

Substance Profile for The Challenge Oxirane, (chloromethyl)- (Epichlorohydrin) CAS No. 106-89-8

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 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:

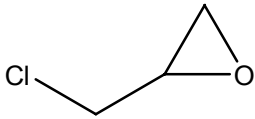
- that were found to meet all of the ecological categorization criteria, including persistence, bioaccumulation potential and inherent toxicity to aquatic organisms (PBiT), and that are known to be in commerce, or of commercial interest, in Canada, and/or
- that were found either to meet the categorization 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 epichlorohydrin was identified as a high priority for action as it was determined to have a high potential for exposure to individuals in Canada (GPE or IPE), and is considered to present a high hazard to human health. 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

CAS Registry Number	106-89-8
Inventory names	Oxirane, (chloromethyl)-; 1-chloro-2,3-epoxypropane; epichlorohydrin; copolymer of oxirane, (chloromethyl)-; propane, 1-chloro-2,3-epoxy-
Other names	(±)-Epichlorohydrin; (chloromethyl)ethylene oxide; (chloromethyl)oxirane; (RS)-epichlorhydrin; α-epichlorohydrin; γ-Chloropropylene oxide; 1,2-epoxy-3-chloropropane; 2,3-epoxypropyl chloride; 2-(chloromethyl)oxirane; 2-chloropropylene oxide; 3-chloro-1,2-epoxypropane; 3-chloro-1,2-propylene oxide; 3-chloropropene-1,2-oxide; 3-chloropropylene oxide; chloropropylene oxide; glycerol epichlorohydrin; glycidyl chloride; J 006; NSC 6747
Chemical group	Discrete organics
Chemical sub-groups	Halogenated alkyl epoxides
Chemical formula (NCI)	C ₃ H ₅ ClO
Chemical structure	
SMILES	O(C1CC1)Cl
Molecular mass (NCBI)	92.5239 g/mol

Based on information submitted by the 11 companies that notified this substance to the Domestic Substances List, 2,240 tonnes of epichlorohydrin were in commerce in 1986 for a variety of uses from a wide range of sectors, including (but not limited to) the following categories: adhesive/binder/sealant/filler; organic chemical intermediate; formulation component (including polymers); solvent/carrier; pharmaceuticals; plastics and synthetic resins; plating and surface finishing.

Potential uses of epichlorohydrin in Canada include use in production of epoxy resins, elastomers, synthetic glycerine, wet strength resins, anion-exchange resins, flocculants, and cationic polymers.

Epichlorohydrin can also be used as a cross-linking agent for starches (used in consumer products such as powder coating inside latex gloves, surface coating mixtures, and drug delivery systems). Although cross-linked food starch is, probably, not made in North America, it may be imported into Canada.

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

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
Oxirane, (chloromethyl)-
(Epichlorohydrin)
CAS No. 106-89-8

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA, 1999), Health Canada undertook to categorize all 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) 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.

Epichlorohydrin is considered to meet the criteria for GPE under SimET and for high hazard under SimHaz. This document summarizes the currently available information used to support the inclusion of this substance in the Challenge.

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 Intermediate (IPE) or Lowest Potential for Exposure (LPE), based on criteria for quantity and nature of use (Health Canada, 2003).

Results of the Application of SimET

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

Nomination Information for DSL

Quantity in Commerce

The quantity of epichlorohydrin reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 2,240,000 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-86 was 11.

Use Codes and Description

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

- 4 Adhesive/binder/sealant/filler
- 10 Chemical intermediate - organic
- 21 Formulation component
- 36 Polymer, component of a formulation
- 44 Solvent/carrier
- 52 Adhesive and Sealant Production
- 76 Organic Chemicals, Industrial
- 77 Organic Chemicals, Specialty
- 83 Pharmaceuticals
- 87 Plastics and Synthetic Resins
- 88 Plating and Surface Finishing
- 92 Rubber Products

Potential Uses in Canada

The additional information below on potential uses of epichlorohydrin was identified through searches of the available scientific and technical literature.

