Canadian Soil Quality Guidelines for the Protection of Environmental and Human Health

DIISOPROPANOLAMINE

This fact sheet provides Canadian soil quality guidelines for diisopropanolamine (DIPA) for the protection of environmental and human health (Table 1). A supporting scientific document is also available (CCME 2006).

Background Information

DIPA ($C_6H_{15}NO_2$; CAS 110-97-4) is used in a number of commercial, industrial, and household applications. It is known under a variety of synonyms, including bis(2-hydroxypropyl)amine, 1,1'-iminobis(2-propanol) and 1,1'-iminodipropan-2-ol. It has a molecular weight of 133.19 $g \cdot mol^{-1}$, a density of 0.989 $g \cdot cm^{-3}$ at 25°C, an aqueous solubility of 870,000 $mg \cdot L^{-1}$ at 25°C, a mean K_d in aquifer materials of 2.2 $L \cdot kg^{-1}$, a vapour pressure at 42°C of 2.7 x 10^{-3} kPa, and a Henry's law constant of 1.72 x 10^{-7} $atm \cdot m^{-3} \cdot mol^{-1}$.

In North America, the Dow Chemical Company (Dow) is the dominant DIPA producer. In 1995, US production was estimated by Dow to be approximately 7,000 tons per year. DIPA is available as commercial grade compound (98% pure, containing a maximum of 0.5% water) and as low freezing grade DIPA containing 10 or 15% water.

DIPA applications include cosmetics and personal care products, gas treating, detergents, metalworking fluids, coatings, corrosion inhibitors, and cement applications. Cosmetic and personal care applications of DIPA include the manufacture of lotions, shampoos, soaps, and cosmetics. DIPA is also used together with sulfolane in the Sulfinol™ process to remove hydrogen sulphide and carbon dioxide from a natural gas stream.

Reports on the presence of anthropogenic DIPA in the

Table 1. Soil quality guidelines for DIPA ($mg \cdot kg^{-1}$).

	Land use			
	Agricultural	**Residential/ parkland**	**Commercial**	**Industrial**
Guideline	**180[a]**	**180[a]**	**180[a]**	**180[a]**
SQG_{HH}	460	460	460	460
Limiting pathway for SQG_{HH}	Groundwater check (drinking water)	Groundwater check (drinking water)	Groundwater check (drinking water)	Groundwater check (drinking water)
Provisional SQG_{HH}	NC[b]	NC[b]	NC[b]	NC[b]
Limiting pathway for provisional SQG_{HH}	ND	ND	ND	ND
SQG_E	180	180	180	180
Limiting pathway for SQG_E	Groundwater check (aquatic life)	Groundwater check (aquatic life)	Groundwater check (aquatic life)	Groundwater check (aquatic life)
Provisional SQG_E	NC[c]	NC[c]	NC[c]	NC[c]
Limiting pathway for provisional SQG_E	ND	ND	ND	ND
Interim soil quality criterion (CCME 1991)	No value	No value	No value	No value

Notes: NC = not calculated; ND = not determined; NA = not applicable; SQG_{HH} = soil quality guideline for human health; SQG_E = soil quality guideline for environmental health.

[a]Data are sufficient and adequate to calculate an SQG_{HH} and an SQG_E. Therefore, the soil quality guideline is the lower of the two and represents a fully integrated guideline for this land use, derived in accordance with the draft revised soil protocol (CCME 2003).

[b]Because data are sufficient and adequate to calculate an SQG_{HH} for this land use, a provisional SQG_{HH} is not calculated.

[c]Because data are sufficient and adequate to calculate an SQG_E for this land use, a provisional SQG_E is not calculated.

The guidelines in this fact sheet are for general guidance only. Site-specific conditions should be considered in the application of these values. The values may be applied differently in various jurisdictions. The reader should consult the appropriate jurisdiction before application of the values.

environment are limited to data collected at sour gas processing facilities in western Canada (CAPP 1997; Wrubleski and Drury 1997). At these facilities, a maximum soil DIPA concentration of 1,480 mg·kg^{-1} was measured in clay-rich till. No studies were found that had detected DIPA as a naturally-occurring compound in the environment.

