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

SULFOLANE

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

Background Information

Sulfolane ($C_4H_8SO_2$; CAS 126-33-0) is a solvent used for gas treatment in a number of industrial processes. It is known under a variety of synonyms and trade names including bondelane A, 2,3,4,5-tetrahydrothiophene-1,1-dioxide, and tetramethylene sulfone. It has a molecular weight of 120.17 $g \cdot mol^{-1}$, a density of 1.276 $g \cdot cm^{-3}$ at 15°C, an aqueous solubility of 1,266,000 $mg \cdot L^{-1}$ at 20°C, a log K_{oc} of 0.07, a mean K_d in aquifer materials of 0.08 $L \cdot kg^{-1}$, a vapour pressure at 20°C of 1.33 x 10^{-3} kPa, and a Henry's law constant of 8.9 x 10^{-10} $atm \cdot m^{-3} \cdot mol^{-1}$.

The total worldwide production of sulfolane is estimated at between 18,000 and 36,000 tons per year. Commercially, sulfolane is available as anhydrous sulfolane and as sulfolane containing 3% deionized water.

Sulfolane is widely used for gas treatment processes including: sour gas sweetening, hydrogen selenide removal from gasification of coal, shale, or tarsands; olefin removal from alkanes; nitrogen, helium, and argon removal from natural gas; atmospheric CO_2 removal in nuclear submarines; ammonia and H_2S removal from waste streams; and H_2S, hydrogen chloride (HCl), nitrous oxide (N_2O), and CO_2 removal from various streams. In addition to gas treatment, sulfolane is also used as a polymer solvent, polymer plasticizer, polymerization solvent, and in electronic/electrical applications (Kirk-Othmer 1999).

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

	Land use			
	Agricultural	**Residential/ parkland**	**Commercial**	**Industrial**
Guideline	**0.8**[a]	**0.8**[a]	**0.8**[a]	**0.8**[a]
SQG_{HH}	0.8	0.8	0.8	0.8
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	210	210	430	430
Limiting pathway for SQG_E	Soil Contact	Soil Contact	Soil Contact	Soil Contact
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; SQG_{HH} = soil quality guideline for human health; SQG_E = soil quality guideline for environmental health.

Guideline values in this table apply to soil analyses presented on a dry weight basis (i.e., mg sulfolane per kg dry weight soil).

[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.

Reports on the presence of anthropogenic sulfolane in the environment are limited to data collected in the vicinity of sour gas processing facilities in Western Canada (CAPP 1997; Wrubleski and Drury 1997). The maximum measured sulfolane concentrations in groundwater were 800 mg·L^{-1} in shallow till and 88 mg·L^{-1} in bedrock. The only report of sulfolane occurring naturally in the environment was in a composite sample of a sponge (*Batzella sp.*) and tunicate (*Lissoclinum sp.*) which contained approximately 50 mg·kg (dry·weight)$^{-1}$ sulfolane (Barrow and Capon 1992).

Environmental Fate and Behaviour

Laboratory studies indicate that the major physical and chemical processes that determine the transport and distribution of sulfolane in soil and water are adsorption and leaching. Sulfolane is poorly adsorbed to soil and has a high aqueous solubility and low volatility. Sulfolane is highly mobile in the subsurface.

Sorption of sulfolane to soil particles is low with sulfolane partitioning preferentially into porewater (Luther et al. 1998). The high aqueous solubility of sulfolane, in combination with the low K_{oc} and K_d, provides the potential for high concentrations of sulfolane to be present in soil porewater. Volatilisation of sulfolane is minimal due to the low Henry's law constant.

Biodegradation of sulfolane has been investigated in an activated sludge system, in wastewater treatment, in laboratory microcosm studies using contaminated aquifer sediments, and as part of a natural attenuation study in natural wetlands. Most studies have demonstrated that sulfolane biodegrades in nutrient-enriched aerobic microcosms from a variety of sulfolane-contaminated environmental samples (Fedorak and Coy 1996). Data from microcosm and field studies indicate that under typical groundwater conditions (aerobic or anaerobic, but very low in nutrients, particularly phosphate), sulfolane degradation may be very slow or non-existent. However, under conditions typical of surface water (aerobic, sufficient nutrients) it has been shown that sulfolane degradation can be relatively rapid, with complete removal occurring after 5 to 11 weeks (CCME 2006).

