonium salts, and virtually 100% of dissolved DNOC will be in the ionized form at environmentally relevant pHs (pH 6–8). Based on this information, Environment Canada reviewed the use of DNOC salts to determine if they should also be included in this screening

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assessment. The sodium, potassium and ammonium salts of DNOC are not on the Domestic Substances List (DSL), although DNOC sodium salt is on the Non-Domestic Substances List (NDSL). If a company were intending to manufacture or import these substances, they would be considered to be new to Canada and subject to notification under the New Substances Notification Regulations. Therefore, the ecological screening assessment focused on the uses of DNOC, but a review of the fate and effects of its salts was also carried out.

DNOC used to be registered as a pesticide under the *Pest Control Products Act* (PCPA); however, its registration was discontinued in December 1990. Three of the DNOC salts (sodium, ammonium and potassium) have been used as pesticides internationally but were never registered under the PCPA in Canada.

Manufacture, Importation and Use of DNOC

Globally, DNOC is used mainly in the plastics industry as an inhibitor of polymerization in styrene and aromatic vinyl products; it is also used as an intermediate in the synthesis of fungicides, dyes and pharmaceuticals (IPCS, 2000; UNEP/FAO, 2002).

Two Canadian companies reported manufacture or import of DNOC in 1986, with amounts in the range of 100–1000 tonnes (Environment Canada, 1990). Historically, DNOC was used in Canada as an antioxidant, corrosion inhibitor, tarnish inhibitor and antiscaling agent, for a total of 99.9% of the Canadian market (Environment Canada, 1990).

An industry survey conducted by Environment Canada resulted in use pattern information for the year 2000 (Environment Canada, 2003a). Under Section 71 of CEPA 1999, this Notice with Respect to Certain Substances on the Domestic Substances List applied to any person who, during the 2000 calendar year, manufactured or imported DNOC, whether alone or in a mixture or in a product, in a total quantity greater than 10 000 kg. The survey indicated that DNOC is not manufactured in Canada; however, between 100 and 1000 tonnes of DNOC were imported in 2000 (Environment Canada, 2003a).

Releases of DNOC

Only one company, located on the St. Clair River near Sarnia, Ontario, reported releases of DNOC to the National Pollutant Release Inventory (NPRI) (Environment Canada, 2003b). Although the facility reported only off-site transfers and no releases to water, air or soil, it was used to develop a conservative scenario to estimate the quantity of DNOC that could be released into the St. Clair River from such a site. It is assumed, in a conservative scenario, that one customer is receiving the total annual import quantity (100–1000 tonnes). The scenario assumes releases of 0.2% of the annual import quantity of DNOC into the St. Clair River, which, based on professional judgement, recognizes routine process losses and waste from equipment cleaning for a substance handled in bulk. This accounts for releases to solid waste and wastewater. Using this percentage results in an estimated annual release of 200–2000 kg. It is further assumed that DNOC is in use throughout the year and that there is continuous release (24 hours per day) over

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the year (350 operating days). Daily releases over a period of 350 days correspond to approximately 0.57–5.7 kg/day. Sewage treatment plant (STP) removal rates were also considered. The STP model (CEMC, 2001) estimated that 27% of DNOC would be removed and that 73% would enter the environment in the form of final wastewater effluent from an STP.

Two main sources of atmospheric nitrophenols (a category that includes DNOC) have been reported in the literature. These include secondary formation by reactions in the troposphere and emissions from automobiles. Researchers have examined the atmospheric occurrence and formation of DNOC (Nojima *et al.*, 1976; Alber *et al.*, 1989; Richartz *et al.*, 1990). DNOC has been shown to form as a secondary pollutant via the reaction of toluene and 2-methylphenol with nitrogen monoxide and hydroxyl radicals. It is difficult to estimate the quantity that may result from the anthropogenic release of precursor species. Direct emission of DNOC from car exhaust is likely only of minor importance. Under experimental conditions, exhaust from an automobile motor was found to contain DNOC at <0.01 ng/m³ (Trempe *et al.*, 1993).

Disposal of DNOC

The NPRI (Environment Canada, 2003b) reported that amounts of up to 2 tonnes of DNOC and its salts were annually “transferred for disposal” by Nova Chemicals (Table 2). For all years before 2002, the methods of treatment were biological, such as biooxidation, and incineration or thermal. For the year 2002, disposal was to a landfill.

Table 2: NPRI data for DNOC and its salts (all reporting is for the Nova Chemicals plant in Sarnia, Ontario)

Year	Transfers for disposal (tonnes)	Biological treatment (tonnes)	Incineration (tonnes)	Landfill (tonnes)
2002	1.49			1.49
2001	0.01	0.01		
2000	0.25	0.03	0.22	
1999	0.02	0.02		
1998	0.68	0.04	0.64	
1997	0.36	0.06	0.3	
1996	2.00	0.08	1.92	
1995	0.03	0.03		
1994	0.04	0.04		

Environmental Fate and Partitioning

Environmental fate analysis integrates information on the chemical behaviour of the substance with the properties of the receiving environment. The objective of fate analysis is to determine the multimedia distribution of the substance after its release into the environment. This includes consideration of the persistence and bioaccumulation of the substance in the environment.