Environmental Fate and Behaviour in Soil

Laboratory studies have shown that the major physical and chemical process that determines the transport and distribution of DIPA in soil and water is cation exchange. DIPA acts as a weak base in soil pore water and other aqueous systems. Its pKa value of 8.9 indicates that DIPA becomes more protonated at pH values less than 8.9 (Kim et al. 1987). Dissolving DIPA in water may increase the pH of the water. The protonated form of DIPA is strongly sorbed to the clay minerals in soil. DIPA has a high aqueous solubility and low volatility. The mobility of DIPA in the subsurface is controlled by its sorption to soil.

Sorption of DIPA by aquifer materials is relatively independent of organic carbon content, but a strong function of cation exchange capacity (Luther et al., 1998). The soil-water distribution coefficient (K_d) for DIPA in equilibrium with pure montmorillonite (16 to 42 L·kg^{-1}) was much higher than for humus-rich soil (2.0 L·kg^{-1}). The mean K_d in soils and aquifer materials was 2.2 L·kg^{-1}. Luther et al. (1998) reported DIPA retardation coefficients of 3.2, 5.3, and 12 for weathered sandstone, weathered shale/sandstone, and clay-rich till, respectively. These values indicate that, particularly in the presence of clay-rich sediments, DIPA migration can be significantly retarded relative to groundwater flow velocity.

The biodegradation of DIPA has been investigated in acclimated sewage sludge, refinery wastewater, laboratory microcosm studies using contaminated and uncontaminated aquifer materials, and as part of a natural attenuation study in natural wetlands. Most studies have demonstrated that DIPA biodegrades in aerobic microcosms from a variety of DIPA-contaminated environmental samples, so long as nutrients (N and P) are not limiting. Degradation half-lives in aerobic conditions with sufficient nutrients range from less than 1 day to 5 weeks. Under anaerobic conditions, DIPA biodegradation was confirmed to occur at 28°C under NO_3^-, Mn^{4+}, and Fe^{3+} reducing conditions. At 8°C, evidence of anaerobic degradation under NO_3^-, Mn^{4+}, and Fe^{3+} reducing conditions was observed in a limited number of microcosms.

Behaviour and Effects in Biota

Soil Microbial Processes

Specific studies designed to address the effect of DIPA on nitrogen fixation and nitrification, carbon cycling, or nitrogen mineralization have not been conducted. However, a number of biological fate studies have been conducted to determine the biodegradation rate of DIPA by indigenous soil bacteria. These studies provide some constraint on the DIPA concentration at which soil-dwelling bacteria are viable. A study by Greene et al. (1999) provided evidence that DIPA was readily degraded by mixed populations of indigenous bacteria in fine-textured soil contaminated with up to 350 mg·L^{-1} DIPA.

Terrestrial Plants

CAPP (2001) determined the toxicity of DIPA to four species of terrestrial plants (lettuce (*Lactuca sativa*), carrot (*Daucus carota*), alfalfa (*Medicago sativa*), and timothy (*Phleum pratense*)) using four soils with differing texture, organic carbon content, and cation exchange capacity. The endpoints measured were emergence, biomass, root length, and shoot length. For all four plant species, the most sensitive endpoint was reduced root length, with the lowest EC_{25} for this endpoint being 130 mg·kg^{-1} for carrot in sand. The highest EC_{25} reported was 18,700 mg·kg^{-1} for reduced emergence of timothy in loam. Plants were generally most sensitive to DIPA in sand and least sensitive in loam.

Terrestrial Invertebrates

CAPP (2001) conducted earthworm toxicity testing using four soils with differing texture, organic carbon content, and cation exchange capacity. The endpoint considered was survival. The lowest LC_{25} value was 800 mg·kg^{-1}, which was obtained in sand. Sand and till soils returned similar toxicity values, which were approximately an order of magnitude more sensitive than values from tests in loam.

Human and Experimental Animal Health Effects

Studies indicate that DIPA is poorly metabolized in mammals. Dow (1985) concluded that DIPA, either ingested or absorbed through skin, will be eliminated rapidly and almost entirely in the urine.

