Substance Profile for The Challenge

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

(AMS)

CAS No. 125351-99-7

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) required the Minister of Health and Minister of the Environment to categorize the approximately 23 000 substances on the Domestic Substances List (DSL). Categorization involved identifying those substances on the DSL that are a) considered to be persistent (P) and/or bioaccumulative (B), based on criteria set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada, 2000), and "inherently toxic" (iT) to humans or other organisms, or b) that present, to individuals in Canada, the greatest potential for exposure (GPE).

Further to this activity, the Act requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that meet the categorization criteria. A screening assessment involves a scientific evaluation of available information for a substance to determine whether the substance meets the criteria set out in section 64 of CEPA 1999. 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 the addition of the substance to the List of Toxic Substances in Schedule 1 of CEPA 1999 and, where applicable, the implementation of virtual elimination of releases to the environment.

A number of substances have been identified by the Ministers as high priorities for action based on the information obtained through the categorization process. This includes substances:

- that were found to meet all of the ecological categorization criteria, including persistence, bioaccumulation potential and inherent toxicity to aquatic organisms (PBiT), and that are known to be in commerce, or of commercial interest, in Canada, and/or
- that were found either to meet the categorization criteria for GPE or to present an intermediate potential for exposure (IPE), and were identified as posing a high hazard to human health based on available evidence on carcinogenicity, mutagenicity, developmental toxicity or reproductive toxicity.

Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting and interpreting the results of an assessment, sufficient data are currently available to conclude whether these substances meet the criteria under section 64 of CEPA 1999.

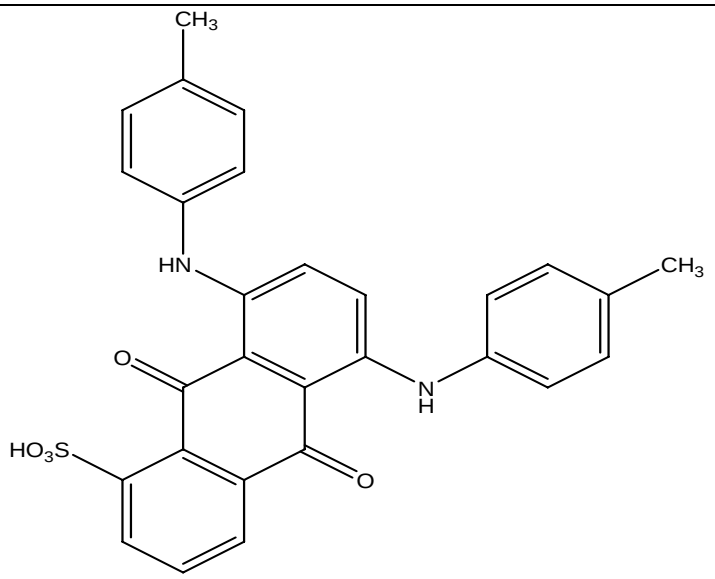
As such, the Ministers have issued a Challenge to industry and other interested stakeholders through publication in Canada Gazette Part I December 9, 2006 to submit, within the timelines stated in the Challenge section of this document, specific information that may be used to inform risk assessment and to develop and benchmark best practices for risk management and product stewardship.

The substance 9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts was identified as a high priority for action as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The technical human health and ecological information that formed the basis for concern associated with this substance is contained in Appendices I and II, respectively.

Substance Identity

For the purposes of this report, this substance will be referred to as AMS, which has been derived from the inventory name 9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts.

CAS Registry Number (NCI)	125351-99-7
Inventory name	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	Organic UVCB
Chemical sub-group	Anthracenediones
Formula of Representative Chemical	$C_{28}H_{22}N_2O_5S$

Structure of Representative Chemical	
SMILES of Representative Chemical	C42=C(C(=O)C3=C(C4=O)C=CC=C3S(=O)(=O)O)C(NC5=CC=C(C)C=C5)=CC=C2NC1=CC=C(C)C=C1
Molecular mass of Representative chemical	498.56 g/mol

Based on information submitted in response to a legal Notice published in 2006 under section 71 of CEPA 1999, AMS was not manufactured in Canada in 2005 in a quantity meeting the 100 kg reporting thresholds. One company reported importing up to 1,000 kg into Canada in 2005 for activities described as Wholesale Trade/Distribution of Chemical (except agricultural) and Allied Products. It can be used as colorant in printing inks, in rubber and plastic products, and in paints, lacquers and varnishes (Environment Canada, 2006).

