Screening Assessment for the Challenge

9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts

Chemical Abstracts Service Registry Number
125351-99-7

Environment Canada
Health Canada

November 2008

Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on 9,10-anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts (AMS), Chemical Abstracts Service Registry Number 125351-99-7. This substance was identified as a high priority for screening assessment and included in the Ministerial Challenge because it was originally found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and is believed to be in commerce in Canada.

The substance AMS was not considered to be a high priority for assessment of potential risks to human health, based upon application of the simple exposure and hazard tools developed by Health Canada for categorization of substances on the Domestic Substances List. Therefore, this assessment focuses on information relevant to the evaluation of ecological risks.

AMS is an organic “unknown or variable composition, complex reaction products, and biologicals” (UVCB) substance that may be used in Canada and elsewhere as a blue colorant dye in textiles, printing inks, rubber, plastic products, paints, lacquers and varnishes. The substance is not naturally produced in the environment. Between 100 and 1000 kg/year of AMS were imported into Canada in 2005 and 2006, for use mainly in the colorants and plastics industry. The quantity of AMS imported into Canada, along with the uses reported for this substance, indicate that it could potentially be released into the Canadian environment.

Based on certain assumptions and reported use patterns, most of the substance is expected to end up in waste disposal sites, but a relatively large fraction may also be released to water. It is not expected to be significantly present in other media.

Based on its physical and chemical properties, AMS does not have the potential to accumulate in aquatic organisms and an empirical acute aquatic toxicity value suggests that the substance is not hazardous to aquatic organisms. When considered together with the low volume of AMS imported into Canada, as well as information on its uses, it is unlikely that AMS is causing ecological harm in Canada. However, AMS does not degrade quickly in the environment. It is expected to be persistent in water, soil and sediments. Therefore, the substance has been determined to meet the persistence criteria as set out in the *Persistence and Bioaccumulation Regulations*.

In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment.

Introduction

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

Based on the information obtained through the categorization process, the Ministers identified a number of substances as high priorities for action. These include substances that

- met all of the ecological categorization criteria, including persistence (P), bioaccumulation potential (B) and inherent toxicity to aquatic organisms (iT), and were believed to be in commerce; and/or
- met the categorization criteria for greatest potential for exposure (GPE) or presented an intermediate potential for exposure (IPE), and had been identified as posing a high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity.

The Ministers therefore published a notice of intent in the *Canada Gazette*, Part I, on December 9, 2006 (Canada 2006), that challenged industry and other interested stakeholders to submit, within specified timelines, specific information that may be used to inform risk assessment, and to develop and benchmark best practices for the risk management and product stewardship of those substances identified as high priorities.

The substance 9,10-anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts was identified as a high priority for assessment of ecological risk as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada.

The Challenge for 9,10-anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts was published in the *Canada Gazette* on May 12, 2007 (Canada 2007). A substance profile was released at the same time. The substance profile presented the technical information available prior to December 2005 that formed the basis for categorization of this substance. As a result of the Challenge, submissions of information were received.

Although 9,10-anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE and high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Under CEPA 1999, screening assessments focus on information critical to determining whether a substance meets the criteria for defining a chemical as toxic as set out in section 64 of the Act, where

> "64. […] a substance is toxic if it is entering or may enter the environment in a quantity or concentration or under conditions that
>
> (*a*) have or may have an immediate or long-term harmful effect on the environment or its biological diversity;
> (*b*) constitute or may constitute a danger to the environment on which life depends; or
> (*c*) constitute or may constitute a danger in Canada to human life or health."

Screening assessments examine scientific information and develop conclusions by incorporating a weight of evidence approach and precaution.

