FOREWORD INTRODUCTION

CHLOROPROPENE

CAS N°: 107-05-1

SIDS Initial Assessment Report for the 4th SIAM (Tokyo, 20-22 May 1996)

Chemical Name: 3-Chloropropene

CAS No: 107-05-1

Sponsor Country: The Netherlands

SIDS Contact Point in Sponsor Country: Mr. Dick Sijm

History: SIDS Dossier and Testing Plan were reviewed at the 3rd SIDS Review Meeting, September 1993. Agreed that no tests were needed.
At the SIAM-3, this chemical was identified as having a potential risk to health, since the occupational exposure could be approximately equal to the calculated level of concern based on animal studies. This was being controlled in the sponsor country.
After the SIAM, some additional exposure information on this chemical was gathered using the proposed OECD format. The revised SIDS Initial Assessment Report in which the additional information has been integrated, was reviewed and discussed at SIAM 4.

Comments:

Deadline for circulation: April 1st 1996
(To all SIDS Contact Points and the OECD Secretaria t)

Date of Circulation: April 1st 1996

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	107-05-1
Chemical Name	3-Chloropropene (Allylchloride)
Structural Formula	CH_2=CH-CH_2-Cl

CONCLUSIONS AND RECOMMENDATIONS

It is currently considered of low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE CONCLUSIONS AND RECOMMENDATIONS

Total European production is approximately 280000 t/a The substance is manufactured by hot chlorination (400-600^{o} C) of propylene. The production process is carried out in a 100% closed system. Allylchloride is predominantly (90% worldwide) used as an intermediate in the manufacture of epichlorohydrin and glycerine. It is also used as an intermediate in the production of allyl derivatives (allyl alcohol, diallyl phthalate, allylamine), in the synthesis of medical derivatives, agricultural chemicals and allyl starches, and as thermosetting resins for varnishes, plastics, and adhesives.

Most important emissions of allylchloride will probably occur to the atmosphere. Allylchloride is volatile (estimated to partition 99.35 and 0.59%, air and water respectively), will be removed rapidly from the atmosphere by photodegradation: half life for the reaction with OH-radicals is less than 1 day and if allylchloride is emitted into water it will rapidly volatilise to the air. Hydrolysis will occur (hydrolysis t ½ of 12 days, pH8), but this is not thought to be an important removal process due to the high volatilisation.

Allylchloride is considered to be toxic to fish, with 24-96 hrs LC_{50}-values ranging from 6.9 to 70 mg/l. Allylchloride is found to be also toxic to fish in a test with a deviating exposure time of 14 days. For daphnids allylchloride does not need to be classified for acute toxicity. The lowest LC_{50}-value of 0.34 mg/l is found in a 48-h study with *Xanopus laevis*. Chronic NOEC values for algae and protozoa are ranging from 6.3 to 8.6 mg/l, and for bacteria of 115 mg/l. For environmental assessment, it is decided to use the LC50 for *Xanopus laevis* to derive a PNEC (i.e. 3.4 µg/l) because clearly chronic data is not available from the most sensitive taxonomic groups.

Allychloride was found to be harmful in acute oral toxicity tests and toxic in inhalation toxicity tests. No overall NOAEL could be established from the oral studies in mice, rats and rabbits.

Inhalation studies have been carried out in mice, rats, rabbits and cats with exposures varying from 5 weeks to 6 months. The target organs were liver, kidneys and lungs and the central nervous system. In a recent adequate study, not focussing on neurotoxicity, with rats the NOAEL was 155 mg/m^3 (duration adjusted: 27 mg/m^3). At higher dose levels slight tubular degeneration in the kidneys of both sexes was observed.

The neurotoxic effects of allylchloride have been studied extensively in mice, rats, rabbits and cats. Allychloride is a neurotoxic agent, which especially damages the peripheral nervous system resulting in a dying-back pattern of axonal degeneration. In the most reliable study a NOAEL for neurotoxicity of 31 mg/m^3 (duration adjusted: 7.38 mg/m^3) has been established.

Reproduction studies have not been carried out with allylchloride. However, effects on the male reproductive system were investigated *in vitro* as well as *in vivo*. Testosterone production was not affected in rat foetal testes *in vitro*. Effects on the male gonads of rats and rabbits were observed *in vivo*. In mice, which survived a single s.c. dose = 496 mg/kg b.w. allylchloride, various degrees of damage in the testes was observed. However, no histopathological effects were found in the testes of rats after subchronic inhalatory exposure to concentrations = 782.5 mg/m^3. In developmental studies with rats and rabbits by the inhalation route a slight delay in skeletal development in rats was observed at maternal toxic doses. In adequately performed studies the NOAEL for foetal/embryo and maternal toxicity was 93 mg/m^3 (duration adjusted: 27.3 mg/m^3).

Based on all available mutagenicity data it can be concluded that allylchloride is mutagenic to bacteria and yeast and induces UDS in human HeLa cells, but not in embryonic testinal cells. Allychloride did not cause chromosome aberrations *in vitro* in mammalian cells. Negative results were obtained in the available *in vivo* tests.

IARC (1987) concluded that there is inadequate evidence for the carcinogenicity of allylchloride to experimental animals. Allychloride was classified in group 3.

The PEC/PNEC ratio for aquatic organism according to the USES model is 0.006 and 1.4 E-6 for the local and regional scenario, respectively, both indicating no risk for the aquatic environment.

Using the data for the Shell Pernis plant in the USES model the MOS between the overall NOAEL and the data for indirect exposure for the local scenario is 230 indicating no concern for human safety following indirect exposure.

Occupational exposure to allylchloride will occur during production, processing and transportation. For most plants workplace measurements ensure that exposure limits are below the current MAC/TLC of 3.13 mg/m^3. This value can be considered as a best worst-case Estimated Human Exposure ($EHE_{best\ worst\text{-}case}$) for production. At normal operation the Margin of Safety between the $EHE_{best\ worst\text{-}case}$ and the overall NOAEL of 31 mg/m^3 is sufficient. However, the data available for processing are insufficient to draw a firm conclusion about the Margin of Safety.

NATURE OF FURTHER WORK RECOMMENDED

Appropriate action on setting occupational exposure limits could be taken by the individual national authorities.

FULL SIDS SUMMARY

CAS NO: 107-05-1		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point	NA	other	-135°C
2.2	Boiling Point	NA	ASTM D 1078	43-49°C (at 1013 hPa)
2.3	Density	NA	other	.0936 kg/l
2.4	Vapour Pressure	NA	other	395 hPa at 20°C
2.5	Relative vapour density	NA	other	2.6 (air = 1)
2.6	Partition Coefficient (Log Pow)	NA	other (HPLC)	2.1
2.7	Water Solubility	NA	other	3600 mg/l at 20°C
2.8	Henry Coefficient	NA	calculated	835 $Pa.m^3$/mol at 20°C
2.9	Flash point	NA	ASTM D 56	-32°C (closed cup)
2.11	Explosive limits in air	NA	other	3.2-11.2 vol% in air
2.12	Auto-ignition temperature	NA	ASTM D 2155	391°C
ENVIRONMENTAL FATE/BIODEGRADATION				
3.1.1	Photodegradation	NA	other (measured)	in air $T_{1/2}$ = 9 hour (with O_3-radicals) $T_{1/2}$ = 11 hour (with OH-radicals)
3.1.2	Stability in Water	NA	other (measured)	Evaporation $T_{1/2}$ = 27 minutes at 25°C Hydrolysis $T_{1/2}$ = 12 days at 20°C and pH8
3.2	Monitoring data	NA	NA	Background concentration: In air = < 16 ng/m^3 -64 ng/m^3 (in USA, 1982) In water = < 0.1 ug/l (Germany, 1983) = < 5 ug/l (Japan, 1977)
3.3	Transportation and Distribution	NA	Calculated (fugacity level I)	In air = 99.35% In water = 0.59%
3.5	Biodegradation	NA	MITI test	readily biodegradable
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Carassius auratus*	other	LC_{50} (24-h) = 10 mg/l
		Lebistus reticulates	APHA	LC_{50} (96-h) = 51 mg/l
		Lepomis macrochirus	APHA	LC_{50} (96-h) = 42 mg/l
		Leuciscus idus melanotus	other	LC_{50} (48-h) = 70 mg/l
		Oryzias latipes	other	LC_{50} (48-h) = 6.9 mg/l
		Pimephales promelas	APHA	LC_{50} (96-h) = 20 mg/l
		Peocilia reticulata	Other	LC_{50} (14-d) = 1.2 mg/l
4.2	Acute Prolonged Toxicity to Aquatic Invertebrates	*Daphnia magna*	other	EC_{50} (24-h) = 250 mg/L