THE CHALLENGE

Respecting direction under section 76.1 of CEPA 1999, and in the absence of additional relevant information as a result of this Challenge, the Ministers are predisposed to conclude, based on a screening assessment, that this substance satisfies the definition of toxic under section 64 of CEPA 1999. As such, the Ministers are prepared to then recommend to the Governor in Council that this substance be added to the List of Toxic Substances in Schedule 1 of CEPA 1999, with the intent of initiating the development of risk management measures taking into account socio-economic considerations.

If it is determined that the substance meets the virtual elimination criteria in subsection 77(4) of CEPA 1999, then subsequent risk management activities will be based on the objective of eliminating the release of any measurable quantity of the substance to the environment. In the absence of further information on existing management practices for a substance, actions would be proposed based on the assumption of worst-case practices. The management actions being considered for such substances at this time include prohibition through regulations, of the manufacture, use, sale, offer for sale and import of this substance, except for those activities controlled under the *Pest Control Products Act* and/or the *Food and Drugs Act.*

Exceptionally, should no information be identified to indicate that this substance is in commerce in Canada, the Ministers will conclude, based on a screening assessment, that this substance does not satisfy the definition of toxic under section 64 of CEPA 1999. However, given the properties of this substance, there is concern that new activities for the substance that have not been identified or assessed under CEPA 1999 could lead to the substance meeting the criteria set out in section 64 of the Act. Therefore it would be recommended that this substance be subject to the Significant New Activity provisions specified under subsection 81(3) of the Act, to ensure that any new manufacture, import or use of this substance in quantities greater than 100 kg/year is notified, and that ecological and human health risk assessments are conducted as specified in section 83 of the Act prior to the substance being introduced into Canada.

Section 71 Notice

Under the Challenge, information deemed necessary for improved decision making may be gathered by the Minister of Environment using section 71 of CEPA 1999. This information may be used for the purpose of assessing whether a substance is toxic or is capable of becoming toxic as defined under section 64 of CEPA 1999, or for the purpose of assessing whether to control, or the manner in which to control a substance.

The information mandated through the notices may relate to, among other things; quantity of the substance imported, manufactured, used, or released, concentrations, suppliers, customers, as well as types of uses of the substance.

Copies of the section 71 notice and guidance on how to comply with it are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca), or from the contact provided below.

Opportunity to Submit Additional Information to Inform Screening Assessment

The Ministers of Health and Environment are inviting the submission of additional information for consideration during screening assessment of this substance. Data of the types described in the following paragraphs are considered most relevant, although other submitted information will be considered.

Data on the persistence, bioaccumulation, and potential for toxicity of the substance to organisms in different environmental media – Through the categorization exercise, available experimental data were collected up to December 2005. Where acceptable experimental data were not available, Quantitative Structure Activity Relationships (QSARs) or read across data were used to fill the data gaps. Since experimental data are preferred, interested parties have an opportunity to provide new or additional relevant experimental study information on the persistence, bioaccumulation, and potential for toxicity of this substance to organisms in different environmental media (air, water, sediment, soil). Efforts should focus on providing data for the endpoints for which quality experimental data does not already exist, as demonstrated by the information summarized in Appendix II of this document. As submitted data will be evaluated for completeness and robustness, it is recommended that stakeholders follow the guidance for test protocols and alternative approaches for test data, as described in Section 8 of the "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers".[1]

Data on the toxicity of the substance to human health - Through the categorization exercise, the high health priorities for action were those substances identified by various agencies as representing a high health hazard on the basis of potential to induce cancer, and/or adversely affect reproduction and development, two critical determinants of the health of Canadians of all ages. The hazard classifications used were those developed by national or international agencies in which large numbers of substances have been classified for endpoint-specific hazard based on original review and critical evaluation of data, assessments of weight of evidence and extensive peer review. Interested parties have an opportunity to provide new or additional relevant experimental study information on the toxicity of the substance to human health which could inform the screening assessment.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