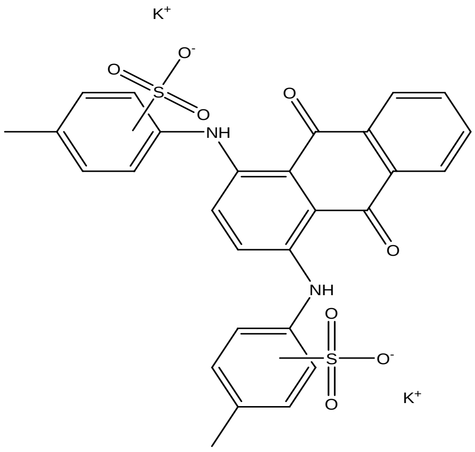
This screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to February 2008 for ecological sections of the document. Key studies were critically evaluated; modelling results may have been used to reach conclusions. When available and relevant, information presented in hazard assessment from other jurisdictions was considered. The screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies and lines of evidence pertinent to the conclusion.

This screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. The critical information and considerations upon which the assessment is based are summarized below.

Substance Identity

For the purposes of this report, this substance will be referred to as AMS, which has been derived from the DSL inventory name 9,10-anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts. Other names and identifying characteristics of the substance are presented in Table 1.

Table 1. Substance identity

Chemical Abstracts Service Registry Number (CAS RN)	**125351-99-7**
Name on Domestic Substances List (DSL)	**9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts**
Other name	*1,4-Di-(4-methylanilino)anthraquinone, sulfonated, potassium salts*
Chemical group (DSL stream)	Organic UVCB
Chemical sub-group	Anthracenediones
Formula of representative chemical [a]	$C_{28}H_{20}N_2O_8S_2.2K$
Structure of representative chemical [a]	
Simplified Molecular Input Line Entry System (SMILES) of representative chemical [a]	O=C(C3=C2C=CC=C3)C1=C(NC5=CC=C(C)C=C5S(=O)([O-])=])=O)=C1C2=O.[K+].[K+]
Molecular mass of representative chemical [a]	654.79 g/mol

[a] This structure differs from that used for Categorization, since a more representative chemical structure was identified from analysis of information gathered from the CEPA section 71 notices for the 2006 calendar year (Environment Canada and Health Canada. 2007). This information indicated that the chemical structure of benzenesulfonic acid, 2,2'-[(9,10-dihydro-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-methyl-, dipotassium salt (CAS RN 83044-88-6) is similar to that of AMS. The difference between these two chemical structures is the fact that AMS does not define the position of the sulfonate groups (Table 3). A new set of quantitative structure-activity relationship (QSAR) estimates for persistence were generated using this new chemical structure.

Physical and Chemical Properties

Table 2 contains experimental and extrapolated physical and chemical properties of AMS that are relevant to its environmental fate.

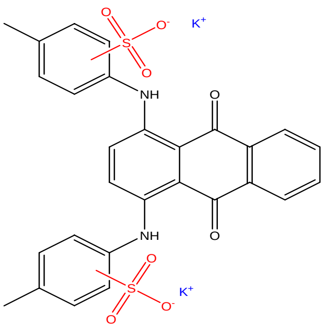
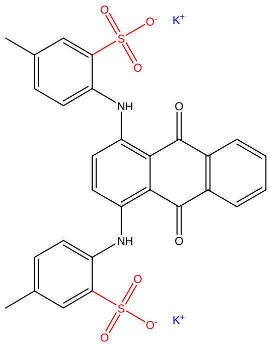
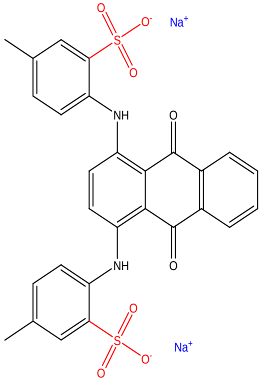
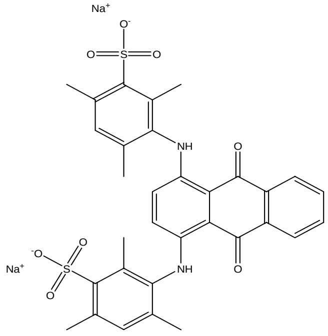
Table 2. Physical and chemical properties for AMS