Production of epoxy resins based on bisphenol A-diglycidyl ether (BADGE) accounts for more than 75% of epichlorohydrin consumption in other countries. These epoxy resins are used in surface coatings, structural composites, adhesives, for potting and encapsulation, and other minor applications.

Epichlorohydrin is also used to produce phenoxy resins used mostly in surface coatings. Production of synthetic glycerine accounts for about 10% of epichlorohydrin production. Glycerine is used as an ingredient or processing aid in cosmetics, toiletries, personal care, drugs, and food and beverages.

The third major use of epichlorohydrin is in the production of elastomers, particularly rubber with resistance to extreme conditions (Dow, 2006; Solvay S.A., 2006). Epichlorohydrin is used to produce wet strength resins, e.g. polyamide-epichlorohydrin

resin for use in paper products such as tissues and filters and cellulose products used in food and beverages such as sausage casings and tea bags (US EPA, 1985). Anion-exchange resins and flocculants, produced using epichlorohydrin as a reactive ingredient, are used in drinking water and wastewater treatment and in the production of food and beverages (WHO, 2004).

Epichlorohydrin is used to produce cationic polymers which are surfactants in hair care products and detergents. Resins produced from epichlorohydrin are used in the textile industry as dye fixatives, sizing agents and anti-static agents.

Epichlorohydrin is a cross-linking agent for starches. Cross-linked starch hydrogels may be used in consumer products such as powder coating inside latex gloves, surface coating mixtures and drug delivery systems. Although cross-linked food starch is probably not made in North America, it may be imported into Canada (NTP, 2005).

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

Epichlorohydrin is considered to be a potentially high hazard substance based on its classification for carcinogenicity by the European Commission, United States National Toxicology Program (NTP), International Agency for Research on Cancer (IARC), and United States Environmental Protection Agency (US EPA).

The following classifications for carcinogenicity of epichlorohydrin are available:

The European Commission has classified epichlorohydrin as Category 2 for carcinogenicity (Substance which should be regarded as if carcinogenic to man) (European Commission, 2002 and 1993, ESIS, 2006).

The US NTP considers epichlorohydrin to be “reasonably anticipated to be a human carcinogen based on sufficient evidence of carcinogenicity in experimental animals” (NTP, 2005).

IARC has classified epichlorohydrin as Group 2A (Agent is probably carcinogenic to humans) due to inadequate evidence for the carcinogenicity in humans but sufficient evidence for the carcinogenicity in experimental animals (IARC, 1999).

The US EPA conducted a weight of evidence assessment of the carcinogenicity of Dimethyl sulfate and classified it as a Group B2 carcinogen (Probable human carcinogen). This conclusion was based on inadequate human data. “Multiple studies in rats and mice administered epichlorohydrin by various routes were positive. As epichlorohydrin is a strong alkylating agent, tumors are produced at the site of application” (US EPA, 1994).

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; however, as a result of the combination of the severe hazard properties of these substances and their high potential for exposure to humans, evaluation of the need for preventative and protective actions is required.

References

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Appendix II
Ecological Information to Support The Challenge for
Oxirane, (chloromethyl)-
(Epichlorohydrin)
CAS No. 106-89-8

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.

Physical and Chemical Properties

Tables 1a and 1b contain experimental and modelled physical-chemical properties of epichlorohydrin which are relevant to its environmental fate.

Table 1a: Experimental physico-chemical properties for epichlorohydrin

Property	Value/Units	Reference
Boiling point (BP)	116.5 °C; 117 °C	Plunkett, 1987; SRC PHYSPROP Database, 2003
Melting point (MP)	-57.2 °C; -26 °C	Howard, 1989; SRC PHYSPROP Database, 2003
log K _{ow}	0. 3; 0.45	Howard, 1989; Deneer <i>et al.</i> , 1988
Vapour pressure (VP)	1600 Pa (*12 mm Hg at 20 °C); 2192 Pa (*16.4 mm Hg at 25 °C)	Verschueren, 1983; Daubert & Danner, 1985
Water solubility (WS)	*65900 mg/L (at 25 °C)	Yalkowsky & Dannenfelser, 1992