[1] "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers (version 2005)", Government of Canada, Available from http://www.ec.gc.ca/substances/nsb/eng/cp_guidance_e.shtml

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[2] "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers (version 2005)", Government of Canada, Available from http://www.ec.gc.ca/substances/nsb/eng/cp_guidance_e.shtml

Opportunity to Submit Additional Information on Current Uses and Existing Control Measures to Inform the Risk Management Approach for this Substance

The Ministers of Health and Environment are inviting the submission of additional information that is deemed beneficial by interested stakeholders, relating to the extent and nature of the management/stewardship of substances listed under the Challenge.

Organizations that may be interested in submitting additional information in response to this invitation include those that manufacture, import, export or use this substance whether alone, in a mixture, in a product or in a manufactured item.

Additional information is being invited in the following areas:

- Import, manufacture and use quantities
- Substance and product use details
- Releases to the environment and spill management
- Current and potential risk management and product stewardship actions
- Existing legislative or regulatory programs controlling/managing the substance
- Information to support the development of a regulatory impact assessment.

A questionnaire is available which provides a detailed template as an example for the submission of this information. Guidance on how to respond to the challenge questionnaire is also available. Interested stakeholders are invited to provide available additional information, recognizing that not all questions in the questionnaire may be relevant to a particular substance, use, or industrial sector.

Copies of the questionnaire and associated guidance are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca)**,** or from the contact provided below.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

Request for Documents and Submission of Information

Documents and instructions may be requested from the following contact. Information in response to the above Challenge must be submitted to this address.

DSL Surveys Coordinator
Place Vincent Massey, 20th Floor
351 Saint Joseph Boulevard
Gatineau QC K1A 0H3
Tel: 1-888-228-0530/819-956-9313

Fax: 1-800-410-4314 / 819-953-4936
Email: DSL.surveyco@ec.gc.ca

Appendix I
Human Health Information
to Support The Challenge for
9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-,
sulfonated, potassium salts
(AMS)
CAS No. 125351-99-7

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA, 1999), Health Canada undertook to categorize substances on the Domestic Substances List (DSL) to identify those representing the greatest potential for human exposure (GPE) and those among a subset of substances considered persistent (P) and/or bioaccumulative (B) by Environment Canada that are also considered to be "inherently toxic" to humans.

In order to efficiently identify substances that represent the highest priorities for screening assessment from a human health perspective, Health Canada developed and applied a Simple Exposure Tool (SimET) to the DSL to identify those substances that meet the criteria for GPE, Intermediate Potential for Exposure (IPE) or Low Potential for Exposure (LPE), and a Simple Hazard Tool (SimHaz) to identify those substances that pose a high or low hazard.

AMS is considered to meet the criteria for LPE under SimET and does not meet the criteria for high hazard under SimHaz. This document summarizes the currently available information on which the SimET and SimHaz results are based.

Exposure Information from Health Related Components of DSL Categorization

SimET was developed and used to identify substances on the DSL considered to represent GPE. This approach was based on three lines of evidence: 1) the quantity in commerce in Canada, 2) the number of companies involved in commercial activities in Canada (i.e., number of notifiers), and 3) the consideration by experts of the potential for human exposure based on various use codes. The proposed approach was released for public comment in November 2003 and also enabled designation of substances as presenting an IPE or LPE, based on criteria for quantity and nature of use (Health Canada, 2003)

Results of the Application of SimET

AMS has been determined to be LPE based on a consideration of the DSL nomination information listed below.

Nomination Information for DSL

Quantity in Commerce

The quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 1,100 kg

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was fewer than 4.