Property	Type	Value	Temperature (C°)	Reference
Physical state	Experimental	Blue powder	-40 to 40	MSDS 2003
Boiling point (ºC)	Read-across [a]	>150	n/a	ETAD 1995
Decomposition point (ºC)	Experimental	>170	n/a	MSDS 2003
	Read-across [a]	>300	n/a	ETAD 1995
Vapour pressure (Pa)	Read-across [a]	10^{-8} to 10^{-10}	25	ETAD 1995; Baughman and Perenich 1988
Henry's Law constant (Pa·m^3/mol)	No information available			
Log K_{ow} (Octanol-water partition coefficient; dimensionless)	Read-across [a]	<3	25	Anliker et al. 1981; Anliker and Moser 1987
Log K_{oc} (Organic carbon-water partition coefficient – L/kg; dimensionless)	No information available			
Water solubility (mg/L)	Experimental	30 000	20	MSDS 2003
	Read-across [a]	>10 000	25	ETAD 1995

[a] The extrapolated values used for substances in the disulfonic acid dyes group are based on evidence on disulfonic acid dyes submitted to Environment Canada under the *New Substance Notification Regulations* and/or available evidence from other disulfonic acid dye analogues (e.g., ETAD 1995).

At the Environment-Canada-sponsored Quantitative Structure–Activity Relationship (QSAR) Workshop in 1999 (Environment Canada 2000), many structural classes of pigments and dyes were identified by Environment Canada and other invited modelling experts as "difficult to model" using QSARs. The inherent properties of many of the structural classes of dyes and pigments (including acid and disperse dyes) are not amenable to model prediction because they are considered "out of the model domain of applicability" (e.g., structural and/or property parameter domains). Therefore Environment Canada reviews the applicability of QSAR models to dyes and pigments on a case-by-case basis to determine the domain of applicability. Environment Canada has considered it inappropriate to use QSAR models to predict the physical and chemical properties of AMS and has consequently used a “read-across” approach to determine the approximate physical and chemical properties in Table 2. These properties were subsequently used for further modelling in this assessment.

Table 3. Structural analogues of AMS

<table>
<tr>
<td>i.
9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts
(CAS RN 125351-99-7)</td>
<td>ii.
Benzenesulfonic acid, 2,2'-[(9,10-dihydro-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-methyl-, dipotassium salt
(CAS RN 83044-88-6)</td>
<td>iii.
Benzenesulfonic acid, 2,2'-[(9,10-dihydro-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-methyl-, disodium salt
(CAS RN 4403-90-1)</td>
<td>iv.
Benzenesulfonic acid, 3,3'-[(9,10-dihydro-9,10-dioxo-1,4 anthracenediyl)diimino]bis[2,4,6-trimethyl-, disodium salt
(CAS RN 4474-24-2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td colspan="4">- The difference between the chemical structures of *i.* (AMS) and *ii.* is that *i.* does not define the position of the sulfonate groups.
- Structures *ii.* and *iii.* are respectively the potassium and the sodium salt of the same substance.
- The difference between the chemical structures of *i.* (AMS) and *iv.* is the two additional methyl groups at the ortho position of the aromatic ring for *i.* and the fact that *ii.* does not define the position of the sulfonate groups.
- Chemical Abstracts Service Registry Numbers 83044-88-6, 4474-24-2 and 4403-90-1 are very good ecotoxicological analogues of CAS RN 125351-99-7 (AMS).</td>
</tr>
</table>

When available, empirical data from analogues listed in Table 3 were used as values or supporting values for the weight of evidence.

Sources

AMS is not reported to be naturally produced in the environment.