Uptake of sulfolane 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 sulfolane-impacted wetland were included in the study (CAPP 1999, 2000; Headley et al. 1999a,b). Analytical results indicated highly variable sulfolane 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. The maximum measured sulfolane concentration in water within the wetland was 185 mg·L^{-1}, and concentrations measured in the plants were as high as 256 mg·kg^{-1}.

Behaviour and Effects in Biota

Soil Microbial Processes

Specific studies designed to address the effect of sulfolane 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 sulfolane by indigenous soil bacteria. Studies by Fedorak and Coy (1996) and Kim et al. (1999) provide evidence that sulfolane is readily biodegradable at concentrations up to 2,000 mg·L^{-1} in soil porewater.

Terrestrial Plants

CAPP (2001) determined the toxicity of sulfolane 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 and organic carbon content. The endpoints measured were emergence, biomass, root length, and shoot length. Komex (1999) also assessed the toxicity of sulfolane to lettuce seed emergence in artificial soil. EC_{25} values, corrected to reflect analytically measured concentrations, ranged widely from 114 mg·kg^{-1} for reduced biomass of timothy in sand to 8,800 mg·kg^{-1} for reduced emergence of alfalfa in loam. Plants were generally most sensitive to sulfolane in till and least sensitive in loam.

Terrestrial Invertebrates

CAPP (2001) conducted acute (14 day) earthworm mortality tests using four soils with differing texture and organic carbon content. Komex (1999) also assessed the 14 day mortality endpoint for earthworms in artificial soil. LC_{25} values, corrected to reflect analytically measured concentrations, ranged from 665 mg·kg^{-1} in till to 4,500 mg·kg^{-1} in loam. Overall, sand, till and artificial soil returned similar toxicity values, which were approximately an order of magnitude lower than values from tests in loam.

Human and Experimental Animal Health Effects

Sulfolane is rapidly and readily absorbed via the oral and inhalation routes, but poorly absorbed via the dermal route of administration (Andersen et al. 1976; Ursin et al. 1995). Andersen et al. (1976) showed that sulfolane was rapidly distributed throughout the body and then slowly removed from plasma with a half-life of 3.5 to 5 hours. Low doses of sulfolane are readily metabolized in laboratory animals (Andersen et al. 1976).

There was minimal evidence of acute toxicity from sulfolane administered by various routes in rats, mice, guinea pigs, and rabbits. Studies by Andersen et al. (1976) indicated little variation between the LD_{50} of oral, parenteral, and subcutaneous administered doses (which ranged from 1,240 to 3,500 $mg·kg^{-1}·bw$ per day) for these four species. The intravenous LD_{50} values were lower, ranging from 632 to 1,094 $mg·kg^{-1}·bw$ per day. Regardless of the route of administration or species, sulfolane produced toxic signs indicative of central nervous system (CNS) stimulation or depression (dependent on dose).

Three studies have examined the chronic or sub-chronic toxicity of sulfolane to laboratory animals. Andersen et al. (1977) conducted subchronic (90 day) inhalation toxicity studies with rats, guinea pigs, beagle dogs, and squirrel monkeys. Toxic effects including leukopenia, increased plasma transaminase activity, convulsions, vomiting, and death were seen at higher concentrations. These toxic effects were not found in any of the test species on exposure to concentrations of 20 $mg·m^{-3}$ or lower. The inhalation exposure concentration of 20 $mg·m^{-3}$ was considered the NOAEL.

Zhu et al. (1987) reported the results of a six month study of the chronic toxicity of sulfolane administered orally to guinea pigs (which had just stopped breast-feeding) at dose levels of 0.25, 2.5, 25, and 250 $mg·kg^{-1}$ bw. Pathological examinations indicated a significant increase in fatty deposits in the liver tissue for the 2.5, 25, and 250 $mg·kg^{-1}$ bw exposure groups. Shrinkage of spleen white pulp and decreasing cell counts in spinal marrow were also noted in these three dose groups. No biochemical or pathological changes were found in the 0.25 $mg·kg^{-1}$ bw dosage group, which was determined to be the NOAEL.

Huntingdon Life Sciences (HLS 2001) exposed rats to sulfolane in their drinking water for 13 weeks at concentrations of 0, 25, 100, 400, and 1,600 $mg·L^{-1}$. The sulfolane exposure was reported to be well-tolerated, with the only adverse effects being a nephropathy in male rats at the two highest doses, and reduced white blood cell counts in females in the three highest dose groups. The NOAEL in female rats was 2.9 $mg·kg^{-1}·bw$ per day (equivalent to 25 $mg·L^{-1}$ sulfolane in drinking water) based on reduced white blood cell counts.