Use Codes and Description

The following DSL use codes have been identified for the substance:

13 Colourant - pigment/stain/dye/ink

Hazard Information from Health Related Components of DSL Categorization

Simple Hazard Tool (SimHaz)

SimHaz is a tool that has been used to identify, among all of the approximately 23 000 substances on the DSL, those considered to present either high or low hazard to human health based on formalized weight of evidence criteria and/or peer review/consensus of experts. This tool has been developed through extensive compilation of hazard classifications of Health Canada and other agencies and consideration of their robustness based on availability of transparent documentation of both process and criteria (Health Canada, 2005)

Results of the Application of SimHaz

AMS has not been classified for hazard by any of the agencies considered under the SimHaz tool and therefore does not meet the criteria for high hazard under SimHaz.

Uncertainties

SimET and SimHaz have been developed as robust tools for effectively identifying substances from the DSL that are considered to be human health priorities for further consideration. It is recognized that they do not include a number of elements normally considered in a human health risk assessment such as a comprehensive characterization of exposure and hazard, a comparison of exposure metrics to hazard metrics and a detailed analysis of uncertainties

References

Health Canada. 2003. Proposal for Priority Setting for Existing Substances on the Domestic Substances List under the Canadian Environmental Protection Act, 1999: Greatest Potential for Human Exposure..
http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/existsub/exposure/greatest_potential_human_exposure-risque_exposition_humaine_e.pdf

Health Canada. 2005. Proposed Integrated Framework for the Health-Related Components of Categorization of the Domestic Substances List under CEPA 1999 http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/contaminants/existsub/framework-int-cadre_e.pdf

Appendix II
Ecological Information
to Support The Challenge for
(9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts)
(AMS)
CAS No. 125351-99-7

Introduction

The information in this document will form the basis of a screening assessment under section 74 of CEPA, 1999. Data relevant to an ecological screening assessment were identified in original literature, review documents, commercial and government databases prior to December 2005. Properties and characteristics may also have been estimated using Quantitative Structure Activity Relationship (QSAR) models. In addition, an industry survey was conducted for the year 2005 through a Canada Gazette Notice issued pursuant to section 71 of CEPA 1999 (Environment Canada, 2006). This Notice requested data on the Canadian manufacture and import of the substance.

Physical and Chemical Properties of Representative Structure

There is no empirical physical-chemical property data available.
Table 1 contains modelled physical-chemical properties of a representative structure of AMS which are relevant to its environmental fate.

Table 1. Physical and chemical properties for a representative structure of AMS.

Property	Type	Value	Reference
Boiling Point	Modelled	732.66◦C	MPBPWIN v1.41
Melting Point	Modelled	321.28 ◦C	MPBPWIN v1.41
log Kow	Modelled	5.53	Kowwin v.1.67
log Koc	Modelled	4.459	PCKOCWIN v.1.66
Vapour Pressure	Modelled	4.973×10^{-19} Pa	MPBPWIN v1.41
Vapour Pressure	Modelled	3.73×10^{-21} mm Hg	MPBPWIN v1.41
Henry's Law Constant	Modelled	6.96×10^{-18} Pa –m^3/mole (6.87×10^{-23} atm-m^3/mole)	HenryWin v3.10
Water solubility	Modelled	1.08×10^{-5} mg/L	WSKOWWIN v1.41

Manufacture, Importation and Uses

Manufacture and Importation

In Canada, no manufacture of AMS was reported in response to a CEPA section 71 survey notice for the 2005 calendar year in a quantity meeting the 100kg reporting threshold. One company reported import of this substance in the 100-1,000 kg/year range (Environment Canada, 2006). Similar quantities were reported to the DSL during the calendar year 1986 (see Appendix I).

The Substances in Preparations in Nordic Countries (SPIN) database indicated AMS was used in Sweden during 1999 – 2004. However, quantities were not specified (SPIN, 2000).

Uses

There are 3 categories of potential uses for AMS that have been identified or suggested in Canada and worldwide:

1. Pigment for colouring printing inks;
2. Paint, lacquers and varnishes; and
3. Colorant in manufacture of rubber and plastic products (SPIN, 2000; Environment Canada, 2006).

Similar uses were reported to the DSL during the calendar year 1986 (see Appendix I).