Information gathered from the CEPA 1999 section 71 notices for the 2005 and 2006 calendar years indicate that AMS was not manufactured in Canada in a quantity meeting the 100 kg reporting threshold (Canada 2006b; Environment Canada and Health Canada. 2007. For the 2005 and 2006 calendar years, the same Canadian company reported importing this substance in the 100–1000 kg/year range. In addition, for the 2006 calendar year, two Canadian companies identified a stakeholder interest in AMS (Environment Canada and Health Canada. 2007).

According to the Substances in Preparations in Nordic Countries database (SPIN 2006), AMS was used in Sweden in the years 1999–2004. However, information on exact use quantities and use patterns is not open to the public.

Uses

The company that reported importing AMS into Canada in response to a CEPA section 71 survey notice for the 2005 and 2006 calendar years indicated the following North American Industry Classification System (NAICS) code: 418410 “Chemical (except Agricultural) and Allied Product Wholesaler-Distributors. This Canadian industry sector comprises establishments primarily engaged in wholesaling industrial and household chemicals, cleaning compounds and preparations, plastics resins, plastic basic forms and shapes, and industrial gases.”

This NAICS code is consistent with the DSL use codes that were identified for AMS in 1986.

The information above suggests that AMS may have widespread uses, particularly as a blue colorant dye.

Releases to the Environment

AMS is not naturally released into the environment from natural sources.

The company that reported importing this substance in the 2006 did not indicate any releases of this chemical to the environment.

Mass Flow Tool

To estimate release of AMS to the environment at different stages of its life cycle, a mass flow tool was used. For each identified type of use of the substance, the results of the tool include the estimated proportion and quantity of release to the different environmental media as well as the proportion of the substance chemically transformed or sent for waste disposal. Assumptions and input parameters used in making these estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers’ websites and technical databases. Of particular relevance are emission factors, which are generally expressed as the fraction of a substance released to the environment, particularly during its manufacture, transformation, and use associated with industrial processes. Sources of such information include emission scenario documents (often developed under the auspices of the

Organisation for Economic Co-operation and Development – OECD), and default assumptions used by different international chemical regulatory agencies.

Based on the tool results (Table 4), of the total quantity of the substance that is in commerce, most ends up in waste disposal sites (60.56%), but a significant percentage is predicted to be released to water (37.58%). Another 1.85% of the substance is lost by transformation, which indicates destruction or modification of the structure of the substance after its disposal (e.g., incineration).

Table 4. Estimated releases and losses of AMS to environmental media, transformation and distribution to management processes, based on the mass flow tool[1]

Fate		**Proportion of the mass (%)**	**Major life cycle stage involved**
Releases to environment			
	To soil	0.0	Use
	To air	0.01	Processing and use
	To water	37.58	Processing
Process			
	Loss by transformation	1.85	Use
	Transferred to waste disposal sites (e.g., landfill)	60.56	Waste management (e.g., landfill)
	Managed as hazardous waste	n/a	Waste management (e.g., landfill)

[1] For AMS, information from the following OECD emission scenario documents was used to estimate releases to the environment and distribution of the substance, as summarized in this table: OECD 2004; OECD 2006. Values presented for releases to environmental media do not account for possible mitigation measures that may be in place in some locations (e.g., partial removal by sewage treatment plants). Specific assumptions used in derivation of these estimates are summarized in Environment Canada 2007a

Based on the above, the largest release of AMS is to water associated with the processing and use stage of its life cycle. Note that the mass flow tool assumes no releases from waste disposal sites.

Environmental Fate

Based on its physical and chemical properties (Table 2) AMS is expected to partition predominantly to water.

According to the mass flow tool results presented in Table 4, most of AMS is released to water during processing and so a release scenario to water seems to be the most relevant for Canada.

If released into water, AMS will tend to stay in water, based upon its high water solubility value (30 000 mg/L).

AMS may enter soil through waste water treatment plant sludge, which may be used for soil enrichment, or through the disposal of sludge, coloured textiles, papers and leather substrates in landfills. Volatilization from dry or moist soil surfaces seems to be an unimportant fate process based upon the low estimated vapour pressure. If released to soil (from products), AMS is expected to migrate to the water phase of the soil (e.g., groundwater) or undergo surface runoff.