Sulfolane has never been assessed by mammalian cancer bioassays. The structurally related compound, 3-sulfolene was assessed by the National Cancer Institute and was found to be negative in a gavage carcinogenicity study in Osborne-Mendel rats and B6C3F1 mice (NCI 1978).

Mutagenicity and genotoxicity assays have been conducted by Shell (1982) and Phillips (1984). Sulfolane was not mutagenic in bacteria or yeast, and showed no evidence of being capable of producing structural alterations *in vitro* such as chromosomal aberrations in primary rat liver cultures or SCE (Chinese hamster ovary cells). On the other hand, there is one report of a positive response at the highest dose in a mouse lymphoma assay, but no clear dose-response. Based on the criteria described, there is insufficient evidence to conclude that sulfolane is genotoxic.

No reliable long-term reproductive or developmental toxicity studies have been conducted on sulfolane. Teratogenic effects of sulfolane were observed in pregnant mice after oral administration at doses of 93, 280, and 840 $mg·kg^{-1}$ bw. Skeletal changes were found at the highest treatment level (840 $mg·kg^{-1}$ bw) but not at lower exposures (Zhu et al. 1987). However, as this dose is approximately half of the LD_{50}, it is unclear whether this response represents a true teratogenic response, or simply the effects of a near-lethal dose on the pregnant mother.

A human tolerable daily intake (TDI) was derived from the HLS (2001) study. The NOAEL of 2.9 $mg·kg^{-1}·bw$ per day in female rats in this study was divided by an uncertainty factor of 300 (10 each for intra- and interspecies variation, and 3 for the aggregate of database limitations and subchronic to chronic extrapolation), to give a TDI of 0.0097 $mg·kg^{-1}·bw$ per day. The HLS (2001) study was selected over the Zhu et al. (1987) study because of concerns with the quality of the latter study, and over the Andersen et al. (1977) study based on a more applicable route of administration.

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

For sulfolane, the soil contact guideline was calculated based on a species sensitivity distribution of EC25 plant and invertebrate 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 50 $mg \cdot L^{-1}$ for sulfolane. 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 soil contact guideline was the lowest of the ecological guidelines/check values for sulfolane, 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 sulfolane, the CCME (2003) protocol was used together with the human tolerable daily intake of 0.0097 $mg \cdot kg^{-1} \cdot bw$ per day to calculate the human ingestion guideline. The ground water guideline for drinking water was calculated using the CCME (2003) protocol and the source guidance value for groundwater (SGVG) of 0.09 $mg \cdot L^{-1}$ (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 Sulfolane

The soil quality guidelines for sulfolane 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_{HH}, which is based on the protection of groundwater for drinking water (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 draft revised soil protocol (CCME 2003). There was no interim guideline for sulfolane 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 sulfolane (mg·kg^{-1} dry weight).

	Land Use			
	Agricultural	**Residential/ parkland**	**Commercial**	**Industrial**
Recommended Guideline	**0.8**[a]	**0.8**[a]	**0.8**[a]	**0.8**[a]
Human health guidelines/check values				
SQG_{HH}	**0.8**	**0.8**	**0.8**	**0.8**
Soil ingestion guidelines	660	660	2 400	41 000
Inhalation of indoor air check	NC	NC	NC	NC
Off-site migration check	—	—	—	9 000
Groundwater check (drinking water)	0.8[b]	0.8[b]	0.8[b]	0.8[b]
Produce, meat, and milk check	NC	NC	—	—
Environmental health guidelines/check values				
SQG_E	**210**	**210**	**430**	**430**
Soil contact guidelines	210	210	430	430
Soil and food ingestion guideline	NC[c]	—	—	—
Nutrient and energy cycling check	NC[c]	NC[c]	NC[c]	NC[c]
Off-site migration check	—	—	—	3 000
Groundwater check (aquatic life)	450	450	450	450
Interim soil quality criterion (CCME 1991)	No value	No value	No value	No value

Notes: NC = not calculated; ND = not determined; NA = not available; 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]The groundwater check for drinking water is the lowest of the human health guidelines and check values.

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

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