Acute data on the mammalian toxicity of DIPA using single dose exposures are available on four species of laboratory animal from four studies. Acute LD_{50} values range from 2,120 to 8,000 mg·kg^{-1}·bw·day^{-1}.

The subchronic toxicity of DIPA following oral administration via water or food has been reported in four animal studies. Dow (1984) exposed rats to DIPA in drinking water over a period of two weeks. The authors reported a NOAEL of 600 mg·kg^{-1}·bw·day^{-1} for this study. Toxic effects observed at higher doses included weight loss, altered clinical biochemical parameters, inflammation and degeneration of kidney and urinary bladder, and liver atrophy. Konishi et al. (1991) reported the results of an 18 week study in which Wistar rats received 1% DIPA mixed with their powdered diet and showed no evidence of renal toxicity. BIBRA (1991) reported that rats given 5,000 mg·kg^{-1}-·bw·day^{-1} for seven days produced no evidence of toxic effects. Toropkov (1980) reported a threshold of 0.22 mg·kg^{-1}·bw·day^{-1} for toxic effects in guinea pigs for less than chronic exposures.

Yamamoto et al. (1989) reported the results of a chronic study that found no increase in the incidence of tumours observed in target organs of Wistar rats fed 1% DIPA (w/v) in food for a period of 94 weeks. The dosage of DIPA was 156 mg per animal per day. This was interpreted to indicate that chronic (lifetime) exposure to 391 mg·kg^{-1} bw day^{-1} of DIPA was not carcinogenic (Yamamoto et al. 1989), and this concentration may be considered the NOAEL from this study.

Yamamoto et al. (1989) also investigated the effect of providing nitrite in drinking water in conjunction with 1% DIPA (w/v) in food for a period of 94 weeks. At a nitrite concentration of 0.3%, (but not at 0.15%), tumours appeared in every expected target organ. Yamamoto et al. (1989) suggest their results provide evidence that endogenous nitrosation of environmental nitrosatable amines can be a potential risk factor for human cancer development.

The genotoxicity of DIPA has not been extensively investigated. However, one study in *Salmonella* was negative (Mortelmans et al. 1986). An unpublished report found that DIPA did not produce chromosomal aberrations in rat lymphocytes with or without metabolic activation at exposures of 313 to 5,000 mg·L^{-1} (Dow 1994 in BASF 1994). There were no other published reports in the literature.

Based on the NOAEL of 391 mg·kg^{-1}·bw·day^{-1} in rats in the chronic Yamamoto et al. (1989) study, and using an uncertainty factor of 1000 (ten each for intra- and interspecies variation, and an additional ten-fold factor to reflect inadequacies in the database and the possibility of endogenously produced N-nitrosobis(2-hydroxypropyl)amine), a provisional TDI of 0.39 mg·kg^{-1} ·bw·day^{-1} was established.

Guideline Derivation

Canadian soil quality guidelines are derived for different land uses following the process outlined in CCME (2003) using different receptors and exposure scenarios for each land use (Table 1). Detailed derivations for DIPA soil quality guidelines are provided in CCME (2006).

Soil Quality Guidelines for Environmental Health

The environmental soil quality guidelines (SQG_E) are based on soil contact using data from toxicity studies on plants and invertebrates. In the case of agricultural land, soil and food ingestion are considered for livestock. To provide a broader scope of protection, a nutrient and energy cycling check and a groundwater check for aquatic life are calculated. For industrial land use, an off-site migration check is also calculated (Table 2).

DIPA acts as a weak base, and sufficient concentrations of DIPA in soil in the absence of available buffering capacity could raise the pH of soil pore water to unacceptable levels. Accordingly, a pH check was also calculated for this compound (Table 2). A pH check is not included in the CCME (2003) protocol, but is included here to address an issue specific to DIPA and a small number of other compounds. Details are provided in CCME (2006).

For each land use, the lowest of the environmental health guidelines or check values that are calculated is recommended as the SQG_E.