Air is not considered to be an important medium for AMS because of the low volatility of this substance, based on its low predicted vapour pressure.

Persistence and Bioaccumulation Potential

Environmental Persistence

There are no reliable empirical biodegradation data available for this substance.

ETAD (1995) states that, with some exceptions, dyes are considered essentially non-biodegradable under aerobic conditions. Repeated evaluation of ready and inherent biodegradability using accepted screening tests (e.g., OECD) have confirmed this assumption (Pagga and Brown 1986; ETAD 1992). Based on the chemical structure of AMS, there is no reason to suspect that biodegradation will be other than that described for dyes in ETAD (1995). The modelled data presented in Table 5 support this assumption of non-degradability.

Once released into the environment, AMS is thus expected to be persistent in all media. AMS is not expected to be found in the air compartment; however, the oxidation half-life of 0.06 days (Table 5) demonstrates that any AMS in air could be rapidly oxidized. AMS is not expected to react, or react appreciably, with other photo-oxidative species in the atmosphere, such as O_3 and NO_3, nor is it likely to degrade via direct photolysis. Therefore, it is expected that reactions with hydroxyl radicals will be the most important fate process in the atmosphere for this chemical. With a half-life of 0.06 days via reactions with hydroxyl radical, AMS is not persistent in air.

Table 5. Modelled data for persistence of AMS

Medium	Fate process	Degradation value	Degradation endpoint	Reference
Air	Atmospheric oxidation	0.06	Half-life (days)	AOPWIN 2000
Air	Ozone reaction	Not reactive	Half-life (days)	AOPWIN 2000
Water	Biodegradation	>182 (recalcitrant)	Half-life (days)	BIOWIN 2000 (USM)
Water	Biodegradation	0 (does not biodegrade fast)	Probability	BIOWIN 2000 MITI Non-linear
Water	Biodegradation	Not readily biodegradable	Weighted 6 model assessment	BIOWIN 2000
Water	Biodegradation	Out of acceptable domain of model	Probability	TOPKAT 2004
Water	Biodegradation	2.9%	BOD (MITI 301C)	CATABOL c2004-2008
Water	Anaerobic biodegradation	0 (does not biodegrade fast)	Probability	BIOWIN 2000
Sediment	Biodegradation	>728 (recalcitrant)	Half-life (days)	Based on the modelled half-life in water[1]
Soil	Biodegradation	>182 (recalcitrant)	Half-life (days)	Based on the modelled half-life in water[1]

[1] Values were derived from the modelled half-life in water using the extrapolation factors of Boethling et al. (1995): $t_{1/2\ water} : t_{1/2\ soil} : t_{1/2\ sediment} = 1:1:4$.

For estimating degradation in water, soil and sediment, a QSAR weight-of-evidence approach (Environment Canada, 2007a) was applied using the models shown in Table 5. Based on these results AMS can be considered persistent in water (half-life ≥ 182 days). To estimate a half-life in soils and sediments, an approach has been developed using Boethling's extrapolation factors (Boethling et al. 1995), which involves estimating the half-life in these media from that estimated for water ($t_{1/2\ water}$: $t_{1/2\ soil}$:$t_{1/2\ sediment}$ = 1: 1: 4). Therefore, in soils and sediments, the half-lives for AMS are expected to exceed 182 days and 365 days, respectively.

The weight of evidence based on the data described above indicates that AMS meets the persistence criteria for water and soil (half life ≥ 182 days) and sediment (half-life ≥ 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

There are no empirical bioaccumulation data available for this substance.

The log K_{ow} data presented in the read-across in Table 2 suggest that this substance does not have the potential to bioaccumulate in the environment.