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Level III fugacity modelling (CEMC, 2002) predicts the following fate for DNOC (estimated for the neutral form of DNOC) released into different media:

- With releases solely to water (as would be expected from the stated use), the majority of DNOC would remain in water (99%), with a minor amount partitioning to sediments (1%). Loss of the substance from the aquatic environment at steady state will be mainly a result of transport (~55% advection) out of the “unit world” and degradation (~45%).
- With emissions solely to air, the majority of DNOC would partition to soil (91%) and water (7%).
- With releases solely to soil, the majority of DNOC would remain in soil (98%), with some transfer to water (2%).

The following information was considered in evaluating whether DNOC meets the criteria for persistence and bioaccumulation as defined under the *Persistence and Bioaccumulation Regulations* of CEPA 1999:

- *Persistence:*
 - a) in air, estimated half-life of 8 hours to 129 days (U.S. EPA, 1986b; Atkinson, 1987; Howard *et al.*, 1991);
 - b) in surface water, half-life ranges from 3 to 5 weeks (Mill and Mabey, 1985; Kelly *et al.*, 1994; IPCS, 2000);
 - c) in sediments, half-life is estimated to be 150 days (EPI version 3.11);
 - d) in soil, half-life ranges from 14 hours to less than 2 months (Callahan *et al.*, 1979; HSDB).
- *Bioaccumulation:*
 - a) bioaccumulation factor (BAF) of 25 calculated for DNOC (Gobas and Arnot, 2003).

Persistence criteria are half-lives of greater than or equal to 2, 182, 365 and 182 days for air, water, sediment and soil, respectively.

Bioaccumulation criteria are BAFs or bioconcentration factors (BCFs) of greater than or equal to 5000 or a log K_{ow} of greater than or equal to 5.0.

Based on the *Persistence and Bioaccumulation Regulations*, DNOC is persistent in air and not bioaccumulative.

Environmental Concentrations

Atmosphere and Precipitation

No monitoring data for DNOC in the atmosphere or precipitation in Canada were identified. Monitoring data from other countries are summarized in Table 3.

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Table 3: Concentrations of DNOC in the atmosphere and precipitation

Location	Sampling period	No. of samples	Detection limit ¹ (µg/L)	Mean concentration (µg/L) ²	Reference
Denmark	October–November 2001	5	ns	[0.07–3.2 ng/m ³]	Bossi and Andersen, 2003
The Netherlands	2000–2001	18	ns	>0.1	Duyzer and Vonk, 2002
Italy, Milan	November 1998	12	ns	[600–7200], rainwater	Belloli <i>et al.</i> , 2000
Germany, Bavaria, rainwater	1995–1998	ns	ns	[0.1–2.4] (approximated from graph)	Schüssler and Nitschke, 2001
Germany, Bavaria	July 1998 – March 1999	>100	ns	3.4 [0.5–4.2], fogwater	Römpp <i>et al.</i> , 2001
Germany, Hanover, rain and snow	1988	ns	0.1–1.0	Qualitatively identified	Alber <i>et al.</i> , 1989
England, Great Dun Fell	April–May 1993	6	ns	0.7 [0.26–2.13], cloudwater	Lüttke and Levsen, 1997
Germany, Mount Brocken	June 1994	6	ns	4.2 [0.1–10], cloudwater	Lüttke <i>et al.</i> , 1999
Switzerland, Dübendorf, rain sample and ambient air	March–November 1985	3	ns	0.05 µg/m ³ , ambient air [0.95–1.6 µg/L], rain	Leuenberger <i>et al.</i> , 1988

¹ ns = not specified.

² Unless otherwise specified. The range of values is indicated in square brackets, if available (e.g. [minimum–maximum]).

DNOC has been detected in atmospheric air and precipitation at a number of locations in Europe, and the presence of nitrated phenols in rain is not explained solely by input from pesticide applications (Leuenberger *et al.*, 1988). DNOC has been shown to partition favourably from the gas phase into the aqueous phase, and it is not surprising that the substance has been found in rainwater (Schwarzenbach *et al.*, 2003). DNOC was detected in Denmark, even though the substance has not been used for the last 10 years (Danish Environmental Protection Agency, 2001). The concentrations found in rain in Denmark are of the same order of magnitude as have been detected in England, Germany and Switzerland.

As no atmospheric or precipitation monitoring data for DNOC in Canada could be located, a series of release scenarios were developed to estimate the amount of DNOC that could be released into receiving waters in Canada as a result of rainfall scavenging of DNOC in the atmosphere. The scenarios incorporated precipitation data for 12 Canadian cities, an estimate of the amount of DNOC in rainwater and a calculation of runoff from built-up and natural areas into the receiving STPs. It was assumed that the rain event that would result in DNOC being removed from the atmosphere would be a heavy rainfall and that DNOC would be washed out in the early stages of the rain event and not over the length of the rainfall. The concentration of DNOC used in the scenario is based on precipitation values from Europe that were considered realistic possible levels of DNOC in air in Canada. The mean concentration of DNOC in cloudwater from

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northern Germany (4.2 µg/L) was selected. It was assumed that rainwater would be released as a point source from an STP, but that it would not undergo STP treatment, as STP removal efficiency during a storm event is likely to be poor. The highest concentrations of DNOC were estimated in receiving waters from the STPs in London, Ontario (0.0023 mg/L), Guelph, Ontario (0.0023 mg/L), and Granby, Quebec (0.0025 mg/L).

