ACRYLONITRILE
ECOLOGICAL FATE AND EFFECTS PROFILE

CAS No. 107 - 13 - 1

Prepared for

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by

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1.0 SUMMARY

Acrylonitrile is an important industrial chemical intermediate used in the production of acrylic and modacrylic fibers and other important chemicals and resins and is released as fugitive emissions and in wastewater during its production and use.

It is soluble in water and is also volatile. Direct photolysis of acrylonitrile in aquatic environments is unlikely. Volatilization is a major environmental transport process for acrylonitrile. Acrylonitrile can be volatilized from aquatic and terrestrial systems and transported in the atmosphere as a vapor or adsorbed to particulate. Although acrylonitrile can return to aquatic and terrestrial systems in precipitation, photooxidation in the troposphere is a significant environmental fate process. Hydrolysis and sorption probably are not important fate processes under natural conditions.

If released in wastewater, acrylonitrile will slowly evaporate (half-life 1-6 days) and also biodegrade (complete degradation in approximately 1 week in receiving water in which microorganisms would be acclimated). There is very little information of acrylonitrile on movement, fate and persistence in water.

If released to the atmosphere, it will degrade primarily by reacting with photochemically produced hydroxyl radicals. The half-life for this process is 3.5 sunlit days under relatively clean atmospheric conditions to somewhat over a day with smog.

If spilled on land, acrylonitrile will volatilize rapidly due to its high vapor pressure and poor adsorption to soil or to organic sediment.

Acrylonitrile is acutely moderate toxic to aquatic organisms. There is also no evidence that acrylonitrile at 5.0 ppm exposed to medaka (*Oryzias latipes*) for 28 continuous days was carcinogenic or caused any significant chronic toxic effects. Based on the relatively low value of the octanol/water partition coefficient (Log K_{ow} = -.92) and bioconcentration factor (48) for acrylonitrile, it is not expected that acrylonitile will strongly accumulate in the tissue of aquatic organisms. However, the toxic effects of acrylonitrile to terrestrial wildlife are unknown. In addition, its toxicity to plants and algae is also not available. Algae are extremely important in the functioning of aquatic and terrestrial ecosystems because they serve as a foundation of most aquatic and terrestrial food chains. Algae also aid in transforming organic wastes to stable effluents

Bioaccumulation of acrylonitrile is not expected to be a significant process. Acrylonitrile is biodegraded by sewage sludge, but there may be an insufficient population of microorganisms in the water column and insufficient contact time for biodegradation to be effective in surface waters.

There is no information on the effects of acrylonitrile on microorganisms, which play a dominant role in transformations of biotic and manufactured chemical wastes. Microorganisms also serve many important functions associated with the major biogeochemical cycles, e.g., carbon, nitrogen and sulfur.

2.0 ENVIRONMENTAL FATE

2.1 Environmental Fate Data

TYPE OF FATE	DATA	REFERENCE
Hydrolysis	N.A.[1]	
Water Solubility	7.2% at 0°C; 7.9% at 40°C	WHO, 1983
	7.35 % at 20°C	Merck, 1989
	74,000 ppm at 25°C	Yalkowsky, 1989
Photolysis - soil	N.A.	
Photolysis - water	An initial conc. of 10 mg/L: only 46% remained after 24 hr; 19% after 48 hr and 5% after 96 hr.	NRC, 1980
	Half-life = 1-6 days	Going *et al*., 1979
Photolysis - air	Half-life = 9 to 10 hours	USEPA, 1983
	Under a 12-hr sunlight days, degrades by reaction with hydroxyl radicals with a reaction half-life of 3.5 hours.	HSDB, 1999
	Half-life of 3.5 days under relatively clean atmospheric conditions and 1 day with smog	Edney *et al*., 1983
Sorption/desorption (K_d)	Not expected to adsorb onto organic sediment (no K_d was provided)	USEPA, 1982