A reliable log K_{ow} for AMS could not be estimated using predictive models. A range of QSAR bioaccumulation predictions were obtained from the various QSAR models considered for AMS. However, these QSAR predictions for AMS are not considered reliable. The main reason for the lack of reliability of these QSAR bioaccumulation predictions is the high water solubility potential of anionic dyes like AMS, which is not accounted for in these predictions.

Anionic dyes, in general, will have low log K_{ow} values (< 3.0) and high water solubility (> 2000 mg/L). This pattern has been observed based on data from previous bioconcentration and partition studies with dyes (ETAD 1995). The high water solubility of AMS (Table 2) provides an indication that AMS has a low potential to bioaccumulate or bioconcentrate in aquatic biota.

Another reason for the low bioaccumulation potential of AMS is its high degree of dissociation under typical environmental conditions. Perrin et al. (1981) and Lee et al. (1990) suggest a decrease of only 0.11 unit in the pKa for organic acids and bases with a change in ionic strength (μ) from 0 to 0.1. Ionic strength for aqueous phases in the environment typically ranges from 0.001 to 0.14. Therefore, overall effects from pH and pKa changes due to ionic strength upon speciation are likely to be minimal. This suggests that the "salt" form is likely to behave as either the ionized or the neutral species depending on the pH and the pKa of the chemical. The degree of dissociation is dependent on the pKa (estimated to be ~<1), therefore AMS is expected to be highly dissociated under typical environmental conditions. This high degree of dissociation is a likely reason for the low bioaccumulation potential for this substance.

The weight of evidence indicates that AMS does not meet the bioaccumulation criterion (BCF, BAF ≥ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

In the Aquatic Compartment

There are few empirical ecotoxicity data available for AMS and therefore data from a close chemical analogue (CAS RN 4474-24-2) were also considered. Based on the available experimental evidence (Table 6) and the analysis of functional groups, AMS is not expected to cause harm to aquatic organisms at relatively low concentrations (e.g., acute $LC_{50} < 1$ mg/L).

Table 6 Empirical data for aquatic toxicity for AMS and a chemical analogue

CAS RN	Test organism	Type of test	Duration (hours)	Endpoint	Value (mg/L)	Reference
4474-24-2	*Oncorhynchus mykiss (Salmo gairdneri)* [rainbow trout]	Acute	48	LC_{50}[1]	75	Sandoz 1977
	Bacteria (activated sludge)	Respiration inhibition	3	IC_{50}[2]	>1.000	Clariant 1989
125351-99-7	*Poecilia reticulata* (guppy)	Acute	96	LC_{50}[1]	14.3	BMG 1996

[1] LC_{50} – The median or nominal lethal concentration (LC_{50}) is the concentration of a substance that is estimated to be lethal to 50% of the test organisms.

[2] IC_{50} – The concentration of a substance that is estimated to cause inhibition of 50% of the test organisms.

Experience with new dyes at Environment Canada and the United States Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) has shown that, in general, the number of sulphonic acid groups determines potential for toxicity. Dyes with one or two sulphonic acid groups have shown moderate to high acute toxicity (<1-10 mg/L) to some aquatic biota, while dyes with more than two sulphonic acid groups have shown very low acute (>100 mg/L) and chronic (>10 mg/L) toxicity to most aquatic biota. Furthermore, Environment Canada has generally found anionic dyes to be of low toxicity regardless of the number of acid groups, but some exceptions have been found (e.g., when a reactive functional group is not hindered). Therefore, AMS as an anionic dye with two sulphonic acid groups and no reactive functional group is expected to have a low to moderate toxicity to aquatic organisms.

An empirical acute toxicity study on *Poecilia reticulata* (guppy) (Table 6) found a 96-hour LC_{50} of 14.3 mg/L indicating that AMS is not hazardous to aquatic organisms at relatively low concentrations (i.e., $LC/EC_{50}s > 1$ mg/L) (Appendix I). This conclusion is also supported by another empirical acute toxicity study for an analogue of AMS (CAS RN 4474-24-2) on *Salmo gairdneri, oncorhynchus mykiss* (rainbow trout) (Table 6) which found a 48-hour LC_{50} of 75 mg/L.