Releases, Fate, and Presence in the Environment

Releases

AMS is not naturally produced in the environment. Data concerning the environmental releases in Canada are not available. Since AMS is not manufactured in Canada, there is no release to waste water effluent during the production phase. According to its major applications in printing inks, paints, and as plastic colorants, it is possible that AMS may be released to the environment in a dispersive manner. It is assumed that the predominant release route is through use of such products, and to a lesser degree at the end of their life cycle from landfills. The de-inking process for paper recycling and residue rinse during the processing phase, could lead to release through wastewater treatment plants (STPs). The STP treatment and leaching from landfills may lead to soil (through land application of sewage sludge) and ground water exposures.

Fate

The high log K_{ow} and log K_{oc} values indicate this substance will likely partition to soil and sediments. Indeed, the results of the Level III Fugacity modelling indicate that if AMS is released equally to the three major environmental compartments (air, water, and soil), it

will partition in water, soil, and sediments, with the latter two being the predominant compartments (Table 2).

Table 2. Results of the Level III fugacity modelling (EPIWIN V3.12)

	Fraction of Substance Partitioning to Each Medium (%)			
Substance Released to:	**% in Air**	**% in Water**	**% in Soil**	**% in Sediment**
Air (100%)	0.00	1.11	88.80	10.10
Water (100%)	0.00	9.93	0.00	90.10
Soil (100%)	0.00	0.01	99.90	0.07
Air, water, soil (33.3% each)	0.00	3.93	60.40	35.70

If the substance is released solely to air, a vapour pressure of 4.973×10^{-19} Pa and Henry's Law constant of 6.87×10^{-23} atm-m^3/mole indicate that the amount that remains in air will be negligible. The major two media where AMS will partition are soil and sediment (> 98 %) and a very small amount will partition in water (~ 1.11 %) due to the substance's low water solubility.

If released to soil, AMS is expected to have high adsorptivivity to soil (i.e. expected to be immobile) based upon estimated log K_{oc} of 4.459. Volatilization from dry or moist soil surfaces seems to be an unimportant fate process based upon the low estimated Henry's Law constant and vapour pressure. Therefore, if released to soil, AMS will mainly remain in this environmental compartment, which can be illustrated by the results of the Level III fugacity modelling (Table 2).

If released into water, AMS is expected to strongly adsorb to suspended solids and sediment based upon high value of estimated K_{oc}. Volatilization from water surfaces is expected to be an unimportant fate process based upon this compounds' estimated Henry's Law constant. Thus, if water is a receiving medium, AMS is expected to mainly remain in sediments and, to some extent, in water (Table 2).

Presence in the Environment

No monitoring data relating to the presence of the substance in environmental media (air, water, soil, sediment) have yet been identified.

Evaluation of P, B and iT Properties

Environmental persistence

Once released into the environment, AMS appears to be relatively persistent in water, soil and sediments. The Level III Fugacity model indicates negligible partitioning of the substance into air. For the small amount of AMS that may partition into air, the predicted atmospheric oxidation half-life of 0.05337day (Table 3) demonstrates that in air, it is likely to 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 0.053 days via reactions with hydroxyl radical, a representative structure of AMS is not persistent in air.

Table 3. Modelled persistence data for a representative structure of AMS

Medium	Fate Process	Degradation Value	Degradation Endpoint	Reference
Air	Atm. oxidation	0.053	Half-life (days)	AOPWIN v1.91
Air	Ozone reaction	Not Reactive	Half-life (days)	AOPWIN v1.91
Water/Soil	Biodegradation	60	Half-life (days)	BIOWIN v4.02 , Ultimate survey
Water/Soil	Biodegradation	0	Probability	TOPKAT Probability Aerobic Biodegradation v.6.1
Water/Soil	Biodegradation	0.0001	Probability	BIOWIN v4.02 , MITI Non-linear Probability

For estimating degradation in water, soil and sediment, a QSAR weight-of-evidence approach (ESD, 2006a) was applied using the models shown in Table 3. Based on these results shown in table 3, the estimated timeframe for biodegradation indicates that, the representative structure of AMS can be considered as persistent in water and soil because the half-life from the BIOWIN Ultimate survey model is 60 days and both BIOWIN v4.02 (Non-Linear) and TOPKAT Probability Aerobic Biodegradability (v6.1) is less than 0.2 (ESD, 2006a).