* Original values reported in non-SI units

Table 1b: Modelled physico-chemical properties for epichlorohydrin

Property	Value/Units	Model
Boiling point (BP)	99 °C	MPBPWIN v1.41
Melting point (MP)	-65.5 °C	MPBPWIN v1.41
Henry's Law constant (HLC)	0.27 Pa · m ³ /mole (2.621×10 ⁻⁶ atm · m ³ /mole); 5.7 Pa · m ³ /mole (5.621×10 ⁻⁵ atm · m ³ /mole)	HenryWin v3.10
log K _{oc}	0.652	PCKOCWIN v1.66
log K _{ow}	0.63	KOWWIN v1.67
Vapour pressure (VP)	2386 Pa (17.9 mm Hg)	MPBPWIN v1.41
Water solubility (WS)	50630 mg/L	WSKOWWIN v1.41

Manufacture, Importation, and Uses

Available information is presented in Appendix I.

Releases, Fate and Presence in the Environment

Releases

The National Pollutant Release Inventory (NPRI) contains information on annual releases of chemicals. Throughout the years 1994-2001, there were reported releases of epichlorohydrin into the Canadian environment. Within this period, the release volumes were as follows:

- 1994-1996: 127-133 kg/year (two locations);
- 1997-1999 and 2002-2005: ≤ 4 kg/year (one location);
- 2000-2001: 594 kg/year (one location).

Possible differences between the large reported use quantities in 1986 and the relatively low NPRI release data in 1994-2005 could be due to a decrease in use or due to very effective management of this substance (e.g. application of new low- or no-release technologies), or both, during the past 10 years.

In addition, it should also be acknowledged that only facilities that meet established reporting criteria are required to report to the NPRI.

Fate

Aquatic fate

Based on the estimated $\log K_{oc}$ value of 0.65 (Table 1b), epichlorohydrin is not expected to adsorb to suspended solids and sediments. Volatilization from water surfaces, based upon the estimated Henry's Law constants of $(2.6-5.6) \times 10^{-5} \text{ atm} \cdot \text{m}^3/\text{mole}$ (Table 1b), is expected to be moderate. Thus, if water is a receiving medium, epichlorohydrin is expected to mainly remain in water and, to some extent, partition to air as indicated by the results of Level III Fugacity modelling (Table 2).

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

Receiving media	% in Air	% in Water	% in Soil	% in Sediment
Air (100%)	83.7	12.7	3.6	0.02
Water (100%)	2.3	97.4	0.1	0.18
Soil (100%)	3.9	18.9	77.1	0.04
Air, water, soil (33.3% each)	11.6	43.5	44.8	0.08

Terrestrial fate

Based on the estimated log K_{oc} value of 0.65 (Table 1b), epichlorohydrin is not expected to adsorb to soil and, therefore, is expected to have very high mobility in this environmental compartment. Volatilization of epichlorohydrin from moist soil surfaces is expected to be an important fate process given estimated Henry's Law constants of $(2.62-5.62) \times 10^{-5} \text{ atm} \cdot \text{m}^3/\text{mole}$. The potential for volatilization of epichlorohydrin from dry soil surfaces may exist based upon experimental and estimated vapour pressure values of 12-18 mm Hg (Tables 1a and 1b).

Atmospheric fate

According to a model of gas/particle partitioning of semi-volatile organic compounds in the atmosphere (Bidleman, 1988), epichlorohydrin having a vapour pressure of 12-18 mm Hg (Tables 1a and 1b) is expected to exist solely as a vapour in the ambient atmosphere. This chemical may also be removed from the atmosphere by wet deposition processes, considering the very high water solubility of this chemical (51-66 g/L, Tables 1a and 1b).

Presence in the Environment

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

Evaluation of P, B and iT Properties

Environmental Persistence

Vapour-phase epichlorohydrin is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals. The half-life for this reaction in air is estimated to be ~24 days (Table 3a), calculated from its experimental rate constant of $4.4 \times 10^{-13} \text{ cm}^3/\text{molecule} \cdot \text{sec}$ (Atkinson, 1989). The AOPWIN model predicted a very similar half-life value of ~19 days (Table 3b).