A range of aquatic toxicity predictions were obtained from the various QSAR models considered for AMS and its analogues. However, as with bioaccumulation, these QSAR ecotoxicity predictions for AMS are not considered reliable.

The available empirical ecotoxicity information indicates that AMS is moderately toxic to aquatic organisms (acute toxicity 10-100 mg/L).

In Other Environmental Compartments

Because AMS could be released to soil from waste disposal of products that degrade and release AMS, it would be desirable to obtain toxicity data for soil organisms. However, no suitable ecological effects studies were found for this compound in media other than water.

Ecological Exposure Assessment

No data concerning concentrations of AMS in environmental media (air, water, soil, sediment) in Canada have been identified. Environmental concentrations are, therefore, estimated from available information, including estimated substance quantities, release rates and receiving water bodies.

Environment Canada conducted quantitative evaluations of exposure and of ecological effects for this substance, as further considerations within the weight of evidence.

The Industrial Generic Exposure Tool – Aquatic (IGETA) (Environment Canada 2007b) was used to determine whether there is a potential risk associated with AMS by comparing the conservative predicted environmental concentration (PEC) in the aquatic environment with a predicted no-effect concentration. The result is a risk quotient based on an industrial non-site-specific scenario. This simple model represents a point-source discharge from an industry, its dilution in a small watercourse and calculation of a risk quotient for that scenario.

A very conservative PEC was calculated using the following **equation (1)**:

$$\text{PEC} = \frac{\text{I} \times \text{L} \times (1-\text{R}) \times 1000}{\text{D} \times (\text{F} + \text{S}) \times 86\,400}$$

Where:

PEC = Predicted environmental concentration (mg/L)
I = Maximum mass imported into (or manufactured in) an industrial complex linked with a discharge point (400 kg/year)
L = Losses by processing (100%).

R = Removal rate of the sewage treatment plant (0%).
1000 = Conversion of units (kg/m^3 to mg/L)
D = Days of release of the substance from site (150 days/year).
T = Transformation of unit (1000) (default value)
F = Flow of the receiving watercourse (0.65 m^3/s)
S = Flow of the effluent from the sewage treatment plant (0.04 m^3/s)
86 400 = Number of seconds in one day (sec)

Based on this equation, the PEC in receiving waters is 0.0447 mg/L (Environment Canada 2008).

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine various supporting information and develop conclusions based on a weight-of-evidence approach and using the precautionary principle as required under section 76.1 of CEPA 1999.

Although AMS is expected to be persistent in water, soil and sediment, it is expected to have a low bioaccumulation potential. The relatively low importation volumes of AMS, along with information on its uses, indicate relatively low potential for releases into the Canadian environment. It has also been demonstrated to have a moderate potential for toxicity to aquatic organisms.

A risk quotient analysis, integrating very conservative estimated potential exposures with potential for adverse environmental effects, was performed for the aquatic medium. A risk quotient was calculated to determine whether there are ecological risks in Canada.

Equation (1) presented above was used to estimate the PEC of 0.0447 mg/L. A predicted no-effect concentration (PNEC) was derived from the acute toxicity value of 14.3 mg/L for the guppy, by dividing this value by an assessment factor of 100 (10 to account for interspecies and intraspecies variability in sensitivity and 10 to estimate a long-term no-effects concentration from a short-term LC_{50}) to give a PNEC of 0.143 mg/L. The resulting conservative risk quotient (PEC/PNEC) = 0.0447 / 0.143 = 0.313.

The calculated risk quotient is less than 1. Given that IGETA provides a conservative estimate of exposure, this result indicates a low potential for ecological harm to the aquatic environment resulting from local exposure from a point-source industrial release. The low risk quotient indicates that there is a 100-fold margin of safety, to account for possible errors associated with calculation of the PEC and PNEC.