Aquatic Concentrations

No recent aquatic monitoring data for DNOC in Canada were identified. Older data on levels of DNOC in Canadian waters as well as in other countries are summarized in Table 4.

Table 4: Concentrations of DNOC in surface water

Location	Sampling period ¹	No. of samples ¹	Detection limit ¹ (µg/L)	Mean concentration ^{1,2} (µg/L)	Reference
Italy, River Po	January 1994 – December 1996	ns (samples were taken at 15-day intervals during the sampling period)	0.1	nd	Davi and Gnudi, 1999
Germany, Elbe River	1994	ns	0.05	[ns– 0.06]	Pietsch <i>et al.</i> , 1995
Denmark, Hølvads Rende area, soil water, drainage water, stream water	October 1989 – December 1991	ns	ns	0.005 (soil water) nd (drainage water) [0.02–0.16] (stream water)	Mogensen and Spliid, 1995
Denmark, Bolbo Bæk area, soil water, stream water	April 1990 – December 1991	ns	ns	0.005 (soil water) 0.16 (stream water)	Mogensen and Spliid, 1995
Denmark, four ponds	November 1989 – December 1990	ns	ns	[nd–0.64]	Mogensen and Spliid, 1995
The Netherlands, Meuse River and Rhine River; Slovakia, Danube River and Nitra River	ns	4	0.4	nd	Brouwer and Brinkman, 1994
Germany, Bavaria, Mount Ochsenkopf and University of Bayreuth campus	Fall 1988	ns	1.98	[nd–12.5]	Richartz <i>et al.</i> , 1990
Point source					
Ontario, St. Clair River near Sarnia (industrial area)	1979	24	1	[nd–10]	Munro <i>et al.</i> , 1985

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Location	Sampling period ¹	No. of samples ¹	Detection limit ¹ (µg/L)	Mean concentration ^{1,2} (µg/L)	Reference
Ontario, St. Clair River near Sarnia (industrial area)	1980	25	1	nd	Munro <i>et al.</i> , 1985
Ontario, St. Clair River near Sarnia, industrial effluent, process/sewer water, township ditch water ³	1979	119	1	[nd–10 000]	Munro <i>et al.</i> , 1985
Ontario, St. Clair River near Sarnia, industrial effluent, process/sewer water, township ditch water ³	1980	61	1	nd	Munro <i>et al.</i> , 1985
United States, California groundwater	ns	ns	ns	ns–35	Hallberg, 1989
Italy, Taranto, surface seawater contaminated by oil refinery or iron and steel factory wastes	ns	2	0.017	[0.030–0.065]	Cardellicchio <i>et al.</i> , 1997
Unspecified location, oil refinery effluent, paper mill effluent	ns	ns	0.5	nd	Paterson <i>et al.</i> , 1996

¹ ns = not specified; nd = not detected.

² The range of values is indicated in square brackets, if available (e.g., [minimum–maximum]).

³ Mean concentration in effluent is presented as an indication of resulting exposure. This value was not included in the section on releases of DNOC, as details on effluent quantities and release rate were not provided.

As no recent Canadian surface water monitoring data were identified, aquatic exposure estimates were modelled. The scenario uses the ChemSim model (Environment Canada, 2003c) to predict estimated exposure values. ChemSim model runs were done for three river flow estimates and two loading rates (calculated in the section on releases of DNOC), for a total of six model runs. As indicated in the release scenario, it is assumed that DNOC is in use throughout the year and that there is continuous release (24 hours per day) over the year (350 operating days). Two estimates of low river flow (2.5th and 10th percentiles) were selected to derive Estimated Exposure Values (EEVs) under low-flow conditions. The 50th-percentile flow value was also selected to estimate EEVs under more typical conditions. The maximum concentration of DNOC at 20 m downstream of the reporting facility with a worst-case scenario release of 5.7 kg/day and a 2.5th-percentile river flow is estimated to be less than 0.006 mg/L. If STP treatment is considered, an EEV of 0.0014 mg/L is estimated.

Sediment, Sewage Sludge and Soil

Monitored soil, sediment and sludge concentrations of DNOC are summarized in Table 5. The high flow and velocity of the St. Clair River rapidly dilute and disperse the substance.

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Therefore, loadings of DNOC do not appear likely to cause significant exposure to benthic organisms, as only a minor amount of DNOC is expected to partition to sediments (1%). Based on the results of modelling, at a release rate of 5.7 kg/day, 0.057 kg/day (or 1%) would be available to be adsorbed onto sediments.