4.3	Toxicity to Aquatic Plants e.g. algae	*Mycrocystis aeruginosa*	other	TGK (8-d) = 8.2 mg/l (~ NOEC)
		Scenedesmus quadricauda	other	TGK (8-d) = 6.3 mg/l (~ NOEC)
4.4	Toxicity to bacteria	*Pseudomonas putida*	other	TGK (16-h) = 115 mg/l (~ NOEC)
		Nitrifying bacteria	other	NOEC (2.5-h) = 120 mg/l
		Nitrifying bacteria	other	EC_{75} (2-4 h) = 180 mg/l
4.5	Toxicity to protozoa	*Chilomonas paramaecium*	other	TGK (48-h) = 8.6 mg/l (~ NOEC)
		Entosiphon sulcatum	other	TGK (72-h) = 8.4 mg/l (~ NOEC)
		Uronema parduczi	other	TGK (20-h) = > 240 mg/l (~ NOEC)
4.6	Toxicity to amphibia	*Xenopus laevis*	other	LC_{50} (48-h) = 0.34 mg/l
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	other	LD_{50} = 450-700 mg/kg b.w.
		Mouse	other	LD_{50} = 425-550 mg/kg b.w.
		Rabbit	other	LD_{50} = 300 mg/kg b.w.
5.1.2	Acute Inhalation Toxicity	Rat	other	LC_{50} (2-6 h) = 3200-11800 mg/m^3
		Mouse	other	LC_{50} (2-6 h) = 2500-11500 mg/m^3
		Rabbit	other	LC_{50} (2-h) = 22500 mg/m^3
		Guinea pig	other	LC_{50} (2-h) = 5800 mg/m^3
		Cat	other	LC_{50} (2-h) = 10500 mg/m^3
5.1.3	Acute Dermal Toxicity	Rabbit	other	LD_{50} = 2026 mg/kg b.w.
5.2	Corrosiveness/ Irritation			
	skin and eye irritation	Rabbit	other	slightly irritating
5.4	Repeat Dose Toxicity (inhalation)	Rabbit	other	NOAEL (3 m) = 155 mg/m^3 (50 ppm) (d.a. = 27 mg/m^3)
5.5	Genetic Toxicity In Vitro			
A.	Bacteria Test (Gene mutation)	*Salmonella typhimurium*	plate inc. assay	2 tests negative, 1 positive in TA1535 with S9
			spot test	2 tests positive (in TA1535 with S9) (in TA1535 with and without S9)
			liquid susp. assay	positive in TA100 without S9
		Escherichia coli	spot test	positive with and without S9

B.	Non-Bacterial In Vitro Test (Gene mutation)	*Streptomyces coelicolor*	plate inc. assay spot test	positive for both forward and reverse mutation positive for both forward and reverse mutation
		Aspergillus nidulans	plate inc. assay spot test	negative negative
		Saccharomyces cerevisiae	liquid susp. assay	positive both wit h and without S9
C.	Non-Bacterial In Vitro Test (Chromosomal aberration)	*Aspergillus nidulans*	other	increase in haploid segregants and diploid non-disjunctional sectors
		Rat liver RL1	other	negative
		Human Hela S3	H_3-thymidine incorp.	positive UDS
	DNA Modifying Activity			
		Escherichia coli	other	positive in pol A_1
5.6	Genetic Toxicity In Vivo	Rat/CD	micronucleus test dominant lethal assay	negative
		Rat/DC	sperm abnormality	negative
		Mouse/B6C3F1	SLRL test	negative
		Drosophila melanogaster		negative
5.7	Carcinogenicity (oral)	Rat & Mouse/B6C3F1	other	according to IARC the rat study was inadequate for evaluation. In mice a nonsignificant increase in the incidence of squamous-cell papillomas and carcinomas of the fore stomach was observed
	Carcinogenicity (dermal)	Mouse/Ha: IRC		tumour incidence was not enhanced
5.8	Developmental Toxicity/Teratogenicity (inhalation)	Rat & Rabbit	other	no irreversible structural changes were observed, embryotoxicity occurred at maternal toxic dose levels (NOAEL for embryotoxicity for both rats and rabbits 93 mg/m^3 d.a. 27.3 mg/m^3
5.9	Experience with Human Exposure	Females	occupational	toxic polyneuropathy, slowly improving after removal from exposure
5.10	Other studies Neurotoxicity	Rat	other	NOAEL 32 mg/m^3 = 7.4 mg/m^3 duration adjusted

SIDS Initial Assessment Report

1. IDENTITY

Chemical name:	3-chloro-1-propene
Synonym:	allylchloride; 1-chloro-2-propene, 2-propenyl chloride; 3-chloropropene; 3-chloropropylene; 3-chloro-1-propylene; alpha-chloropropylene; chlorallylene; chloroallylene; propene, 3-chloro-; CAL; monochloropropylene
Cas-number:	107-05-1
Empirical formula:	C_3H_5Cl
Structural formula:	CH_2=CH-CH_2-Cl
Molecular weight:	76.53
Degree of purity:	> 97% (m/m)
Impurities:	hexa-1,5-diene (0.3% w/w) 1-chloropropene (0.2% w/w) 1-chloropropane (0.2% w/w)

2. EXPOSURE

2.1 General discussion

2.1.1 Production quantity

In the Netherlands allylchloride is produced at Pernis. During 1990-1992 the yearly production ranged from 10000 - 50000 tonnes. In 1985 the total European production (3-4 producers) of allylchloride was 280000 tonnes (Eureco, 1990).
In the US 190000 tonnes were produced in 1979 (HSDB). Three Japanese companies also manufacture allylchloride: the 1982 production ranged from 30000-40000 tonnes (IARC, 1985).

2.1.2 Production

There are 5 production sites in Europe. The following companies produce and/or process allylchloride: Solvay S.A., Dow Deutschland Inc., Shell Nederland Chemie B.V., Solvay Alkali GmbH.
The substance is manufactured by hot chlorination (400-600 °C) of propylene, purification will occur by fractionated distillation. The production process is carried out in a 100% closed system (Eureco, 1990).

2.1.3 Uses

Main type of category is non dispersive use, closed systems (Solvay, 1994).
Allylchloride is predominantly (90% worldwide) used as an intermediate in the manufacture of epichlorohydrin and glycerine (Eureco, 1990).
It is also used as an intermediate in the production of allyl derivatives (allyl alcohol, diallyl phthalate, allylamine) and in the synthesis of medical derivatives, agricultural chemicals and allyl starches. In the UK major uses of 3-chloropropene are in the preparation of sulphonates, xanthates, intermediates for the production of high-performance resins (HSE, 1997).
Hawley (1971) also mentioned the use as thermosetting resins for varnishes, plastics, and adhesives.

2.2 Environmental exposure

2.2.1 Relevant exposure properties

Vapour pressure:	395 hPa at 20 °C
Water solubility:	3600 mg/l at 20 °C
Octanol-water partition coefficient:	log K_{ow} = 2.1 (experimentally determined)
Henry coefficient:	835 Pa.m^3/mol at 25 °C (calculated)
Biodegradation:	Results from biodegradation tests are equivocal. A modified MITI test indicates a borderline case of ready biodegradability: 55-69% based on BOD after 28 days. It is unknown whether the 10 day time-window was reached (>60% degradation within 10 days). In another test degradation of allylchloride was shown: BOD was 14 and 25% of ThOD after 5 days with non-adapted and adapted seed, respectively. This test is not equal to a standard OECD test for ready-biodegradability. However, when it is assumed that in the MITI test the 10 day time-window has probably been reached, it can be concluded that allylchloride can be degraded in the environment. Based on the information available the compound is considered readily biodegradable.
Hydrolysis:	A half-life in water of 12 days at pH of 8 and 20 °C has been determined. After hydrolysis of allylchloride allyl alcohol is formed which is readily biodegradable (Krijgsheld, 1984).

Photolysis:	Allylchloride will react with ozone or hydroxyl (OH) radicals in the atmosphere. It is well established that the OH radical is the dominant reactive species in the degradation of organic compounds in the atmosphere (Atkinson, 1985). Assuming an OH radical concentration of 10^6 molecules/cm^3 a half life of 11 hours can be calculated. The value of 10^6 molecules/cm^3 may be regarded as a typical value for the Northern Hemisphere (de Leeuw, 1993). Reaction of allylchloride with OH radicals leads to the formation of the OH-haloalkene adduct. The subsequent reactions of this adduct under atmospheric conditions is unknown, however. It should be realized that the value of 0.80 days is an underestimation as allylchloride may also react with ozone and NO_3 radicals.
1 ppm	3.13 mg/m^3.