To estimate a half-life in sediments, an approach has been developed using Boethling's extrapolation factors (Boethling et al., 1995), which involves estimating the half life in sediment from that estimated for water ($t_{1/2\ water}$: $t_{1/2\ sediment}$ = 1:4). Therefore, in sediments, the half-life for AMS is expected to exceed 365 days.

The long-range transport potential (LRTP) of AMS from its point of release to air is estimated to be low according to the model prediction presented in Table 4. The TaPL3 model was used to estimate Characteristic Travel Distance (CTD), defined as the maximum distance traveled by 63% of a substance; or in other words, the distance that 37% of the substance may travel beyond. Beyer et al (2000) have proposed CTD's of >2000 km as

representing high LRTP, 700-2000 km as moderate, and <700 km as low. Based on the result shown in Table 4, AMS is expected to remain primarily in areas close to its emission sources.

Table 4. Model Predicted Characteristic Travel Distance (CTD) for a representative structure of AMS

Characteristic Travel Distance	Model (Reference)
479 km	TaPL3 (CEMC, 2003)

The modelled data (Tables 3) demonstrate that the representative structure of AMS meets the persistence criteria (half-lives in soil and water greater or equal to 182 days and/or half-lives in sediment greater or equal to 365 days) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000; Environment Canada, 2003).

Potential for bioaccumulation

There are no empirical bioaccumulation data available for this substance. The modelled log K_{ow} value for AMS indicates that this substance has the potential to bioaccumulate in the environment.

The Modified GOBAS BAF middle trophic level model produced BAF values from 112200 L/kg wet weight, indicating that this substance has the potential to bioconcentrate and biomagnify in the environment. The GOBAS BCF and BCF OASIS models also provide a weight-of-evidence to support the bioconcentration potential of the substance.

Table 5. Modelled bioaccumulation data for a representative structure of AMS

Test Organism	Endpoint	**Value** (wet weight, L/kg)	Reference
Fish	BAF	112200	Gobas BAF T2MTL (Arnot & Gobas, 2003)
Fish	BCF	13800	Modified Gobas BCF 5% T2LTL (Arnot & Gobas, 2003)
Fish	BCF	38000	OASIS, 2005
Fish	BCF	5*	BCFWIN v2.15

* Default value for sulfonate class.

The modelled bioaccumulation values do not take into account the metabolism potential of the substance.

The weight of evidence indicates that AMS meets the bioaccumulation criterion (BCF, BAF ≥ 5000) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada 2000).

Ecological Effects

In the Aquatic Compartment

There are no empirical ecotoxicity data available for this substance. The QSAR model suggests that this substance causes harm to aquatic organisms at relatively low concentrations (e.g., acute LC50 < 1 mg/L).

Table 6. Modeled aquatic toxicity values for a representative structure of AMS

Organism	Endpoint	Duration	Concentration (mg/L)	Reference
Fish	LC50	14 d	0.0056*	ECOSAR v. 0.99h Neutral Org. SAR, with safety factor

*This value has a safety factor of 100, because AMS is predicted to be a reactive chemical, more toxic than a neutral organic. This value was used as pivotal inherent toxicity value for categorization.

There is modelled evidence that the substance causes harm to aquatic organisms at relatively low concentrations (e.g. acute LC50≤1mg/L) [Table 6]. A range of aquatic toxicity values were obtained from the various QSAR models considered, however none provided reliable toxicity estimates for the representative structure of AMS as the predictions indicated that acute effects would be expected beyond the range of bioavailability. Therefore, following the weight of evidence approach for combining QSARs to determine the pivotal inherent toxicity value, the ECOSAR Neutral Organic fish14 days LC50 equation was used (ESD, 2006a). A safety factor of 100 was applied to the estimated toxicity for the representative structure of AMS as it was predicted, by ASTER, to have a mode of action other than narcosis (U.S. EPA, 1999).
These results indicate that the representative structure of AMS is highly hazardous to aquatic organisms (i.e. acute LC/EC50 ≤ 1.0 mg/L).