Table 5: Concentrations of DNOC in soil, sediment and sludge

Location	Sampling period ¹	No. of samples ¹	Detection limit ¹ (ng/g)	Mean concentration ^{1,2} (ng/g)	Reference
Ontario, old urban parkland soil	ns	60	100	Ontario typical range <W ³	OMEE, 1994
Ontario, rural parkland soil	ns	101	100	Ontario typical range <W ³	OMEE, 1994
Canada, agricultural soil	ns	30	50	nd	Webber, 1994
11 sites across Canada, sludge samples	September 1993 – February 1994	12 samples/site	ns	nd	Webber and Nichols, 1995
Sediment, artificial islands, Beaufort Sea	ns	ns	ns	<10 (dry weight)	Fowler and Hope, 1984
Canadian municipal sludges	1980–1985	15	ns	[1200–1500] (dry weight)	Webber and Lesage, 1989
Poland, Holy Cross mountains, soil	July 3–6, 1996	8	1	nd	Migaszewski, 1999
Italy, Taranto, sediment contaminated by oil refinery or iron and steel factory wastes	ns	2	ns	nd	Cardellicchio <i>et al.</i> , 1997

¹ ns = not specified; nd = not detected.

² The range of values is indicated in square brackets, if available (e.g., [minimum–maximum]).

³ <W is a qualifier, given to indicate that the sample may contain the analyte but the level would probably not exceed the laboratory method detection limit (MDL). W is approximately one-third to one-fifth of the MDL (OMEE, 1994).

DNOC was detected in 13% of Canadian municipal sludges sampled during the period 1980–1985 at concentrations ranging from 1200 to 1500 ng/g dry weight, with a median concentration of 1300 ng/g dry weight (Webber and Lesage, 1989). It was not detected (detection limit not stated) in sludge or sludge compost from various locations in Canada sampled in 1993–1994 (Webber and Nichols, 1995).

DNOC was not detected (method detection limit = 100 ng/g) in 101 samples of “rural parkland” soil or in 60 samples of “old urban parkland” soil in Ontario (OMEE, 1994). Similarly, DNOC was not detected (detection limit = 50 ng/g) in agricultural soil from various locations across Canada (Webber, 1994).

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DNOC was not detected in fish composites (detection limit not stated) from the United States (DeVault, 1985).

As indicated in the section on environmental fate and partitioning, DNOC has a relatively low bioaccumulation potential. However, as will be seen in the section on effects characterization, results of repeated oral dose toxicity studies indicate that mammals may be fairly sensitive to DNOC. Therefore, wildlife exposure to DNOC from food and water has been estimated.

An EEV for wildlife was estimated based on a calculation of the total daily intake of the substance by mink and otter. An energetics model based on the general exposure model for wildlife from the U.S. Environmental Protection Agency's (EPA) Exposure Factors Handbook (U.S. EPA, 1993) was used.

$$TDI = \left[FMR \left(\frac{C_i \cdot P_i}{GE_i \cdot AE_i} \right) \right] \cdot Pt$$

where:

- TDI = total daily intake (mg/kg-bw per day)
- FMR = normalized free metabolic rate of wildlife receptor of interest (250 kcal/kg-bw per day for mink and river otter)
- C_i = concentration of contaminant in the i th prey species (mg/kg-bw) (see below)
- P_i = proportion of the i th prey species in the diet (unitless) (default = 35% for mink; 100% for otter)
- GE_i = gross energy of the i th prey species (default = 850 kcal/kg-bw prey)
- AE_i = assimilation efficiency of the i th prey species by the wildlife receptor (default = 0.91)
- Pt = proportion of the time the receptor spends in the contaminated area (= 9% for mink and 0.06% for otter).

The model incorporated the metabolic rate of the wildlife receptors of interest (mink and otter), the proportion of food uptake by the receptors and the amount of time the animals spend in the contaminated area (St. Clair River), which is based on the typical habitat range of the wildlife receptors.

The concentration of the substance in a fish (C_i) must be estimated based on the highest EEV_{water} and a BAF. The BAF was estimated using the Modified Gobas Model (Gobas and Arnot, 2003). The BAF represents a benthic/pelagic food chain and estimates the accumulation from all sources in a mid-trophic-level fish that would typically be eaten by a mammalian piscivore.

$$C_i = EEV_{\text{water}} \cdot BAF$$

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where:

C_i = concentration in a prey fish (mg/kg-bw)
 EEV_{water} = EEV calculated for surface water (mg/L) (see section on aquatic concentrations)
 BAF = bioaccumulation factor for substance (L/kg) (see section on environmental fate and partitioning).

$$C_i = 0.0014 \cdot 25 = 0.035$$

The model estimated EEVs of 0.0004 mg/kg-bw per day and 0.000 007 mg/kg-bw per day for mink and otter, respectively.

Effects Characterization

Biotic Effects

Key studies of the toxicity of DNOC to organisms in different environmental media are presented in Tables 6 to 9. Studies primarily on the acute toxicity of DNOC to microorganisms, aquatic invertebrates, insects, terrestrial invertebrates and vertebrates were located in the literature. No acute or chronic marine toxicity data were identified.