2.2.2 Release and sources

Allylchloride may be released into the atmosphere during its manufacturing and use.
Since production and processing occurs in 100% closed systems no high emissions to the atmosphere are expected.
Diurnal urban air samples collected in the USA were found to contain only several ng/m^3 with a highest concentration of 64 ng/m^3 found in Pittsburg, PA. (IARC, 1985). Allylchloride concentrations in surface water in Japan (site unknown) and in Europe (river Rhine) were below the detection limit: <0.5 ug/l and <0.1 ug/l respectively.

2.2.3 Partitioning and fate

Allylchloride is soluble in water and soluble in acetone, benzene and methanol and very soluble in diethylether, ethanol and chloroform. The substance can react violently with acids, bases such as ammonia and amines, metals and their alloys.

Allylchloride can be considered as a volatile compound. Results from Mackay level 1 calculations indicate that 99.35% and 0.59% will partition into air and water, respectively (Annex 1).

Most important emissions of allylchloride will probably occur to the atmosphere. Allylchloride will be removed rapidly from the atmosphere by photodegradation: half life for the reaction with OH-radicals is less than 1 day.
If allylchloride is emitted into water it will rapidly volatilize to the air. Model calculations for a river indicate a half life of approx. 3 hours. Under experimental conditions which included 250 ml vessels, concentration of 1 mg/l, 200 rpm stirring of a solution, still air, solution depth of 6.5 cm, the half life was approx. 30 minutes (Dilling, 1977). Allylchloride present in the water phase will biodegrade in a Waste Water Treatment Plant or in surface water, as the compound can be considered as readily biodegradable. Hydrolysis does occur, but will not be an important removal process due to the high volatilization rate and the relatively slow half life for hydrolysis of 12 days at a pH of 8.

2.3 Consumer exposure

There will be no significant consumer exposure due to its use as an intermediate.

2.4 Occupational exposure

2.4.1 Manufacture

Occupational exposure can occur during production, processing and transportation. The occupational exposure is predominantly being controlled by process enclosure, the provision of local exhaust ventilation (LEV) and personal protective equipment (PPE).

In the Netherlands workplace monitoring data are available for the Shell Pernis production plant. Data were obtained during normal operation, maintenance stops and shut down from 1980-1991. All data relate to exposure by inhalation and an 8 hour working period. Mean allylchloride concentrations range from 0.2 to 2.89 mg/m^3.

At a German production site a 24-hour air monitoring (GC) is used to ensure that exposure levels of allylchloride stay below the applicable workplace exposure limits of 3 mg/m^3 (Dow, 1994).

Emission of Solvay production plants to the atmosphere was less than 0.1% of the production; no waste water discharges during production occur (Solvay, 1994).

At processing sites in three UK background atmospheric levels of airbourne allylchloride ranging from non-detectable to 10.5 mg/m^3 were found using colorimetric indicator tubes. Time-weight average (TWA) full-shift personal and area samples were found to be less than 0.06 mg/m^3 at another processing location in UK (EHC, 1997).

Exposure data from processing sites in France were reported for several industrial activities and are listed in the table below. These data are found in a governmental data base and could not be checked, and should therefore not be used in the risk assessment (Diderich, 1995).

Industrial activity	type (n)	results
storage & transport	sampl. of ambient air (2)	8 mg/m^3; 63 mg/m^3
mixing, compressing, moulding, reaction	sampl. of ambient air (49)	< 0.3 – 33 mg/m^3 50 percentile: 3 mg/m^3 90 percentile: 19 mg/m^3
bottling, barreling, reeling, dosing	sampl. of ambient air (2)	0.7 mg/m^3; 4 mg/m^3

The occupational exposure limits (MAC/TLV) for most European countries, US and Japan are 1 ppm (3 mg/m^3), with an occupational short term exposure limit value of 2 ppm (6 mg/m^3). These values are well below the odour threshold value ranging from 3-6 ppm (9-18.5 mg/m^3).

2.4.2 Use

Allylchloride is used as an intermediate predominantly in the production of epichlorohydrine and also glycerine.
In Australia allylchloride is used as a lab. reagent.
In Sweden the substance is used as a raw material in the production of polyallylether. These products go into paint and lacquers. Exposure occurs only during maintenance. In 1993 about 889-906 tonnes was used in manufacturing 3 products (SPR, 1995).

3. TOXICITY

3.1 Ecotoxicity

For assessing the quality of aquatic ecotoxicological studies special attention has to be paid to the way test concentrations are maintained in the test solution due to the volatile properties of allylchloride. First of all a study has to meet several requirements with respect to experimental design. Most of these requirements are stated in test-guidelines like the OECD Test Guidelines. Secondly, special precautions have to be taken for concentration maintenance. In many studies it is reported how the problem of evaporation is dealt with. However, in other studies no special precautions are taken or are not reported. The quality of studies can be ranked as follows from high to low reliability:

- flow-through, static and semi-static studies in which measured concentrations are reported,
- static and semi-static studies in which the test vessels are closed properly and the concentrations are not measured,
- static and semi-static studies where the test vessels are not closed, no analysis of test concentration is carried out (or nothing is reported thereof).

3.1.1 Acute toxicity to fish

Carassius auratus	24-h LC_{50} = 10 mg/l
Carassius auratus, 1-2 g	96-h LC_{50} = 21 mg/l (soft water)
Lebistus reticulates, 0.1-0.2g	96-h LC_{50} = 51 mg/l (soft water)
Lepomis macrochirus, 1-2 g	96-h LC_{50} = 42 mg/l (soft water)
Leuciscus idus melanotus	48-h LC_{50} = 70 mg/l
Oryzias latipes	48-h LC_{50} = 6.9 mg/l
Pimephales promelas, 1-2 g	96-h LC_{50} = 20 mg/l (soft water)
Pimephales promelas, 1-2 g	96-h LC_{50} = 24 mg/l (hard water)
Poecilia reticulata	14-d LC_{50} = 1.2 mg/l

All 96-h tests were static tests and were performed according to APHA Standard Methods (1960). Results were based on nominal concentrations. It is unknown whether the test vessels were closed. Due to the volatile properties of allylchloride these tests are considered as less reliable.
More reliable are the 24 hrs test with *C. auratus* (measured value) and the 48 hrs test with *O. latipes* (renewal 8-16 hrs), although exposure times are relatively short. Most suitable and also reliable is the 14 days test with *P. reticulata* in which the test solutions were renewed every 24 hrs.

3.1.2 Acute toxicity to daphnids

Daphnia magna, 24-h old	24-h EC_{50} = 250 mg/l

A standardized procedure was followed according to Bringmann and Kühn. Test glasses were covered with filtration paper. This is probably insufficient to prevent volatilization.
Therefore this test can be considered as less reliable.

3.1.3 Toxicity to algae

Microcystis aeruginosa	8-d NOEC = 8.2 mg/l
Scenedesmus quadricauda	8-d NOEC = 6.3 mg/l

Tests according to Bringmann and Kühn. TGK (Toxische Grenzkonzentration) values were established and are blessed on total biomass. As percentage effect at the TGK is 3-5% these values are regarded as NOECs. Test vials were adequately closed with metal caps.

3.1.4 Other ecotoxicological information

Toxicity to bacteria

Pseudomonas putida	16-h NOEC = 115 mg/l (total biomass)
Nitrification	2.5-h NOEC = > 120 mg/l
Nitrification	2-4-h EC_{75} = 180 mg/l

Test with *P. putida* according to Bringmann and Kühn. It is unknown whether a closed system was used. The tests on nitrification may be contradictory. However, no information is available on the concentration-effect relationship for the test resulting in an EC_{75} of 180 mg/l. Both tests were carried out using activated sludge. Different results may be caused by different samples taken from waste water treatment plants.

Toxicity to protozoa

Chilomonas paramecium	48-h NOEC = 8.6 mg/l
Entosiphon sulcatum	72-h NOEC = 8.4 mg/l
Uronema parduczi	20-h NOEC = > 240 mg/l

Tests according to Bringmann and Kühn. Test vials were adequately closed with metal caps.

Toxicity to amphibia

Xenopus laevis, 3-4 w old	48-h LC_{50} = 0.34 mg/l

The test was performed with at least 5 concentrations. No replicas were used. Test was carried out in covered glass basins. Results are based on nominal concentration. The test can be considered as reliable.