In Other Media

No effects studies for non-aquatic non-mammalian organisms were found for this compound.

Potential to Cause Ecological Harm

Evidence that a substance is highly persistent and bioaccumulative as defined in the Persistence and Bioaccumulation Regulations of CEPA 1999 (Government of Canada, 2000) together with evidence of toxicity and commercial activity provides a significant indication of its potential to be entering the environment under conditions that may have harmful long term ecological effects (ESD, 2006b). Substances that are persistent remain in the environment for a long time, increasing the potential magnitude and duration of exposure. Substances that have long half-lives in mobile media (air and water) and partition into these media in significant proportions have the potential to cause widespread contamination. Releases of small amounts of bioaccumulative substances may lead to high internal concentrations in exposed organisms. Highly bioaccumulative and persistent substances are of special concern, since they may biomagnify in food webs, resulting in

very high internal exposures, especially for top predators. Evidence that a substance is both highly persistent and bioaccumulative, when taken together with other information (such as evidence of toxicity at relatively low concentrations, and evidence of uses and releases) may therefore be sufficient to indicate that the substance has the potential to cause ecological harm.

The volume of AMS imported into Canada was over 100 kilograms per year. The quantities of AMS contained in imported printing, painted materials, and coloured plastics are not available. The dispersive use of AMS indicates potential for releases into the Canadian environment. Once released in the environment, because of its resistance to degradation, AMS will remain in water, sediment and soil for long times. As it persists in the environment, it will likely bioaccumulate and may be biomagnified in trophic food chains. It has also demonstrated relatively high toxicity. This information suggests that AMS has the potential to cause ecological harm in Canada.

Uncertainties

The uncertainties exist in the conclusions reached in this document because all P, B, iT evaluations are based on modelled data. There were no empirical studies available relating to the persistence, bioaccumulation and toxicity of AMS. The information on environmental concentrations or monitoring data in Canada and long term low level exposure of AMS is also lacking.

The experimental or predicted concentrations, associated with inherent toxicity for aquatic organisms, may have an additional source of uncertainty in some situations, e.g. where these concentrations exceed the solubility of the chemical in water (either experimental or predicted). Given that concentrations for both the toxicity and water solubility often vary considerably (up to several orders of magnitude), it is acknowledged that these uncertainties exist.

Regarding toxicity, based on the predicted partitioning behaviour of the substance, the significance of soil and sediments as important media of exposure is not well addressed by the effects data available. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures, although the water column may not be the medium of primary concern based on partitioning estimates.

There is also uncertainty associated with basing the overall conclusion that AMS may be causing ecological harm, solely on information relating to its persistence, bioaccumulation, relative toxicity and use pattern. Typically quantitative risk estimates (i.e., risk quotients or probabilistic analyses) are important lines of evidence when evaluating a substance's potential to cause environmental harm. However, when risks for persistent and bioaccumulative substances such as AMS are estimated using such quantitative methods, they are highly uncertain and are likely to be underestimated (ESD, 2006b). Given that long term risks associated with persistent and bioaccumulative substances cannot at present be reliably predicted, quantitative risk estimates have limited relevance. Furthermore, since

accumulations of such substances may be widespread and are difficult to reverse, a conservative response to uncertainty (that avoids underestimation of risks) is justified.

Dyes are generally not considered to be model-difficult because of lack of inclusion in ecotoxicity model training sets. Such structures are treated as routine organic chemicals that are predictable by current models. Rather, the water solubility of these substances is difficult to ascertain, and the uncertainty, therefore, resides in determining their bioavailability. Since the predictions of inherent toxicity of the representative structure of AMS derived from QSAR models indicated that acute effects would be expected beyond the range of bioavailability, additional uncertainty is recognized with predicting the inherent toxicity using a generic narcotic equation with an application factor (ESD, 2006a). The results of this approach indicate that the representative structure of AMS can harm organisms at low exposure concentrations.

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