



This fact sheet provides Canadian water quality guidelines for Diisopropanolamine (DIPA) for the protection of agricultural water uses (Table 1). A scientific supporting document is also available (Environment Canada 2005).

### 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  $\times 10^{-3}$  kPa, and a Henry's law constant of 1.72  $\times 10^{-7}$   $atm \cdot m^3 \cdot mol^{-1}$ .

In North America, the Dow Chemical Company (Dow) is the dominant DIPA producer. In 1995, the 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<sup>TM</sup> process to remove hydrogen sulphide and carbon dioxide from a natural gas stream.

Reports on the presence of anthropogenic DIPA in the environment are limited to data collected at sour gas processing facilities in western Canada (CAPP 1997; Wrubleski and Drury 1997). The maximum measured DIPA concentration in groundwater was 590  $mg \cdot L^{-1}$  in a shallow till aquifer (Greene et al. 1999). No studies were found that had detected DIPA as a naturally-occurring compound in the environment.

### Environmental Fate and Behaviour

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. 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  $L \cdot kg^{-1}$ ) was much higher than for humus-rich soil (2.0  $L \cdot kg^{-1}$ ). The mean  $K_d$  in soils and aquifer materials was 2.2  $L \cdot kg^{-1}$ . 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 is significantly retarded relative to groundwater flow velocity.

**Table 1. Water quality guidelines for DIPA for the protection of agricultural water uses (Environment Canada 2005).**

Use	Guideline value ( $mg \cdot L^{-1}$ )
Irrigation water	2 <sup>a</sup>
Livestock water	NRG <sup>b</sup>

<sup>a</sup>Interim guideline.

<sup>b</sup>No recommended guideline.

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  $\text{NO}_3^-$ ,  $\text{Mn}^{4+}$ , and  $\text{Fe}^{3+}$  reducing conditions. At 8°C, evidence of anaerobic degradation under  $\text{NO}_3^-$ ,  $\text{Mn}^{4+}$ , and  $\text{Fe}^{3+}$  reducing conditions was observed in a limited number of microcosms.

Uptake of DIPA by wetland vegetation was studied as part of a research program to evaluate natural attenuation processes in contaminated wetlands (CAPP 1998, 1999, 2000). Roots, stems, leaves, flower heads, seed heads, and berries of cattail, dogwood, sedge, marsh reed grass, cow parsnip, and smooth brome growing in a DIPA-impacted wetland were included in the study (CAPP 1999, 2000; Headley et al. 1999a,b). Analytical results indicated highly variable DIPA concentrations for different parts of the same species (e.g., roots versus leaves), between different plant species (e.g., cattail leaves versus sedge leaves), and even between different samples of the same part of the same species. Although the maximum measured DIPA concentration in water in the wetland was only  $13 \text{ mg}\cdot\text{L}^{-1}$ , DIPA concentration as high as  $208 \text{ mg}\cdot\text{kg}^{-1}$  were measured in the plants.

## Water Quality Guideline Derivation

The interim Canadian water quality guideline for DIPA for the protection of irrigation water was developed according to the CCME protocol (CCME 1999).

## Irrigation Water

The Canadian water quality guideline for DIPA for irrigation was developed using *Protocols for Deriving Water Quality Guidelines for the Protection of Agricultural Water Uses (Irrigation and Livestock Watering)* (CCME 1999). Irrigation guidelines were calculated for: (1) cereals, tame hays, and pasture crops; and (2) other crops.

Data for two hay/pasture crop species, alfalfa (*Medicago sativa*) and timothy (*Phleum pratense*), and two other crop species, lettuce (*Lactuca sativa*) and carrot (*Daucus carota*), were available for four soil types – loam,

artificial soil, till, and sandy soil (CAPP 2001). Endpoints measured included emergence, root elongation, shoot elongation, and biomass. The data were classified as primary toxicological data. The toxicological data set was sufficient to derive interim guidelines. LOECs, corrected for analytical concentrations, ranged from  $155 \text{ mg}\cdot\text{kg}^{-1}$  for a reduction in root elongation for lettuce and carrot in sand to  $43,300 \text{ mg}\cdot\text{kg}^{-1}$  for timothy emergence in loam.

A species maximum acceptable toxicant concentration (SMATC) was calculated for the most sensitive species/endpoint/soil combination for: (1) cereals, tame hays, and pasture crops; and (2) other crops. The species/endpoint/soil combination resulting in the lowest SMATC was root elongation for lettuce and carrot grown in sand. The acceptable soil concentration (ASC), which is an estimate of the soil concentration that would not result in adverse effects on crops over the course of one growing season, was calculated for this species as the geometric mean of the NOEC ( $77 \text{ mg}\cdot\text{kg}^{-1}$ ) and the LOEC ( $155 \text{ mg}\cdot\text{kg}^{-1}$ ) divided by a safety factor of 10. The ASC for lettuce and carrot was  $30 \text{ mg}\cdot\text{kg}^{-1}$ . The SMATC was calculated by multiplying the ASC for lettuce and carrot ( $11 \text{ mg}\cdot\text{kg}^{-1}$ ) by the soil bulk density ( $1,300 \text{ kg}\cdot\text{m}^{-3}$ ) and the soil bulk volume of a hectare to a depth of 0.15 m ( $100 \text{ m} \times 100 \text{ m} \times 0.15 \text{ m}$ ), and dividing by the irrigation rate ( $1.2 \times 10^7 \text{ L}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$ ) to give an SMATC of  $2 \text{ mg}\cdot\text{L}^{-1}$ . The SMATC for lettuce and carrot, being lower than all other species, was adopted as the interim water quality guideline for irrigation.

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