Table 6: Toxicity of DNOC to aquatic organisms

Organism	Endpoint ¹	Concentration (mg/L)	Reference
Microorganisms			
Bacterium <i>Pseudomonas putida</i>	Toxic threshold, 16-hour EC ₃ (growth)	16	Bringmann and Kühn, 1980
Cyanobacterium <i>Microcystis aeruginosa</i>	Toxic threshold, 72-hour EC ₃ (growth)	0.15	Bringmann and Kühn, 1978
Green alga <i>Scenedesmus quadricauda</i>	Toxic threshold, 7-day EC ₃ (growth)	13	Bringmann and Kühn, 1980
Green alga <i>Scenedesmus subspicatus</i>	96-hour EC ₅₀ (biomass) 48-hour EC ₅₀ (growth rate)	6 12	Sewell <i>et al.</i> , 1995a Sewell <i>et al.</i> , 1995a
Protozoan <i>Entosiphon sulcatum</i>	Toxic threshold, 72-hour EC ₅ (growth)	5.4	Bringmann and Kühn, 1980
Protozoan <i>Chilomonas paramecium</i>	Toxic threshold, 72-hour EC ₅ (growth)	5.4	Bringmann and Kühn, 1981
Protozoan <i>Uronaemia parduezi</i>	Toxic threshold, 72-hour EC ₅ (growth)	0.012	Bringmann and Kühn, 1981
Aquatic plants			
<i>Lemna minor</i>	Specific growth rate, 7-day exposure	0.32	Sloof and Canton, 1983

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Organism	Endpoint ¹	Concentration (mg/L)	Reference
Aquatic invertebrates			
Water flea <i>Daphnia magna</i>	24-hour LC ₅₀	5.7	van der Hoeven, 1984
	14-day LC ₅₀	1.6	van der Hoeven, 1984
	14-day NOEC (reproduction)	0.6	van der Hoeven, 1984
	24-hour LC ₅₀	2.3	Kühn <i>et al.</i> , 1989
	24-hour NOEC (mortality)	1.5	Kühn <i>et al.</i> , 1989
	21-day NOEC (reproduction)	1.3	Kühn <i>et al.</i> , 1989
Water flea <i>Daphnia pulex</i>	48-hour EC ₅₀	0.145	Mayer and Ellersieck, 1986
	3-hour LC ₅₀ (DNOC sodium salt)	3.5	PAN, 2004
Scud <i>Gammarus fasciatus</i>	96-hour LC ₅₀	0.11	Mayer and Ellersieck, 1986
Insects			
<i>Pteronarcys californica</i>	96-hour LC ₅₀	0.32	Mayer and Ellersieck, 1986
Vertebrates (fish)			
Bluegill <i>Lepomis macrochirus</i>	96-hour LC ₅₀	0.95	Sewell <i>et al.</i> , 1995b
	96-hour LC ₅₀	0.36	Mayer and Ellersieck, 1986
Rainbow trout <i>Oncorhynchus mykiss</i>	96-hour LC ₅₀	0.45	Sewell <i>et al.</i> , 1995c
	96-hour NOEC	0.32	Sewell <i>et al.</i> , 1995c
	96-hour LC ₅₀	0.066	Mayer and Ellersieck, 1986
Atlantic salmon <i>Salmo salar</i>	96-hour LC ₅₀	0.20	Zitko <i>et al.</i> , 1976
Bluegill <i>Lepomis macrochirus</i>	96-hour LC ₅₀	0.23	Buccafusco <i>et al.</i> , 1981
Goldfish <i>Carassius auratus</i>	48-hour LC ₅₀ (DNOC sodium salt)	0.45	PAN, 2004
Common carp <i>Cyprinus carpio</i>	13-day NOEC (pH 6.9–9.0)	≤0.25	Ghillebaert <i>et al.</i> , 1995
	13-day NOEC (pH 7.8)	0.5–1.0	
	13-day NOEC (pH 9.0)	no effect	
Common mirror-coloured carp <i>Cyprinus carpio</i>	48-hour LC ₅₀ (DNOC sodium salt)	0.17	PAN, 2004
Medaka high eyes <i>Oryzias latipes</i>	48-hour LC ₅₀ (DNOC sodium salt)	0.20	PAN, 2004

¹ EC = effective concentration; LC₅₀ = median lethal concentration; NOEC = No-Observed-Effect Concentration.

Table 7: Acute toxicity of DNOC to terrestrial plants

Organism	Endpoint ¹	Concentration (mg/L)	Reference
Tobacco <i>Nicotiana glauca</i>	ED ₅₀	0.466	Strube <i>et al.</i> , 1991

¹ ED₅₀ = median effective dose.

Table 8: Acute toxicity of DNOC to terrestrial invertebrates

Organism	Endpoint	Concentration	Reference
Earthworm <i>Eisenia fetida</i>	7-day LC ₅₀	17 mg DNOC/kg of soil	van der Hoeven, 1992
	14-day LC ₅₀	15 mg DNOC/kg of soil	
	14-day NOEC	10 mg DNOC/kg of soil	

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Honey bees <i>Apis mellifera</i>	LD ₅₀ (oral) LD ₅₀ (contact)	2.04 ± 0.25 µg DNOC/bee 406 ± 27µg DNOC/bee	Beran and Neururer, 1955
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Table 9: Toxicity of DNOC to terrestrial vertebrates

Organism	Endpoint	Concentration (mg/kg-bw)	Reference
Japanese quail <i>Coturnix japonica</i>	24-hour LD ₅₀	14.8 (95% CI ¹ 13–17)	Dickhaus and Heisler, 1980
Japanese quail <i>Coturnix japonica</i>	8-day LC ₅₀	106	Til and Kengen, 1980
Pheasants	LD ₅₀	8.4	Janda, 1970
Partridges	LD ₅₀	8.3	Janda, 1970
Rat	90-day LOEL	2.5 (per day)	Den Tonkelaar <i>et al.</i> , 1983

¹ CI = confidence interval.