This compound is not expected to 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, epichlorohydrin meets the persistence criterion in air (half-life ≥ 2 days), as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Table 3a: Experimental persistence values for epichlorohydrin

Medium	Fate Process	Degradation Value	Degradation Endpoint/Units	Reference
Air	Photodegradation	4.4×10^{-13}	Rate constant, $\text{cm}^3/\text{molecule} \cdot \text{sec}$	Atkinson, 1989

Air	Photodegradation	24.3	Half-life, days	Atkinson, 1989
Air	Photodegradation	16	Half-life, hours	Dilling <i>et al.</i> , 1976
Water	Biodegradation	18	*Biodegradation, %	Chemicals Inspection and Testing Institute, 1992
Water	Biodegradation	>40	*Biodegradation, %	Material Safety Data Sheet, 2001
Water	Biodegradation	67.9	*Biodegradation, %	National Institute of Technology and Evaluation
Water	Biodegradation	97	*Biodegradation, %	Popp, 1985
Water	Hydrolysis	6.2	Half-life, days	Piringer, 1980
Water	Hydrolysis	8.2	Half-life, days	Mabey & Mill, 1978

* Test duration: 2-4 weeks

Table 3b: Predicted persistence data for epichlorohydrin

Medium	Fate Process	Degradation Value	Degradation Endpoint	Model
Air	Atm. oxidation	18.95	Half-life (days)	AOPWIN v1.91
Air	Ozone reaction	Non-reactive	Half-life (days)	AOPWIN v1.91
Water	Hydrolysis	126900	Half-life (days)	HYDROWIN v1.67
Water/soil	Biodegradation	15	Half-life (days)	BIOWIN v4.02, Ultimate Survey
Water/soil	Biodegradation	0.521	Probability	BIOWIN v4.02 (MITI Linear)
Water/soil	Biodegradation	0.412	Probability	BIOWIN v4.02 (MITI Non-linear)
Water/soil	Biodegradation	0	Probability	TOPKAT v.6.1

In water, both hydrolysis and biodegradation affect persistence of epichlorohydrin. Hydrolysis half-life of 6.2 days was reported by Piringer (1980), based on the experimental hydrolysis rate constants. Mabey and Mill (1978) cite an experimentally determined rate constant for the hydrolysis of epichlorohydrin ($9.75 \times 10^{-7} \text{ s}^{-1}$ at pH 7 and 20 °C) and estimate a half-life of 8.2 days (Table 3a). These data clearly indicate that abiotic (hydrolytic) degradation of epichlorohydrin should be considered as a significant process, influencing the persistence of this chemical in water. In moist soils, the importance of this process cannot also be ignored.

In contrast to the experimental results on hydrolysis of epichlorohydrin, the modelled result is extremely high: $t_{1/2}=127,000$ days, or ≈ 350 years (Table 3b). It should be, however, noted that according to the guidance from the HYDROWIN model, “The rate constant estimated for the epoxide does not include the neutral hydrolysis rate constant. For some epoxides, the neutral rate constant is the dominant hydrolysis rate at environmental pH. If the neutral rate constant is important, the HYDROWIN estimated rate will underestimate the actual rate”. The HYDROWIN-estimated rate was indeed underestimated and, therefore, hydrolysis half-life was significantly overestimated.

Along with this, it should also be noted that in realistic environmental conditions, reactions between epichlorohydrin and some inorganic anions such as bicarbonate or nitrate can also occur. However, the adducts formed are unstable, and hydrolyse rapidly to 3-chloro-1,2-propanediol and carbonic or nitric acid (Santodonato *et al.*, 1980). Therefore, these anions increase the rate of abiotic transformation of epichlorohydrin.