Conclusion

Based on EC-directive, allylchloride is considered to be toxic to fish, with 24-96 hrs LC_{50}-values ranging from 6.9 to 70 mg/l. Allylchloride is found to be also toxic to fish in a test with a deviating exposure time of 14 days.
For daphnids allylchloride needs not be classified for acute toxicity. The test must be considered as less reliable, however.
The lowest LC_{50}-value of 0.34 mg/l is found in a 48-h study with *Xenopus laevis*. No EC classification for amphibia is estimated yet. Chronic NOEC values for algae and protozoa are ranging from 6.3 to 8.6 mg/l (except the NOEC of >250 mg/l found for *U. parduczi*, and for bacteria of 115 mg/l). No EC classification for chronic effects has been established yet.

3.2 Human toxicity

The kinetics of allylchloride has been studied in rats after oral, inhalatory and intravenous exposure. Allylchloride is rapidly and extensively absorbed by the inhalation and oral routes in rats. No data are available on skin absorption. Unchanged allylchloride is excreted solely in expired air. The main urinary metabolites in the rat following oral dosing are mercapturic acids, demonstrating that gluthathione has a major role in the detoxicification of the substance. Allylchloride is metabolised to expired CO_2 by poorly characterised processes that appear to become saturated as the dose level increases. Faecal excretion of metabolites is not a major route of elimination. There is evidence that biotransformation of allylchloride does not lead to the formation of epichlorohydrin but it does lead to the formation of allylalcohol → acroleine → acrylic acid.

3.2.1 Acute toxicity

Oral rat:	LD_{50} ranging from 450 to 700 mg/kg b.w.
mouse:	LD_{50} ranging from 425 to 500 mg/kg b.w.
rabbit:	LD_{50} = 300 mg/kg b.w.
Inhalation:	LC_{50} (2-6h) ranging from 2.5-22.5 mg/l
Dermal rabbit:	LD_{50} = 2026 mg/kg b.w.
S.C. mice:	LD_{50} = 621 mg/kg b.w.
Skin irritation:	slightly irritating
Eye irritation:	slightly irritating

Conclusion:

Allylchloride was found to be harmful in the acute oral toxicity tests and toxic in the inhalation toxicity tests (the substance is labelled with R 26: very toxic by inhalation) (EC, 1993). Allylchloride is slightly irritating to the skin and eye (EC, 1993).

3.2.2 Repeated dose toxicity

A limited number of oral tests with allylchloride were available. No overall NOAEL could be established from these studies in mice, rats and rabbits. Inhalation studies have been carried out in mice, rats, rabbits and cats with exposures varying from 5 weeks to 6 months. The target organs were liver, kidneys and lungs and the central nervous system. In a recent adequate study, not focussing on neurotoxicity, with rats the NOAEL was 155 mg/m^3 (duration adjusted: 27 mg/m^3). At higher dose levels slight tubular degeneration in the kidneys of both sexes was observed. The neurotoxic effects of allylchloride have been studied extensively in mice, rats, rabbits and cats. Allylchloride is a neurotoxic agent, which especially damages the peripheral nervous system resulting in a dying-back pattern of axonal degeneration. In the most reliable study a NOAEL for neurotoxicity of 31 mg/m^3 (duration adjusted: 7.38 mg/m^3) has been established.

3.2.3 Reproductive toxicity

Reproduction studies have not been carried out with allylchloride.
However, effects on the male reproductive system were investigated *in vitro* as well as *in vivo*. Testosterone production was not affected in rat foetal testes *in vitro*. Effects on the male gonads of rats and rabbits were observed *in vivo*. In mice, which survived a single s.c. dose $\leq$ 496 mg/kg b.w. allylchloride, various degrees of damage in the testes was observed. **However**, no histopathological effects were found in the testes of rats after subchronic inhalatory exposure to concentrations $\geq$ 782.5 mg/m^3. In developmental studies with rats and rabbits by the inhalation route a slight delay in skeletal development in rats was observed at maternal toxic doses. In adequately performed studies the NOAEL for foetal/embryo- and maternal toxicity was 93 mg/m^3 (duration adjusted: 27.3 mg/m^3).

3.2.4 Genetic toxicity

Allylchloride was tested for mutagenicity in a battery of *in vitro* and *in vivo* assays. In the older *in vitro* assays negative results were obtained, probably due to the vaporization of allylchloride. Adequate mutagenicity assays with *Salmonella typhimurium* were positive, with and without metabolic activation. The mutagenicity greatly decreased in the presence of an exogenous activating system. In a spot test with *Escherichia coli* as well as in tests with *Streptomyces coelicolor* both with and without metabolic activation positive results were obtained. Allylchloride was negative in tests with *Aspergillus nidulans*. The substance induces gene conversions in *Saccharomyces cerevisiae* and somatic segregation in *Aspergillus nidulans*. No significant compound-related chromosome damage was observed in RL_1 cells. Allylchloride induces unscheduled DNA synthesis in human HeLa S3 cells, but not in human embryonic intestinal cells.
No increase in chromosomal aberrations was observed in a cytogenetic test with rats exposed to allylchloride by inhalation. The substance was negative in a dominant lethal assay with rats and in a sperm-abnormality test with mice. Allylchloride did not cause an increase in sex-linked recessive lethal mutations in *Drosophila melanogaster*.

Remark:
The available *in vivo* studies are not performed according to current guidelines: there are no indications that allylchloride did reach the target cells (no toxicity was observed) and the used dose levels are rather low.

Conclusion:
Based on all available mutagenicity data it can be concluded that allylchloride is mutagenic to bacteria and yeast and induces UDS in human HeLa cells, but not in embryonic testinal cells. Allylchloride did not cause chromosome aberrations *in vitro* in mammalian cells. Negative results were obtained in the available *in vivo* tests.

Note:
The mutagenicity in bacterial systems is supported by the direct alkylation of DNA and NBP [4-(p-nitrobenzyl)pyridine] by allylchloride.
Mutagenic effects were observed in photooxidation products of allylchloride and NO_x in the presence of sufficient C_2H_6 (Shepson et al., 1987).

3.2.5 Carcinogenicity

Long-term oral gavage studies were available in mice and rats. In mice a non-significant increase in the incidence of squamous-cell papillomas and carcinomas of the forestomach was observed. The rat study was inadequate for evaluation because of high mortality in the exposed animals (tumour development did not attribute to mortality).
No skin tumours were observed in mice after repeated (3 times/week) dermal administration of allylchloride for 440-594 days. Following i.p. administration (3 times/week for 8 weeks) to mice, a slight increase in the incidence of lung adenomas was observed.

Conclusion:
IARC (1987) concluded that there is inadequate evidence for the carcinogenicity of allylchloride to experimental animals. Allylchloride was classified in group 3.

3.2.6 Any other human related information that is available

After overexposure by inhalation to allylchloride eye irritation, often with orbital pain, is the most frequent complaint. Nose, throat and respiratory irritation have also been reported. Prolonged skin contact can result in erythema and edema; a deep-seated pain (described as bone-ache type) beneath the point of skin contact may occur even following exposure to very small quantities of liquid allylchloride.
After occupational exposure polyneuropathy, adverse effects on the central nervous system as well as reversible liver and kidney damage have been reported. A study investigating the potential adverse effects of allylchloride on male fertility was considered inadequate for evaluation of the effects of allylchloride on semen quality (IARC, 1987).
In limited epidemiological studies no indications for an increased cancer incidence were found. No cytogenetic effects were observed in workers exposed to allylchlorid in combinations with other chlorinated hydrocarbons at levels well below the occupational exposure limits.

4. INITIAL ASSESSMENT

The human and/or environmental profiles presented describe the risk assessment for two scenarios:

Scenario 1: A risk assessment is carried out for a standard environment using the uniform System for the Evaluation of Substances (USES) (RIVM, VROM & WVC, 1994) see Annex 2. In this scenario waste water is discharged to a Sewage Treatment Plant (STP). The PEC is calculated 1000 m from the point of discharge of the effluent. A calculation for a regional model.

Scenario 2: A risk assessment, also carried out with the USES model, using data from the Pernis Plant, see Annex 3.

Assumptions made are:

Overall production:	230000 tonnes/year (rest of Europe)
Estimated production Pernis site:	50000 tonnes/year

Environmental

Acute ecotoxicological data for aquatic organisms are available for amphibia, fish, and daphnids: L(E)C50 values range from 0.34 for *Xenopus laevis* to 250 mg/l for *Daphnia magna*. Chronic data are present for algae, bacteria and protozoa: NOEC values range from 6.3 for *Scenedesmus quadricauda* to >240 mg/l for *Uronema parduczi*. It can be concluded that lower organisms are less sensitive than higher organisms like fish and amphibians. Critical study is the one with *X. laevis* being a factor 3.5 lower than the lowest LC50 for fish, being 1.2 mg/l for *Poecilia reticulata*.