This information suggests that AMS is unlikely to be causing ecological harm in Canada.

Uncertainties in Evaluation of Ecological Risk

The lack of supporting evidence from empirical studies is a source of uncertainty in the bioaccumulation assessment.

The persistence assessment is limited by the lack of experimental biodegradation data, which necessitated generation of model predictions.

The uncertainties also exist because of the lack of information on environmental concentrations (e.g., monitoring data) in Canada for AMS.

Uncertainties are also associated with the fraction of substance in commerce that is released, and with the fraction that is removed in sewage treatment plants.

Regarding toxicity, based on the anticipated release pattern for the substance, the significance of soil as a medium of exposure is not well addressed by the effects data available. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures.

For the exposure assessment, the predicted environmental concentration accounts for concentrations in water only, so exposure through soils, suspended solids and sediments is not considered.

Conclusion

Based on the information presented in this screening assessment, it is concluded that AMS 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.

It is therefore concluded that AMS does not meet the definition of “toxic” as set out in section 64 of CEPA 1999. Additionally, AMS does not meet criteria for bioaccumulation potential but its meets criteria for persistence as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

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Appendix I - Robust Study Summary

Robust Study Summaries Form and Instructions: Aquatic iT				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	Reference: BMG Engineering AG.1996. Study Title: Sandlan Green MF-BL: 96-hour Acute Toxicity to Poecilia reticulate (Guppy). Report Number 512-96. Performed by BMG Engineering AG in December 1996, Zurich, Switzerland.			
2	Substance identity: CAS RN	n/a		125351-99-7
3	Substance identity: chemical name(s)	n/a		Sandolan Gruen MF-BL
4	Chemical composition of the substance	2		
5	Chemical purity	1	Y	
6	Persistence/stability of test substance in aquatic solution reported?	1	Y	
	Method			
7	Reference	1	Y	
8	OECD, EU, national, or other standard method?	3	Y	OECD 203
9	Justification of the method/protocol if not a standard method was used	2		
10	GLP (Good Laboratory Practice)	3	N	Good Scientific Practice
	Test organism			
11	Organism identity: name	n/a		*poecilia reticulata*
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organis	1	Y	
14	Length and/or weight	1	Y	
15	Sex	1		
16	Number of organisms per replicate	1	Y	7
17	Organism loading rate	1	N	
18	Food type and feeding periods during the acclimation period	1	Y	
	Test design / conditions			
19	Test type (acute or chronic	n/a		acute
20	Experiment type (laboratory or field	n/a		laboratory
21	Exposure pathways (food, water, both)	n/a		water
22	Exposure duration	n/a		96 hour
23	Negative or positive controls (specify)	1	Y	negative
24	Number of replicates (including controls)	1	N	
25	Nominal concentrations reported?	1	Y	5
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	1		
28	Were concentrations measured periodically (especially in the chronic test)?	1	N	

29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	
30	Photoperiod and light intensity	1	Y	
31	Stock and test solution preparation	1	Y	
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1		
33	If solubilizer/emulsifier was used, was its concentration reported?	1		
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1		
35	Analytical monitoring intervals	1	Y	
36	Statistical methods used	1	N	
	Information relevant to the data quality			
37	Was the endpoint directly caused by the chemical's toxicity, not by organism's health (e.g. when mortality in the control >10%) or physical effects (e.g. 'shading effect')?	n/a	Y	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
40	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	Y	static
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	Y	
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	
43	Was toxicity value below the chemical's water solubility?	3	Y	
	Results			
44	Toxicity values (specify endpoint and value)	n/a	n/a	LC50=14.3mg/L
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a		NOEC=8mg/L
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a		
47	***Score: ... %***	***75.0***		
48	***EC Reliability code:***	***2***		
49	***Reliability category (high, satisfactory, low):***	***Satisfactory Confidence***		
50	***Comments***			