Experimental data on biological degradation of epichlorohydrin are contradictory. The Chemicals Inspection and Testing Institute (1992) reported a biodegradation value of 18% in a 14-day test (Table 3a). Bridie *et al.* (1979) also present a very low BOD₅ (biochemical oxygen demand in a 5-day test) value of only 3% of the ThOD (theoretical oxygen demand) with non-adapted inoculum; adaptation of the inoculum resulted in increasing BOD₅ value to 14% of ThOD. However, it should be noted that in these two studies, the test durations were 14 days and 5 days, respectively, which is significantly shorter than the typical test duration of 28 days recommended in many methods (e.g. OECD Guidelines for Testing of Chemicals). Therefore, it may be supposed that if the abovementioned tests were continued for a longer period of time (i.e. 28 days), biodegradation of epichlorohydrin would, most likely, be higher.

In contrast to the aforementioned results, the National Institute of Technology and Evaluation (Tokyo, Japan) reported BOD value of ~68% in the 14-day test on biodegradation of epichlorohydrin. In another study, based on the modified OECD confirmatory test, Popp (1985) calculated BOD₃₀ (biochemical oxygen demand in a 30-day test) value of 1180 mg O₂/g epichlorohydrin, which corresponds to 97% of the theoretical oxygen demand. According to the Material Safety Data Sheet issued by The Dow Chemical Company for epichlorohydrin, biodegradation of this chemical under aerobic static laboratory conditions was high: BOD₂₀ or BOD₂₈ values were greater than 40% of the theoretical oxygen demand. In addition, according to the International Program on Chemical Safety (IPCS), epichlorohydrin has been claimed as biodegradable substance.

Studies, where biological degradation of epichlorohydrin was investigated using pure microbial cultures, are also available in the scientific literature. In one study (Wijngaard *et al.*, 1989), three bacterial strains were isolated from freshwater sediment contaminated with chloroorganic compounds. After 6 days of incubation with 4 mM epichlorohydrin as sole carbon source, 5% degradation was observed in the sterile control, while in the test cultures, 80-100% degradation was found. Neilson (1990) and Small *et al.* (1995) also reported that pure microbial cultures were able to rapidly biodegrade epichlorohydrin.

In addition, experimental data show that in soils, epichlorohydrin could easily biodegrade; half-lives were within the range of only 7-28 days, depending on soil pH, temperature, and microbial densities (IUCLID Data Set, 2002).

Thus, considering available experimental data on biodegradation of epichlorohydrin in water and soil and using a weight-of-evidence approach, it may be concluded that this chemical can be considered as biodegradable in these two environmental compartments. Therefore, being easily degradable both chemically (hydrolytically) and biologically, epichlorohydrin can be claimed as not persistent in water and soils.

Similar to the experimental results, modelled data on biological degradation of epichlorohydrin are also contradictory (Table 3b). For example, according to the TOPKAT model, the probability of biodegradation of epichlorohydrin is 0 (zero), which means that this chemical is persistent. The reason for this is that epichlorohydrin has been

included in the training set of this model, and the biodegradation value of 18% (from the Chemicals Inspection and Testing Institute, 1992) was used in the set of experimental data of the model (Loonen *et al.*, 1999); as a result, TOPKAT estimated a probability for biological degradation of epichlorohydrin as zero.

However, according to the ultimate survey of the BIOWIN model, half-life for biodegradation of epichlorohydrin is only 15 days. The relatively high BIOWIN linear and non-linear probabilities for biodegradation of this chemical (0.52 and 0.41, respectively – Table 3b) also indicate that epichlorohydrin should be considered as a substance that is biodegradable in water.

To extrapolate modelled half-life in water to half-lives in soils and sediments, Boethling’s extrapolation factors can be used ($t_{1/2 \text{ water}} : t_{1/2 \text{ soil}} : t_{1/2 \text{ sediment}} = 1 : 1 : 4$, Boethling *et al.*, 1995). Using the BIOWIN’s ultimate survey result ($t_{1/2}=15$ days) and extrapolation factors, it may be concluded that epichlorohydrin is not expected to be persistent in soil and sediments.