X. laevis is not a standard test species. The test has been developed by Slooff and Baerselman (1980). Slooff et al. (1983) showed that the sensitivity of this test organism was comparable to fish. They tested 15 compounds to a.o. 5 fish and 2 amphibian species. The value of 0.34 mg/l for *X. laevis* was determined by De Zwart and Slooff (1987) who tested 33 compounds. They tested 5 halogenated hydrocarbons of which allylchloride and 3-bromopropene were at least a factor 15 more toxic than 1-chloro-3-bromopropane, 1,3-dichloropropane and 3-chloro-2-methylpropene. Especially the difference between 3-chloro-2-methylpropene with a LC50 of 10 mg/l and allylchloride is remarkable. The LC50 of 3-bromopropene of 0.66 mg/l is on the other hand almost equal to allylchloride.
It can be concluded that the value for *X. laevis* cannot be regarded as an outlier.
Although it must be stated that no replicas were used, the test design used a closed system in order to prevent volatilisation, so the test is of sufficient quality. Secondly, the sensitivity of *X. laevis* is comparable to the LC50 value for the fish *P. reticulata* of 1.2 mg/l.

It is decided to use the LC50 for *X. laevis* to derive a PNEC. Assessment factors are used to derive a PNEC: a factor 100-1000 on acute L(E)C50 data and 10 on chronic NOEC data (USES). As acute data are available for several taxonomic groups an assessment factor 100 on the lowest L(E)C50, i.e. for *X. laevis*, is considered sufficient. This leads to a PNEC of 3.4 ug/l. Using a factor 10 on the lowest NOEC, i.e. 6.3 mg/l for *S. quadricauda*, leads to a PNEC of 630 ug/l. However, clearly chronic data are not available from the most sensitive taxonomic groups. Therefore the value of 3.4 ug/l is preferred.

Scenario 1 (Annex 2): The PEC/PNEC ratio for aquatic organisms according to the USES model is 59 for the local scenario, indicating a risk for the aquatic environment. For the regional scenario a PEC/PNEC ratio of 0.0008 is calculated.
Using a NOEC of 115 mg/l a PEC/PNEC ratio of 0.065 for microorganisms in the STP is calculated. The concentration in the aeration tank is used as the PEC.

Scenario 2 (Annex 3) Specific data for the Pernis plant are used in the USES model (Shell, 1994).
The maximum release to air is 50 tonnes/year, which means a release of 140 kg/day. The maximum release to water is $\leq$ 0.5 tonnes/year, which means a maximum release of about 1 kg/day. The WWTP at the Pernis plant has a flow of 1500 m^3/hour. This is equivalent to 240.000 inhabitant equivalents based on a

water use per inhabitant of 150 liter/day. The sludge produced by the WWTP is not applied to soil but burned.
The PEC/PNEC ratio for aquatic organisms according to the USES model is 0.006 and 1.4 E-6 for the local and regional scenario, respectively, both indicating no risk for the aquatic environment.
Using an NOEC of 115 mg/l a PEC/PNEC ratio of 6.5 E-6 is calculated. The concentration in the aeration tank is used as the PEC.

Human

In the extensive data base both animal as well as human studies were available. Not all studies were performed according to current standards, but overall the information is considered acceptable. In the human studies specified exposure data were often lacking.

Indications have been obtained that allylchloride may possess genotoxic activity.
However full evaluation of its genotoxicity is not possible. IARC (1987) has classified allylchloride as a category 3 compound.

The neurotoxic effects observed even at very low doses both in experimental animals and humans are used as the toxicological endpoint. Because of uncertainties in the human exposure data the NOAEL of 31 mg/m^3 obtained from a 34-week neurotoxicity study in rats (exposure: 8h/d, 5d/w), is used as overall NOAEL. The NOAEL corrected for continuous exposure is 7.38 mg/m^3.

Scenario 1 (Annex 2): From the USES model it is calculated that the Margin of Safety (MOS) between the overall NOAEL and the data for indirect exposure for the local scenario is 54.7 and for the regional scenario is 7.6 x 10^5. From these data it can be concluded that there is a rather small margin of safety for the local scenario indicating concern for human safety following indirect exposure.

Scenario 2 (Annex 3): Using the data for the Shell Pernis plant in the USES model the MOS between the overall NOAEL and the data for indirect exposure for the local scenario is 230 indicating no concern for human safety following indirect exposure.

Since it is not likely that significant consumer exposure to allylchloride occurs, it is concluded that there will be no concern for human safety by this exposure route.

Occupational exposure to allylchloride will occur during production, processing and transportation.
Allylchloride is an intermediate produced in "closed systems" mostly on site. Less than 5% of the production is processed off site. Inhalation exposure may occur during normal operation, maintenance and shut down, although respiratory protective devices should then be worn.
For most plants workplace measurements ensure that exposure limits are below the current MAC/TLV of 3.13 mg/m^3. This value can be considered as a best worst-case Estimated Human Exposure ($EHE_{best\ worst\text{-}case}$) for production. Personal air monitoring data, regularly being performed at the Pernis plant since 1980, support this assumption. For processing, however 50% of the ambient air samples from industrial sites in France exceed the MAC of 3 mg/m^3.
At normal operation the Margin of Safety between the $EHE_{best\ worst\text{-}case}$ and the overall NOAEL of 31 mg/m^3 is sufficient.
The data available for processing are insufficient to draw a firm conclusion about the Margin of Safety.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusion

Based upon the available data information local risks were estimated for 2 scenarios. For scenario 1 the initial assessment gave indications for concern for humans following indirect exposure. This risk assessment shows the intrinsic hazard of allylchloride in case no risk reduction measurements are taken. Scenario 2 did not indicate a concern for human safety.
Scenario 1 revealed also the existence of a risk for the aquatic environment.
As with human exposure effective risk reduction measurements, i.e. emission reduction, abolished this risk for the aquatic environment (scenario 2).

5.2 Recommendation

From this initial assessment it is clear that all production plants world wide should take adequate emission reduction measurements, if not already taken. Appropriate action on setting occupational exposure limits could be taken by the individual national authorities.

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ANNEX 1

FUGACITY LEVEL I, II AND III PROGRAMS FOR OECD WORKSHOP:
VERSION 1, JAN. 1992

GENERIC PARAMETERS

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION

Properties of ALLYLCHLORIDE

Temperature deg C	25
Molecular mass g/mol	76.5
Melting point deg C	- 135
Fugacity ratio	1.000E + 00
Vapour pressure Pa	39500
Sub-cooled liquid vapour press Pa	39500
Solubility g/m^3	3600
Solubility mol/m^3	4.706E + 01
Henry's law constant Pa.m^3/mol	839.375
Log octanol-water partition coefficient	2.1
Octanol-water partition-coefficient	125.8925
Organic C-water partition-coefficient	51.61593
Fish-water partition coefficient	6.294626
Air-water partition coefficient	3.386E-01
Soil-water partition coefficient	2.477565
Sedt-water partition coefficient	4.955129
Susp sedt-water partition coefficient	15.48478
Aerosol-air partition coefficient	151.8987
Aerosol Z value	6.127867E-02
Aerosol density kg/m^3	2000
Amount of chemical moles	1307190
Amount of chemical kilograms	100000
Fugacity Pa	3.219104E-05
Total of VZ products	4.061E + 10

Phase properties and compositions

Phase	Air	Water	Soil solids	Sedt solids	Susp sedt	Fish
Volume m^3	1.000E + 14	2.000E + 11	9.000E + 09	1.000E + 08	1.000E + 06	2.000E + 05
Density kg/m^3	1.185413	1000	2400	2400	1500	1000
Depth m	1000	20	.1	.01		
Area m^2	1E + 11	1E + 10	9E + 10	1E + 10		
Area fraction	1	.1	.9	.1		
Frn org carb			.02	.04	.2	
Z $mol/m^3.Pa$	4.034E-04	1.191E-03	2.952E-03	5.903E—3	1.845E-02	7.499E-03
VZ mol/Pa	4.034E + 10	2.383E + 08	2.657E + 07	5.093E + 05	1.845E + 04	1.500E + 03
Fugacity Pa	3.219E-05	3.219E-05	3.219E-05	3.219E-05	3.219E-05	3.219E-05
Conc mol/m^3	1.299E-08	3.835E-08	9.502E-08	1.900E-07	5.939E-07	2.414E-07
Conc g/m^3	9.935E-07	2.934E-06	7.269E-06	1.454E-05	4.543E-05	1.847E-05
Conc ug/g	8.381E-04	2.934E-06	3.029E-06	6.057E-06	3.029E-05	1.847E-05
Amount mol	1298644	7670.241	855.1584	19.00352	.59386	.0482813
Amount kg	99346.3	586.7734	65.41962	1.453769	4.543029E-02	3.69352E-03
Amount %	99.3463	.5867735	6.541962E-02	1.453769E-03	4.543029E-05	3.69352E-06