The most sensitive aquatic vertebrates reported in the literature are rainbow trout (Mayer and Ellersieck, 1986; Sewell *et al.*, 1995c). The authors reported LC₅₀ values of 0.066 and 0.45 mg/L, respectively. The 96-hour LC₅₀ study reported by Sewell *et al.* (1995c) is an unpublished study; however, it was cited in a peer-reviewed report (IPCS, 2000). Atlantic salmon and bluegill are also sensitive, with 96-hour LC₅₀ values of 0.20 mg/L and 0.23 mg/L, respectively (Zitko *et al.*, 1976; Buccafusco *et al.*, 1981).

The effect of DNOC on terrestrial vertebrates (mink and otter) (Critical Toxicity Value [CTV] for wildlife) was calculated using the repeated mammalian (rat) oral dose toxicity data provided for the substance (2.5 mg/kg-bw per day for a 90-day rat dietary exposure study, Lowest-Observed-Effect Level [LOEL]) (Den Tonkelaar *et al.*, 1983). The CTV_{wildlife} is calculated by taking the chronic value (geometric mean of the No-Observed-Effect Level [NOEL] and LOEL) from the rat study and correcting it for body weight of a predictive sentinel species (Sample *et al.*, 1996). In this case, the predictive sentinel species are the piscivorous mammals mink and river otter.

The CTV_{wildlife} is thus calculated as:

$$CTV_{wildlife} = ChV_{ts} \cdot (BW_{ts}/BW_{pss})$$

where:

- ChV_{ts} = chronic value for test species (geometric mean of LOEL [2.5 mg/kg-bw per day] and NOEL [0.25 mg/kg-bw per day] = 0.8 mg/kg-bw per day)
- BW_{ts} = mean body weight of test species (0.35 kg)
- BW_{pss} = body weight of predictive sentinel species (0.807 kg for mink; 6.01 kg for otter) (Martin, 2004).

Therefore, CTV_{wildlife} = 0.8 × (0.35/0.807) = 0.35 for mink and 0.8 × (0.35/6.01) = 0.047 for otter.

The ENEV_{wildlife} is calculated from the CTV_{wildlife} as follows:

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$$\text{ENEV}_{\text{wildlife}} = \text{CTV}_{\text{wildlife}}/\text{AF}$$

where:

$\text{ENEV}_{\text{wildlife}}$ = wildlife Estimated No-Effects Value (mg/kg-bw per day)
AF = application factor (interspecies variation, laboratory to field extrapolation) (10).

Therefore, the $\text{ENEV}_{\text{mink}}$ is 0.035 mg/kg-bw per day, and the $\text{ENEV}_{\text{otter}}$ is 0.0047 mg/kg-bw per day.

Abiotic Effects

Stratospheric Ozone Depletion

The ozone-depleting potential (ODP) of a substance is defined as the ratio of calculated ozone column change for each unit mass of a gas emitted into the atmosphere relative to the depletion calculated for an equal mass of reference gas chlorofluorocarbon-11 (CFC-11), an ozone-depleting substance with an ODP of 1. The formula used to calculate ODP is applicable only for substances with chlorine or bromine atoms. As DNOC does not contain any chlorine or bromine atoms, it has an ODP of zero, and it is concluded that DNOC will not contribute to ozone depletion.

Ground-Level Ozone Formation

To estimate ground-level ozone formation, a Photochemical Ozone Creation Potential (POCP) index is used (Environment Canada, 1996). The POCP is a measure of the relative effectiveness for ozone formation of a unit mass of organic substance compared with that of an equivalent mass of ethene. By definition, ethene has a POCP value of 100.

The episodic ozone formation can be estimated from a reactivity scale based on the rate constant for the hydroxyl–hydrocarbon reaction and the molecular weight of the subject substance relative to those properties of ethene:

$$\text{POCP} = (k_s/M_s) (M_{\text{ethene}}/k_{\text{ethene}}) \times 100$$

where:

k_s = reaction rate constant at 298 K for the reaction with the hydroxyl radical for the substance (3.0×10^{-11} cm³/mol per second)
 k_{ethene} = reaction rate constant at 298 K for the reaction with the hydroxyl radical (8.5×10^{-12} cm³/mol per second)
 M_s = molecular mass of the substance (198.13 g/mol for DNOC)
 M_{ethene} = molecular mass of ethene (28 g/mol).

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The POCP value for DNOC is 50.