Therefore, most of the available data demonstrate that epichlorohydrin does not meet the persistence criteria in soil and water (half-lives ≥ 182 days) and in sediments (half-life ≥ 365 days); however, it does meet the persistence criterion in air (half-life ≥ 2 days), as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Potential for Bioaccumulation

Experimental and modelled $\log K_{ow}$ values of 0.03 and 0.37, respectively (Tables 1a and 1b) suggest that the potential for bioaccumulation of epichlorohydrin in aquatic organisms is low.

Experimental bioaccumulation and bioconcentration factors (BAF and BCF) for this substance are not available. The middle-trophic-level modified Gobas BAF model for fish predicted a BAF of 1 L/kg (Table 4), indicating that substance epichlorohydrin does not have the potential to bioaccumulate in the fish. The three BCF models for fish provide a weight-of-evidence to support a low bioconcentration potential of this substance (BCF=1-15 L/kg, Table 4).

Table 4: Predicted bioaccumulation values for epichlorohydrin

Test Organism	Endpoint/Units	Value	Model
Fish	BAF (wet weight, L/kg)	1	Modified Gobas BAF T2MTL (Arnot & Gobas, 2003)
Fish	BCF (wet weight, L/kg)	1 – 15	OASIS; Modified Gobas BCF 5% T2LTL (Arnot & Gobas, 2003); BCFWIN v2.15

Therefore, all modelled data indicate that the substance epichlorohydrin does not meet the bioaccumulation criteria (BCF/BAF ≥ 5000) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Ecological Effects

In the Aquatic Compartment

Experimental ecotoxicological data provide evidence that at low concentrations, epichlorohydrin is not expected to cause significant harm to aquatic. For fish and water flea, experimental LC50/EC50 values vary within a relatively narrow range of 11-72 mg/L (Table 5a).

Table 5a: Experimental aquatic toxicity values for epichlorohydrin

Test Organism	Endpoint	Test Type	Value (mg/L)	Reference No. (ECOTOX database)
Fish (<i>Carassius auratus</i> , <i>Danio rerio</i> , <i>Lepomis macrochiru</i> , <i>Leuciscus idus melanotus</i> <i>Menidia beryllina</i> , <i>Pimephales promelas</i> , <i>Rasbora heteromorpha</i>)	LC50	Acute	10.6*-72	542; 547; 623; 863; 10432 ; 11037
Water flea (<i>Daphnia magna</i>)	LC50	Acute	21-33.4	5718 ; 12055 ; 69457
Water flea (<i>Daphnia magna</i>)	EC50	Acute	40	707
Algae (<i>Microcystis aeruginosa</i> , <i>Anacystis aeruginosa</i>)	LOEC	NA	5.4-6.0	19121

*LC50=10.6 mg/L – pivotal iT value for categorization

Three models produced a similar range of toxicity values (LC50/EC50=18-59 mg/L) for fish and daphnia, while LC50 values for fish from three other models are in the order of thousands of mg/L (Table 5b).

Table 5b: Modelled aquatic toxicity values for epichlorohydrin

Organism	Endpoint	Duration	Toxicity value (mg/L)	Model
Daphnia	EC50	Acute	58.9	TOPKAT v6.1
Fish	LC50	Acute	17.91	ECOSAR v.0.99g
Fish	LC50	Acute	22.18	AI Expert
Fish	LC50	Acute	1200	TOPKAT v6.1
Fish	LC50	Acute	5961	OASIS Forecast
Fish	LC50	Acute	1939	ECOSAR Neutral Org. SAR

Therefore, based on weight-of-evidence, experimental and modelled ecotoxicological data indicate that epichlorohydrin is expected to pose a moderate (acute or immediate) hazard to aquatic organisms.

In Other Media

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

Potential to Cause Ecological Harm

Based on the available information, epichlorohydrin persists in the environment (in air) and is not bioaccumulative, based on criteria defined in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000). Information on concentrations of this chemical in the environment has not been identified at this time. Experimental ecotoxicological data indicate that epichlorohydrin is expected to pose a moderate acute hazard for aquatic organisms exposed to the chemical in water. Information on potential impacts in other environmental compartments has not been identified.

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