ANNEX 2

USES V1.0 SINGLE SUBSTANCE				
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1				
SUBSTANCE IDENTIFICATION				
Name: allylchloride CAS-No: 107-05-1 EC-notification no.: EINECS no: 203-457-6 Molecular weight: [g.mol-l] 76.53 Mol. Formula: C3H5Cl				
PARAMETER STATUS				
Input parameters defaults used: 37 of 57 Model parameters defaults used: 15 of 15 Intermediate results overwritten: 0 of 57				
INPUT PARAMETERS				
TONNAGE		ACTUAL		DEFAULT
Tonnage national	[tonnes.yr-1]	5e+04	S	0
Tonnage Europe	[tonnes.yr-1]	2.3e + 05	S	0
MAIN CATEGORY				
Production: Ib Intermediates isolated, stored on-site Formulation: Ib Dedicated equipment – cleaning limited Processing: Ib Continuous process				
INDUSTRIAL CATEGORY				
Ind. cat.: 3 Chemical industry: chemicals used in synthesis				
USE CATEGORY				
Primary: 33 Intermediates				
EMISSION RELEVANT DURING LIFE-CYCLE STEP ?		ACTUAL		DEFAULT
Emission production		Yes		No
Emission formulation		No		No
Emission processing		Yes		No
Emission private use		No		No
Emission recovery		No		No
Bypass STP		No		No

USES V1.0 SINGLE SUBSTANCE				
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1				
PHYSICO-CHEMICALS PROPERTIES		ACTUAL		DEFAULT
Melting point	[oC]	-135	S	??
Vapour pressure	[Pa]	3.95e + 05	S	0.001
Octanol-water part. coeff. (10log)	[-]	2.1	S	??
Water solubility	[mg.l – 1]	3600	S	??
Henry's law constant	[Pa.m3.mol-1]	839.7	E	??
Air-water part. coeff.	[l.l-1]	0.3544	E	??
Solids-water part. coeff. in soil	[l.kg-1]	1.501	E	??
Solids-water part. coeff. sediment	[l.kg-1]	1.501	E	??
Solids-water part. coeff. susp. mat.	[l.kg-1]	5.174	E	??
DEGRADATION		ACTUAL		DEFAULT
DT50 photodeg. in air	[d]	0.8	S	160
DT50 hydrolysis in water	[d]	12	S	1e+06
Readily biodegradable		Yes		No
DT50 biodeg. in water	[d]	5	E	??
DT50 biodeg. in soil	[d]	0.2715	E	??
DT50 biodeg. in STP	[d]	0.009627	E	??
BIOACCUMULATION		ACTUAL		DEFAULT
BCF fish	[l.kg-1]	5.885	E	??
BCF worm	[kg.kg-1]	23.19	E	??
BCF stem plant	[kg.kg-1]	0.8989	E	??
BCF root plant	[kg.kg-1]	1.525	E	??
BCF air plant	[m3.kg-1]	0.00519	E	??
BCF meat	[d.kg-1]	3.162e-06	E	??
BCF milk	[d.kg-1]	1e-06	E	??
ECOTOXICITY		ACTUAL		DEFAULT
L (E) C50 for fish	[mg.l-1]	1.2	S	??
L (E) C50 for crustaceans	[mg.l-1]	250	S	??
L (E) C50 for algae	[mg.l-1]	6.3	S	??
L (E) C50 for other aquatic species	[mg.l-1]	0.34	S	??
IC50 for micro-org. in STP	[mg.l-1]	??	D	??
NOEC for micro-org. in STP	[mg.l-1]	115	S	??
NOEC for fish	[mg.l-1]	??	D	??
NOEC for crustaceans	[mg.l-1]	??	D	??
NOEC for algae	[mg.l-1]	6.3	S	??
		ACTUAL		DEFAULT
Consumption rate testspecies	[kg.kg-1.d-1]	0.125	D	0.125

USES V1.0 SINGLE SUBSTANCE				
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1				
TOXICITY DATA FOR MAMMALS		ACTUAL		DEFAULT
LD50	[mg.kg-1 (bw)]	425	S	1
LC50 inhalatory	[mg.m-3]	2500	S	??
NOEC in food	[mg.kg-1]	10	E	??
Oral NOAEL, non-carcinogens	[mg.kg-1.d-1]	1.581	E	1
Is this value a LOAEL?		No		No
Animal test or human study?		Animal		Animal
Subchronic or chronic test?		Subchronic		Subchronic
NOAEL inhalatory	[mg.m-3]	7.38	S	??
Is this value a LOAEL?		No		No
Animal test or human study?		Animal		Animal
Subchronic or chronic test?		Subchronic		Subchronic
ADI or TDI	[mg.kg-1.d-1]	??	D	??
Genotoxic or carcinogenic		No		No
Corrosive or sensitizing		No		No
Toxic to reproduction		No		No
		ACTUAL		DEFAULT
Consumption rate testspecies	[kg.kg-1.d-1]	0.1	D	0.1
Scenario		No consumer exposure		No consumer exposure

INTERMEDIATE RESULTS			
LOCAL EMISSION		OVER-WRITE	CALCULATED
Step with largest emission to water			Production
Release to air	[kg.d-1]		500
Release to waste water	[kg.d-1]		500
Release to surface water	[kg.d-1]		0
Release to soil	[kg.d-1]		0
Number of emission days	[d]		300
Distr. factor emission flux to water	[-]		2
REGIONAL EMISSION		OVER-WRITE	CALCULATED
Release to air	[kg.d-1]		821.9
Release to waste water	[kg.d-1]		1027
Release to surface water	[kg.d-1]		0
Release to agricultural soil	[kg.d-1]		0
Release to industrial soil	[kg.d-1]		0

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1			
CONTINENTAL EMISSION		OVER-WRITE	CALCULATED
Release to air	[kg.d-1]		3781
Release to waste water	[kg.d-1]		4726
Release to surface water	[kg.d-1]		0
Release to agricultural soil	[kg.d-1]		0
Release to industrial soil	[kg.d-1]		0
LOCAL EMISSION FROM STP		OVER-WRITE	CALCULATED
Emission STP to air	[kg.d-1]		123.2
Emission STP to water	[kg.d-1]		11.59
Emission STP to susp. matter	[kg.d-1]		0.01021
Emission STP to sludge	[kg.d-1]		3.109
REGIONAL EMISSION FROM STP		OVER-WRITE	CALCULATED
Emission STP to air	[kg.d-1]		246
Emission STP to water	[kg.d-1]		24.14
Emission STP to susp. matter	[kg.d-1]		0.02117
Emission STP to sludge	[kg.d-1]		6.39
CONTINENTAL EMISSION FROM STP		OVER-WRITE	CALCULATED
Emission STP to air	[kg.d-1]		1028
Emission STP to water	[kg.d-1]		115.7
Emission STP to susp. matter	[kg.d-1]		0.1001
Emission STP to sludge	[kg.d-1]		29.41
LOCAL ENVIRONMENT CONCENTRATIONS		OVER-WRITE	CALCULATED
Conc. influent STP	[mg.l-1]		277.8
Conc. aeration tank STP	[mg.l-1]		7.505
Conc. effluent STP	[mg.l-1]		6.446
Conc. sludge STP	[mg.kg-1]		2713
Conc. air (100m from STP)	[mg.m-3]		0.02812
Conc. air (100m from source)	[mg.m-3]		0.1142
Conc. groundwater	[mg.l-1]		0
Conc. agricultural soil	[mg.kg-1]		0.248
Conc. surface water (episode)	[mg.l-1]		0.2014
Conc. surface water (annual)	[mg.l-1]		0.1655