Although it is recognized that DNOC may have the potential to contribute to ground-level ozone formation, the relative contribution is dependent on the concentration as well as on the reactivity of DNOC relative to other volatile organic compounds (VOCs) in an area. Nevertheless, DNOC is a reactive VOC. VOCs “that participate in atmospheric photochemical reactions” were added as a class to Schedule 1 of CEPA 1999 (List of Toxic Substances) in July 2003 and are subject to a range of risk management activities focusing on total VOCs, rather than on individual compounds. Since VOCs that participate in atmospheric photochemical reactions already appear on Schedule 1, a given existing substance’s ability to participate in photochemical reactions is not used as a basis for concluding that it is toxic under Section 64 of CEPA 1999.

It is further worthy of note that releases of DNOC from non-pesticidal uses are believed to be largely to aquatic systems, with little partitioning to air. The extent and mechanism of possible DNOC formation in the atmosphere from precursor species are not yet well understood.

Global Warming Potential

Global Warming Potential (GWP) is defined as the ratio of calculated warming for each unit mass of a gas emitted into the atmosphere relative to the calculated warming for a reference gas, CFC-11. The GWP for DNOC was estimated to be 7.2×10^{-12} , and therefore DNOC is not expected to contribute significantly to climate change.

Risk Characterization

As part of risk characterization, one line of evidence includes consideration of risk quotients to identify potential for ecological effects. Other factors that affect current or potential risks, such as persistence, bioaccumulation and trends in ambient concentrations, are also considered.

Risk Quotient Analysis

Critical exposure and effects results and risk quotients are summarized in Table 10 and described in more detail below.

Table 10: Summary of data used in risk quotient (RQ) analysis of DNOC

Scenario	EEV	CTV	AF ¹	ENEV	RQ (EEV/ ENEV)
Pelagic organisms					
Industrial release; rainbow trout	0.0014 mg/L	0.26 mg/L	100	0.0026 mg/L	0.54

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Scenario	EEV	CTV	AF ¹	ENEV	RQ (EEV/ ENEV)
Rainfall; rainbow trout	0.0025 mg/L	0.26 mg/L	10	0.026 mg/L	0.096
Soil organisms					
Earthworm	0.1 mg/kg	15 mg/kg dry weight	100	0.15 mg/kg dry weight	0.67
Wildlife consumers					
Mink	0.0004 mg/kg-bw per day	0.35	10	0.035 mg/kg-bw per day	0.011
River otter	0.000 007 mg/kg-bw per day	0.047	10	0.0047 mg/kg-bw per day	0.0015

¹ AF = application factor.

Pelagic Organisms

For pelagic organisms, a risk quotient was developed using the average 96-hour LC₅₀ values of rainbow trout reported by Mayer and Eilersieck (1986) (0.066 mg/L) and Sewell *et al.* (1995c) (0.45 mg/L). The average of the two studies, which is the CTV, is 0.26 mg/L.

For the *industrial release scenario*, if STP treatment is considered (27% removal efficiency), the EEV will be 0.0014 mg/L. Using an application factor of 100 on the CTV to account for acute to chronic extrapolation and intra- and interspecies variations, differently sensitive biological endpoints and laboratory to field extrapolations, the ENEV is calculated to be 0.0026 mg/L.

The risk quotient is therefore calculated as:

$$\frac{\text{EEV}}{\text{ENEV}} = \frac{0.0014 \text{ mg/L}}{0.0026 \text{ mg/L}} = 0.54$$

Even with STP removal considered, this represents a conservative scenario due largely to the very high quantity of DNOC assumed to be used by a single facility.

The maximum EEV under the defined *rainfall scenario* was determined to be 0.0025 mg/L with no STP treatment due to the assumption of a heavy rainfall. As rainfall represents an acute exposure scenario, the application factor does not need to account for acute to chronic extrapolation. Therefore, using an application factor of 10 and the same CTV of 0.26 mg/L for rainbow trout, an ENEV of 0.026 mg/L is calculated. The risk quotient is therefore:

$$\frac{\text{EEV}}{\text{ENEV}} = \frac{0.0025 \text{ mg/L}}{0.026 \text{ mg/L}} = 0.096$$

Soil Organisms

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There are no quantified amounts of DNOC concentrations in Canadian soils. OMEE (1994) did not detect DNOC in 161 soil samples collected from soils in Ontario. The method detection limit of 0.1 mg/kg (100 ng/g) will be used as a surrogate for the level of DNOC in Canadian soil and is selected as the EEV.

One study was located in the literature on the effects of DNOC on terrestrial organisms. The LC₅₀ from a 14-day acute toxicity study on the earthworm is 15 mg/kg of soil. This value is selected as the CTV for exposures of soil organisms to DNOC. Dividing the value by a factor of 100 to account for extrapolation from laboratory to field conditions, acute to chronic ratio and interspecies and intraspecies variations in sensitivity gives an ENEV of 0.15 mg/kg.

The risk quotient for soil organisms is therefore:

$$\frac{EEV}{ENEV} = \frac{0.1 \text{ mg/kg}}{0.15 \text{ mg/kg}} = 0.67$$

Aquatic Wildlife

The EEVs for the mink and river otter were estimated to be 0.0004 mg/kg-bw per day and 0.000 007 mg/kg-bw per day, respectively. The ENEV for the mink was estimated to be 0.035 mg/kg-bw per day, and the ENEV for the river otter was calculated to be 0.0047 mg/kg-bw per day.