For DIPA, the soil contact guideline was calculated based on a species sensitivity distribution of plant and invertebrate EC25 toxicity data. The 25th percentile of this distribution was used as the soil contact guideline for agricultural and residential/parkland land uses and the 50th percentile for commercial and industrial land uses. The groundwater check for aquatic life was calculated based on the CCME (2003) protocol and the freshwater aquatic life guideline which is 1.6 mg·L^{-1} for DIPA. There were insufficient data to calculate the nutrient and energy cycling check or the soil and food ingestion check. Details of the guideline and check value calculations are available in CCME (2006). The groundwater check for aquatic life was the lowest of the ecological guidelines/check values for DIPA, and is recommended as the SQG_E for all land uses (Table 2).

Soil Quality Guidelines for Human Health

Human health soil quality guidelines (SQG_{HH}) are based on human soil ingestion guidelines. Guidelines based on other exposure pathways are considered by the inhalation of indoor air check, off-site migration check, groundwater check for protection of drinking water, and produce, meat and milk check.

For DIPA, the CCME (2003) protocol was used together with the human tolerable daily intake of 0.39 $mg \cdot kg^{-1} \cdot bw$ per day to calculate the human ingestion guideline. The groundwater check for drinking water was calculated using the CCME (2003) protocol and the source guidance value for groundwater (SGVG) of 4 $mg \cdot L^{-1}$ (CCME 2006). There were insufficient data to calculate the produce, meat and milk check, and the inhalation of indoor air check was not calculated due to low volatility and Henry's law constant. Details of the guideline and check value calculations are available in CCME (2006). The groundwater check for drinking water was the lowest of the guidelines that was calculated, and is recommended as the SQG_{HH}.

Soil Quality Guidelines for DIPA

The soil quality guidelines for DIPA are the lower of the SQG_{HH} and SQG_E for each land use. For all land uses, the soil quality guideline is the soil concentration calculated for the SQG_E, which is based on the protection of groundwater for aquatic life (Table 1). Because there are sufficient data to calculate an SQG_{HH} and an SQG_E for each land use, the soil quality guideline represents a fully integrated guideline for each land use, derived according to the soil protocol (CCME 2003). There was no interim guideline for DIPA in CCME (1991). CCME (1996) provides guidance on potential modifications to the final recommended soil quality guidelines when setting site-specific objectives.

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Table 2. Soil quality guidelines and check values for DIPA (mg·kg^{-1}).

	Land Use			
	Agricultural	**Residential/ parkland**	**Commercial**	**Industrial**
Recommended Guideline	**180[a]**	**180[a]**	**180[a]**	**180[a]**
Human health guidelines/check values				
SQG_{HH}	**460**	**460**	**460**	**460**
Soil ingestion guidelines	27,000	27,000	97,000	NA[b]
Inhalation of indoor air check	NC	NC	NC	NC
Off-site migration check	—	—	—	380,000
Groundwater check (drinking water)	460[c]	460[c]	460[c]	460[c]
Produce, meat, and milk check	NC	NC	—	—
Environmental health guidelines/check values				
SQG_E	**180**	**180**	**180**	**180**
Soil contact guidelines	360	360	750	750
Soil and food ingestion guideline	NC[d]	—	—	—
Nutrient and energy cycling check	NC[d]	NC[d]	NC[d]	NC[d]
Off-site migration check	—	—	—	5,100
Groundwater check (aquatic life)	180	180	180	180
pH Check[e]	230	230	230	230
Interim soil quality criterion (CCME 1991)	No value	No value	No value	No value

Notes: NC = not calculated; ND = not determined; NA = not applicable; SQG_E = soil quality guideline for environmental health; SQG_{HH} = soil quality guideline for human health. The dash indicates guideline/check value that is not part of the exposure scenario for this land use and therefore is not calculated.

[a]Data are sufficient and adequate to calculate an SQG_{HH} and an SQG_E. Therefore, the soil quality guideline is the lower of the two and represents a fully integrated guideline for this land use, derived in accordance with the soil protocol (CCME 2003).

[b]Not applicable since the calculated guideline was more than 1,000,000 ppm.

[c]The groundwater check for drinking water is the lowest of the human health guidelines and check values.

[d]Data are insufficient/inadequate to calculate this value.

[e]The pH check is calculated in addition to the standard CCME guidelines and checks due to the potential for DIPA to increase the pH of soil porewater to an unacceptable level, see text for details.

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Excerpt from Publication No. 1299; ISBN 1-896997-34-1

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