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1			
REGIONAL ENVIRONMENT CONCENTRATIONS		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		9.29e-06
Conc. surface water	[mg.l-1]		2.826e-06
Conc. porewater	[mg.l-1]		3.311e-07
Conc. natural soil	[mg.kg-1]		1.475e-08
Conc. agricultural soil	[mg.kg-1]		4.494e-07
Conc. industrial soil	[mg.kg-1]		1.475e-08
CONTINENTAL ENVIRONMENT CONCENTRATIONS		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		1.098e-06
Conc. surface water	[mg.l-1]		3.333e-07
Conc. porewater	[mg.l-1]		4.338e-08
Conc. natural soil	[mg.kg-1]		1.743e-09
Conc. agricultural soil	[mg.kg-1]		5.888e-08
Conc. industrial soil	[mg.kg-1]		1.743e-09
LOCAL: CONCENTRATIONS IN HUMAN INTAKE MEDIA		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		0.1142
Conc. drinking water	[mg.l-1]		0.08277
Conc. fish	[mg.kg-1]		0.9693
Conc. stem of plants	[mg.kg-1]		0.2235
Conc. root of plants	[mg.kg-1]		0.3782
Conc. meat	[mg.kg-1]		9.227e-05
Conc. milk	[mg.kg-1]		2.918e-05
LOCAL: INTAKE BY PREDATORS		OVER-WRITE	CALCULATED
Conc. earthworms	[mg.kg-1]		5.75
Conc. fish	[mg.kg-1]		0.9693
LOCAL: HUMAN INTAKE VIA INDIRECT EXPOSURE		OVER-WRITE	CALCULATED
Intake air	[mg.kg-1.d-1]		0.02446
Intake drinking water	[mg.kg-1.d-1]		0.002365
Intake fish	[mg.kg-1.d-1]		0.0001523
Intake stem of plant	[mg.kg-1.d-1]		0.001277
Intake root of plant	[mg.kg-1.d-1]		0.00067
Intake meat	[mg.kg-1.d-1]		1.582e-07
Intake milk	[mg.kg-1.d-1]		1.576e-07
Total human dose	[mg.kg-1.d-1]		0.02893

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1			
REGIONAL: CONCENTRATIONS IN HUMAN INTAKE		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		9.29e-06
Conc. drinking water	[mg.l-1]		1.413e-06
Conc. fish	[mg.kg-1]		1.655e-05
Conc. stem of plants	[mg.kg-1]		4.522e-07
Conc. root of plants	[mg.kg-1]		6.855e-07
Conc. meat	[mg.kg-1]		3.681e-09
Conc. milk	[mg.kg-1]		1.164e-09
Conc. earthworms	[mg.kg-1]		1.042e-05
REGIONAL: HUMAN INTAKE VIA INDIRECT EXPOSURE		OVER-WRITE	CALCULATED
Intake air	[mg.kg-1.d-1]		1.991e-06
Intake drinking water	[mg.kg-1.d-1]		4.037e-08
Intake fish	[mg.kg-1.d-1]		2.6e-09
Intake stem of plant	[mg.kg-1.d-1]		2.584e-09
Intake root of plant	[mg.kg-1.d-1]		1.214e-09
Intake meat	[mg.kg-1.d-1]		6.311e-12
Intake milk	[mg.kg-1.d-1]		6.286e-12
Total human dose	[mg.kg-1.d-1]		2.037e-06
NEC ECOSYSTEMS		OVER-WRITE	CALCULATED
NEC for micro-organisms	[mg.l-1]		115
NEC for aquatic species	[mg.l-1]		.0034
NEC terrestrial species	[mg.kg-1]		??
NEC predator in food	[mg.kg-1]		1
IF TOXICITY DATA ON TERRESTRIAL ORGANISMS ARE NOT AVAILABLE		OVER-WRITE	CALCULATED
NEC terrestrial species	(eq. part. [mg.kg-1]		0.004615
EXTRAPOLATION FACTORS		OVER-WRITE	CALCULATED
Extrapolation IC50micro to NECmicro	[-]		10
Extrapolation LC50 to NEC	[-]		1000
Extrapolation 3 LC50s to NEC	[-]		100
Extrapolation subchronic NOEC to NEC	[-]		10

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1			
FINAL RESULTS			
MICRO-ORGANISMS IN THE STP (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. micro-organisms	[-]	0.06527	0.06527
Distribution factor of the hazard quot.	[-]	43.72	43.72
Probability PEC/NEC > 1	[-]	0.07923	0.07923
AQUATIC ECOSYSTEM (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. aquatic species	[-]	59.24	59.24
Distribution factor for the hazard quot.	[-]	162.8	162.8
Probability PEC/NEC > 1	[-]	0.9428	0.9428
TERRESTRIAL ECOSYSTEM (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. terrestrial species	[-]	??	??
Hazard quot. terr. species (eq. part.)	[-]	53.73	53.73
PREDATORS (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. fish-eating predators	[-]	0.9693	0.9693
Hazard quot. worm-eating predators	[-]	5.75	5.75
MAN (LOCAL)		INTERMEDIATE	DIRECT
Margin of Safety for man	[-]	54.67	54.67
AQUATIC ECOSYSTEM (REGIONAL)		INTERMEDIATE	DIRECT
Hazard quot. aquatic species	[-]	0.0008312	0.0008312
TERRESTRIAL ECOSYSTEM (REGIONAL)		INTERMEDIATE	DIRECT
Hazard quot. terrestrial species	[-]	??	??
Hazard quot. terr. species (eq. part.)	[-]	9.738e-05	9.738e-05
PREDATORS (REGIONAL)		INTERMEDIATE	DIRECT
Hazard quot. fish-eating predators	[-]	1.655e-05	1.655e-05
Hazard quot. worm-eating predators	[-]	1.042e-05	1.042e-05
MAN (REGIONAL)		INTERMEDIATE	DIRECT
Margin of Safety for man	[-]	7.762e+05	7.762e+05

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1			
MODEL PARAMETERS			
DISTRIBUTION PARAMETERS FOR THE LOCAL MODEL	ACTUAL		DEFAULT
Size of the local STP [eq]	1.2e+04	D	1.2e+04
Dilution factor for STP effluent [-]	32	D	32
Distr. factor for dilution [-]	148	D	148
Distr. factor influent discharge [-]	41	D	41
Amount of sludge applied [kg.ha-1.yr-1]	2000	D	2000
DISTRIBUTION PARAMETERS FOR THE REGIONAL SYSTEM	ACTUAL		DEFAULT
Size of the regional STP [eq]	1e+07	D	1e+07
MAN	ACTUAL		DEFAULT
Daily intake of drinking water [m3.d-1]	0.002	D	0.002
Daily intake of fish [kg.d-1]	0.011	D	0.011
Daily intake of leaf crops [kg.d-1]	0.4	D	0.4
Daily intake of root crops [kg.d-1]	0.124	D	0.124
Daily intake of meat [kg.d-1]	0.12	D	0.12
Daily intake of dairy products [kg.d-1]	0.378	D	0.378
Bioavailability for inhalation [-]	0.75	D	0.75
Bioavailability for oral exposure [-]	1	D	1
Bioavailability for dermal exposure [-]	1	D	1
COUNTRY PARAMETERS			

EXTRAPOLATION FACTORS	ACTUAL
Extrapolation IC50micro to NECmicro [-]	10
Extrapolation LC50 to NEC [-]	1000
Extrapolation 3 LC50s to NEC [-]	100
Extrapolation subchronic NOEC to NEC [-]	10
METEO DATA	ACTUAL
Ave. temp. at the air-water interface [K]	285
Ave. wind speed 10m above surface [m.s-1]	5
DISTRIBUTION PARAMETERS FOR THE LOCAL MODEL	ACTUAL
Distribution factor for flushing factor [-]	2

USES V1.0 SINGLE SUBSTANCE		
Printed on: 22/12/1994 11:15 Country: NL Substance: allylchloride CAS-No: 107-05-1		
DISTRIBUTION PARAMETERS FOR THE REGIONAL SYSTEM		ACTUAL
Total area of the reg. system	[m2]	3.8e+10
Frac. of regional area that is water	[-]	0.125
Frac. of regional area that is nat. soil	[-]	0.415
Frac. of regional area that is agr. soil	[-]	0.45
Frac. of regional area that is ind. soil	[-]	0.01
Mixing depth of the reg. water comp	[m]	3
Sum disch. str. crossing sys. bound	[m3.s-1]	2600
DISTRIBUTION PARAMETERS FOR THE REGIONAL AND THE CONTINENTAL SYSTEM		ACTUAL
Atmospheric mixing height	[m]	1000
Mixing depth sediment compartment	[m]	0.03
Mixing depth compartment of natr. soil	[m]	0.05
Mixing depth compartment of agr. soil	[m]	0.2
Mixing depth compartment of ind. soil	[m]	0.05
Average annual precipitation	[m.s-1]	2.51e-08
Frac. rain water infiltrates soil	[-]	0.4
Frac. rain water that runs off soil	[-]	0.5
Dep. velocity aerosol particles	[m.s-1]	.001
Conc. of biota in surface water	[kg.m-3]	.001
Settling velocity susp. particles	[m.s-1]	2.98e-05
DISTRIBUTION PARAMETERS FOR THE STP MODEL (IN/OUT)		ACTUAL
Waste water per inhabitant	[m3.d-1]	0.15
Surplus sludge per inh. equiv.	[kg.d-1.eq-1]	0.0355
ORGANISMS		ACTUAL
Daily intake of soil by cattle	[kg.d-1]	0.41
Daily intake of grass by cattle	[kg.d-1]	16.9
Daily intake of air by cattle	[m.d-1]	122
Daily ventilation rate	[m3.d-1]	20
Average human bodyweight	[kg]	70