The risk quotients for aquatic wildlife are thus calculated to be:

$$\frac{EEV_{\text{mink}}}{ENEV_{\text{mink}}} = \frac{0.0004 \text{ mg/kg-bw per day}}{0.035 \text{ mg/kg-bw per day}} = 0.011$$

$$\frac{EEV_{\text{otter}}}{ENEV_{\text{otter}}} = \frac{0.000 \text{ 007 mg/kg-bw per day}}{0.0047 \text{ mg/kg-bw per day}} = 0.0015$$

Benthic Organisms

No monitoring data for DNOC in sediments in Canada were identified. IPCS (2000) has stated that if released to water, DNOC is only moderately adsorbed onto aquatic sediments. Level III multimedia fate simulation estimated that only about 1% of DNOC is expected to partition to sediments. It is therefore believed that there will be minimal exposure of benthic organisms to DNOC.

Weight of Evidence Analysis

The risk quotient analyses for pelagic and soil organisms and wildlife have shown that it is unlikely that organisms are currently exposed to concentrations of DNOC above known effect

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thresholds. This conclusion is based on current import levels, the locations where DNOC is being used industrially and the current state of knowledge of its atmospheric chemistry.

A conservative scenario based on concentrations of DNOC in precipitation that could be expected to enter Canadian receiving water indicated that the potential for risk to aquatic organisms from this source is low.

In addition, modelling estimates of industrial releases to the St. Clair River indicate that DNOC is not likely to cause adverse effects on pelagic or benthic organisms. This is based on a conservative release scenario developed for the one company importing the substance that currently reports releases of DNOC to the NPRI, although the company has not reported releases to water.

Although sorption is low at environmentally relevant pHs, little leaching to groundwater has been found, likely due to biodegradation.

Potential sources of release of DNOC to the environment are to air and water. Based on its properties, DNOC is persistent in air but not bioaccumulative. Long-range transport modelling estimates that it will be transported over moderate distances, and a decreasing concentration with increasing latitude is expected.

Proposed Conclusions for the Environment

DNOC meets the criteria for categorization owing to its persistence in air and inherent toxicity to aquatic organisms. DNOC is not bioaccumulative.

When comparing effect thresholds with conservatively estimated exposure values for different media, resultant risk quotients are less than unity. DNOC is believed to be used by a limited range of industrial facilities in Canada.

Based on available data and weight of evidence, it is proposed that DNOC is not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends.

Further Considerations

A release scenario using European monitoring data to determine the effects of concentrations of DNOC in precipitation released to Canadian rivers indicated that there is a low likelihood of risk. This is believed to be a conservative scenario; however, there is significant uncertainty. Studies are in progress in Europe to improve understanding of the extent and mechanisms of formation of DNOC in the atmosphere. As the science evolves or Canadian monitoring data become available, this information could be used in setting priorities on the need for further assessment.

Uncertainties

There are uncertainties associated with development of the ENEVs used in this assessment. However, a moderate number of empirical studies from different sources were identified, which increases confidence in the values. Application factors of 10–100 were used to account for information gaps relating to chronic toxicity, effects in the field and effects on potentially more sensitive species. Effects data were not identified for marine species.

Very few Canadian monitoring data are available for DNOC, and those that were identified were fairly old. To both support the limited amount of empirical data and provide greater insight into the potential range of levels of DNOC in the environment, releases were estimated and fate and exposure were modelled. Entry of DNOC to the environment from two sources was considered — industrial releases and precipitation containing DNOC scavenged from the atmosphere. To address the significant uncertainty in these estimations, conservative assumptions were used to ensure that errors would be protective of the environment.

Although there have not been reports of direct releases of DNOC to water from industrial facilities, a conservative scenario was developed to estimate possible releases from an industrial source. This conservatively assumed an upper-limit estimate of the quantity of DNOC potentially used by a single facility; a slightly conservative estimate of the fraction of substance typically released due to handling practices for a substance used in bulk; and a low-percentile estimate of river flow for the receiving water body used in the scenario. Flow characteristics of the St. Clair River were used in the exposure scenario, as it is believed that the only facility in Canada currently using substantive quantities of DNOC is located near this water body. This river is extremely fast flowing and consequently disperses effluents very rapidly. Were there to be facilities having substantive releases to smaller water bodies, then the assumptions used in this scenario may not be sufficiently protective. However, it is believed that there are currently no other large users of DNOC in Canada.

Estimation of possible exposure from atmospherically generated DNOC in precipitation conservatively assumed that the concentration in the atmosphere in Canada would be similar to that in more heavily populated regions of Europe; that the rainfall event would be particularly heavy; that a high percentage of precipitation from a census subdivision would be released to the receiving river body through a single discharge point; and that there would be no removal of DNOC by the municipal STP. In particular, the assumption that atmospheric concentrations in Canada would be the same as average to high concentrations in Germany, which is much more heavily populated and industrialized, is uncertain. While it is believed that use of monitoring data from Germany in the scenario is conservative, the origins of atmospherically generated DNOC are at present not well understood, and no Canadian atmospheric monitoring data were identified for comparison.

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