Organic Carbon/Water Partition Coefficient (K_{OC})	K_{OC} = 9	Kenaga, 1980; Lyman *et al*., 1982

TYPE OF FATE	DATA	REFERENCE
Octanol/water partition Coefficient (K_{OW})	Log K_{OW} = 0.51; 0.25	Hansch and Leo, 1984; 1985
Bioconcentration - Bluegill Sunfish	BCF - 48 (insignificant)	Barrows *et al*., 1978
	Log BCF = 1.68	Barrows *et al*., 1978
	Half-life in bluegill tissue - 4-7 days	USEPA, 1980
Henry's Law Constant	0.063 at 25°C	Bocek, 1976
	1.03×10^{-4} Atom m^3/mole	Bocek, 1976
	1.38×10^{-4} Atom m^3/mole	Meylan and Howard, 1991
Vapor Pressure	100 mm Hg at 23.6°C	IARC, 1979; Norris, 1967
	110 mm Hg at 25°C	Norris, 1967
	108.5 mm Hg at 25°C	Daubert and Danner, 1985
	Volatilization would occur with expected half-lives of 1-6 days in environmental waters.	HSDB, 1999
Others	if released in wastewater, acrylonitrile will slowly evaporate and also biodegrade (complete degradation in approx. 1wk in receiving water in which microorganisms are acclimated.	HSDB, 1999

[1]N.A. = Not Available

2.2 Summary of Environmental Fate of Acrylonitrile

2.2.1 Environmental Degradation/Bioconcentration: Acrylonitrile is not expected to be persistent in the environment. Because of its high water solubility, high Henry's Law constant and a high vapor pressure. It is not expected for acrylontrile to accumulate in aquatic organisms.

2.2.2 Aquatic Fate: Acrylonitrile is very soluble in water with a water solubility of 7,350 ppm. If released into wastewater, acrylonitrile will slowly evaporate and biodegrade. Degradation occurred in approximately one week in receiving water in which microorganisms were acclimated.

Vapor pressure was reported to be 100 mm Hg at 25°C (Norris, 1967) and volatilization would also occur with expected half-lives of 1-6 days in environmental waters. In humic waters photooxidation by radicals may occur but data in natural systems are not available. Adsorption to sediment or particulate matter is reported to be insignificant; furthermore, a low bioconcentration of 48 (Barrows *et al*., 1978) and a low Log K_{ow} of 0.51 (Hansch and Leo, 1984) indicate that acrylonitrile accumulation in aquatic organisms is also insignificant.

2.2.3 Atmospheric Fate: The estimated atmospheric half-life of acrylonitrile is 9-10 hours (USEPA, 1983) , which is sufficiently long for aerial transport to play a significant role in the distribution of acrylonitrile in the neighborhood of emission sources.

If released to the atmosphere, acrylonitrile will degrade by reaction with hydroxyl radicals with a reaction half-life of 3.5 hours under 12 hour sunlit days (HSDB, 1999). This would be reduced considerably under smog conditions. Since it is relatively long-lived in the atmosphere, considerable dispersion would be expected to occur. Reaction with ozone is probably not significant in relation to hydroxyl radicals.

2.2.4 Terrestrial Fate: No K_d was reported but acrylonitrile is not expected to undergo significant adsorption on organic sediment. Acrylonitrile has high vapor pressure and a low K_{oc} indicating negligible sorption to soil. Thus, if spilled on land, acrylonitrile will evaporate rapidly.

2.2.5 Soil Adsorption and soil Mobility: The K_{OC} for acrylonitrile calculated from the water solubility is 9 (Kenaga, 1980; Lyman *et al*., 1982) indicating that adsorption to soil is insignificant.

2.2.6 Volatilization from Water and Soil: Acrylonitrile is highly volatile (100 mm Hg at 25°C) with a Henry's Law Constant of 0.063 at 25°C (Bocek, 1976). Thus, it is expected that a significant portion of acrylonitrile will be transported from the aquatic environment to the troposphere.

3.0 ENVIRONMENTAL EFFECTS

3.1 Environmental Effects Data

TYPE OF EFFECTS	DATA	REFERENCE
Acute LC_{50} Fathead Minnow (*Pimephales promelas*)	96-hour LC_{50} = 10.1mg/L, Flow through	Henderson *et al*., 1961
	96-hour LC_{50} = 14.3,18.1, 10.1 mg/L static	Henderson *et al*., 1961
Acute LC_{50} Bluegill (*Lepomis macrochirus*)	96-hour LC_{50} =10 mg/L; 11.8 mg/L	Buccafusco, 1981; Henderson *et al*., 1961
Acute LC_{50} Guppy (*Poeculia reticulata*)	96-hour LC_{50} =33,500 µg/L static bioassay	Henderson, 1961

TYPE OF EFFECTS	DATA	REFERENCE
Acute LC_{50} Pinfish (*Lagodon rhomboides*) (saltwater)	24-hour LC_{50} = 24,500 μg/L static bioassay	Kayser, 1982
Acute LC_{50} *Daphnia*	24-hour LC_{50} = 13 mg /L; 48-hour LC_{50} =7.6 mg/L	LeBlanc, 1980
	48-hour LC_{50} = 10.95 mg /L	Randall and Knopp, 1980
Acute Toxicity - marine organisms – Shrimp (*Crangon crangon*)	LC_{50} <10,000 μg/L	Portmann, 1985
Early Life Stage - Bluegill Sunfish (*Lepomis macrochirus*)	LEL[1] = - 9.94 μg/L	DYN, 1985
Chronic Life Cycle – *Daphnia*	NOEL[2] = 3.6 mg/L	USEPA, 1983
Chronic effects to Medaka (*Oryzias latipes*)	not carcinogenic or any significant chronic effects to medaka when exposed to acrylonitrile at 5.0 ppm and 28 days of continuous exposure.	Walker *et al*., 1996
Avian/Terrestrial Wildlife Oral LD_{50} Toxicity	LD_{50} = 93 mg/kg in rats	Merck, 1989
Avian/Terrestrial Wildlife Dietary LC_{50} Toxicity	N.A.	
Chronic Avian/Terrestrial Wildlife Toxicity	N.A.	
Acute Toxicity - Plants or soil Organisms	N.A.	
Bacteria - Toxicity Test	N.A.	
Acute Toxicity to Benthic organisms	N.A.	

[1] LEL = low-effect-level
[2] NOEL = no-observed-effect-level

3.2 Summary of Environmental Effects of Acrylonitrile

3.2.1 Acute Toxicity to Aquatic Organisms: Considerable data on the acute toxicity of acrylonitrile to aquatic organisms are available. The data indicate that acrylonitrile is moderately toxic to freshwater fish, invertebrate and marine fish (LC_{50} 1,000 - 100,000 μg/L).

3.2.2 Acute Toxicity to Benthic Organisms or animals exposed to contaminated sediments: No data available

3.2.3 Acute Toxicity to Terrestrial Wildlife via Oral dose: Based on the acute oral toxicity

data to rats, acrylonitrile is not toxic to wildlife.

3.2.4 Acute Toxicity to Terrestrial Wildlife via Diet or Food: No data available

3.2.5 Acute Toxicity to Plants or Soil Organisms exposed through soil concentrations: No data available

3.2.6 Chronic Toxicity to Aquatic Organisms: Acrylonitrile appears to be moderately toxic (NOEL 3.9 mg/L) to Daphnia in a life cycle study; but it is considered highly toxic (LEL 9.94 µg/L) to bluegill sunfish at egg fry stage. No evidence of carcinogenicity or of any other significant chronic effects was noted when medaka was exposed to acrylonitrile at 5.0 ppm and 28 days of continuous exposure.

3.2.7 Chronic Toxicity to Terrestrial Wildlife via Diet or Food: No data available

3.2.8 Toxicity to Bacteria or Algae: No data available

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