ANNEX 3

USES V1.0 SINGLE SUBSTANCE				
Printed on: 22/12/1994 14:02 Country: NL Substance: allylchloride CAS-No: 107-05-1				
SUBSTANCE IDENTIFICATION				
Name: allylchloride CAS-No: 107-05-1 EC-notification no.: EINECS no: 203-457-6 Molecular weight: [g.mol-l] 76.53 Mol. Formula: C3H5Cl				
PARAMETER STATUS				
Input parameters defaults used: 37 of 57 Model parameters defaults used: 14 of 15 Intermediate results overwritten: 9 of 57				
INPUT PARAMETERS				
TONNAGE		ACTUAL		DEFAULT
Tonnage national	[tonnes.yr-1]	5e+04	S	0
Tonnage Europe	[tonnes.yr-1]	2.3e + 05	S	0
MAIN CATEGORY				
Production: Ib Intermediates isolated, stored on-site Formulation: Ib Dedicated equipment – cleaning limited Processing: Ib Continuous process				
INDUSTRIAL CATEGORY				
Ind. cat.: 3 Chemical industry: chemicals used in synthesis				
USE CATEGORY				
Primary: 33 Intermediates				
EMISSION RELEVANT DURING LIFE-CYCLE STEP ?		ACTUAL		DEFAULT
Emission production		Yes		No
Emission formulation		No		No
Emission processing		Yes		No
Emission private use		No		No
Emission recovery		No		No
Bypass STP		No		No

USES V1.0 SINGLE SUBSTANCE				
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1				
PHYSICO-CHEMICALS PROPERTIES		ACTUAL		DEFAULT
Melting point	[oC]	-135	S	??
Vapour pressure	[Pa]	3.95e + 05	S	0.001
Octanol-water part. coeff. (10log)	[-]	2.1	S	??
Water solubility	[mg.l – 1]	3600	S	??
Henry's law constant	[Pa.m3.mol-1]	839.7	E	??
Air-water part. coeff.	[l.l-1]	0.3544	E	??
Solids-water part. coeff. in soil	[l.kg-1]	1.501	E	??
Solids-water part. coeff. sediment	[l.kg-1]	1.501	E	??
Solids-water part. coeff. susp. mat.	[l.kg-1]	5.174	E	??
DEGRADATION		ACTUAL		DEFAULT
DT50 photodeg. in air	[d]	0.8	S	160
DT50 hydrolysis in water	[d]	12	S	1e+06
Readily biodegradable		Yes		No
DT50 biodeg. in water	[d]	5	E	??
DT50 biodeg. in soil	[d]	0.2715	E	??
DT50 biodeg. in STP	[d]	0.009627	E	??
BIOACCUMULATION		ACTUAL		DEFAULT
BCF fish	[l.kg-1]	5.885	E	??
BCF worm	[kg.kg-1]	23.19	E	??
BCF stem plant	[kg.kg-1]	0.8989	E	??
BCF root plant	[kg.kg-1]	1.525	E	??
BCF air plant	[m3.kg-1]	0.00519	E	??
BCF meat	[d.kg-1]	3.162e-06	E	??
BCF milk	[d.kg-1]	1e-06	E	??
ECOTOXICITY		ACTUAL		DEFAULT
L (E) C50 for fish	[mg.l-1]	1.2	S	??
L (E) C50 for crustaceans	[mg.l-1]	250	S	??
L (E) C50 for algae	[mg.l-1]	6.3	S	??
L (E) C50 for other aquatic species	[mg.l-1]	0.34	S	??
IC50 for micro-org. in STP	[mg.l-1]	??	D	??
NOEC for micro-org. in STP	[mg.l-1]	115	S	??
NOEC for fish	[mg.l-1]	??	D	??
NOEC for crustaceans	[mg.l-1]	??	D	??
NOEC for algae	[mg.l-1]	6.3	S	??
		ACTUAL		DEFAULT
Consumption rate testspecies	[kg.kg-1.d-1]	0.125	D	0.125

USES V1.0 SINGLE SUBSTANCE				
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1				
TOXICITY DATA FOR MAMMALS		ACTUAL		DEFAULT
LD50	[mg.kg-1 (bw)]	425	S	1
LC50 inhalatory	[mg.m-3]	2500	S	??
NOEC in food	[mg.kg-1]	10	E	??
Oral NOAEL, non-carcinogens	[mg.kg-1.d-1]	1.581	E	1
Is this value a LOAEL?		No		No
Animal test or human study?		Animal		Animal
Subchronic or chronic test?		Subchronic		Subchronic
NOAEL inhalatory	[mg.m-3]	7.38	S	??
Is this value a LOAEL?		No		No
Animal test or human study?		Animal		Animal
Subchronic or chronic test?		Subchronic		Subchronic
ADI or TDI	[mg.kg-1.d-1]	??	D	??
Genotoxic or carcinogenic		No		No
Corrosive or sensitizing		No		No
Toxic to reproduction		No		No
		ACTUAL		DEFAULT
Consumption rate testspecies	[kg.kg-1.d-1]	0.1	D	0.1
Scenario		No consumer exposure		No consumer exposure

INTERMEDIATE RESULTS			
LOCAL EMISSION		OVER-WRITE	CALCULATED
Step with largest emission to water			Production
Release to air	[kg.d-1]	140	2500
Release to waste water	[kg.d-1]	1	2500
Release to surface water	[kg.d-1]		0
Release to soil	[kg.d-1]		0
Number of emission days	[d]		300
Distr. factor emission flux to water	[-]		2
REGIONAL EMISSION		OVER-WRITE	CALCULATED
Release to air	[kg.d-1]	140	7534
Release to waste water	[kg.d-1]	1	7534
Release to surface water	[kg.d-1]		0
Release to agricultural soil	[kg.d-1]		0
Release to industrial soil	[kg.d-1]		0

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1			
CONTINENTAL EMISSION		OVER-WRITE	CALCULATED
Release to air	[kg.d-1]	770	3.466e+04
Release to waste water	[kg.d-1]	5	3.466e+04
Release to surface water	[kg.d-1]		0
Release to agricultural soil	[kg.d-1]		0
Release to industrial soil	[kg.d-1]		0
LOCAL EMISSION FROM STP		OVER-WRITE	CALCULATED
Emission STP to air	[kg.d-1]		0.2454
Emission STP to water	[kg.d-1]		0.02322
Emission STP to susp. matter	[kg.d-1]		2.045e-05
Emission STP to sludge	[kg.d-1]	0	0.006218
REGIONAL EMISSION FROM STP		OVER-WRITE	CALCULATED
Emission STP to air	[kg.d-1]		0.2394
Emission STP to water	[kg.d-1]		.02349
Emission STP to susp. matter	[kg.d-1]		2.06e-05
Emission STP to sludge	[kg.d-1]	0	0.006219
CONTINENTAL EMISSION FROM STP		OVER-WRITE	CALCULATED
Emission STP to air	[kg.d-1]		1.088
Emission STP to water	[kg.d-1]		0.1224
Emission STP to susp. matter	[kg.d-1]		0.0001059
Emission STP to sludge	[kg.d-1]	0	0.03111
LOCAL ENVIRONMENT CONCENTRATIONS		OVER-WRITE	CALCULATED
Conc. influent STP	[mg.l-1]		0.02778
Conc. aeration tank STP	[mg.l-1]		0.0007514
Conc. effluent STP	[mg.l-1]		0.0006457
Conc. sludge STP	[mg.kg-1]		0
Conc. air (100m from STP)	[mg.m-3]		5.604e-05
Conc. air (100m from source)	[mg.m-3]		0.03196
Conc. groundwater	[mg.l-1]		0
Conc. agricultural soil	[mg.kg-1]		0.003262
Conc. surface water (episode)	[mg.l-1]		2.018e-05
Conc. surface water (annual)	[mg.l-1]		1.658e-05

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1			
REGIONAL ENVIRONMENT CONCENTRATIONS		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		1.225e-06
Conc. surface water	[mg.l-1]		4.974e-09
Conc. porewater	[mg.l-1]		5.199e-10
Conc. natural soil	[mg.kg-1]		1.946e-09
Conc. agricultural soil	[mg.kg-1]		7.056e-10
Conc. industrial soil	[mg.kg-1]		1.946e-09
CONTINENTAL ENVIRONMENT CONCENTRATIONS		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		1.736e-07
Conc. surface water	[mg.l-1]		6.159e-10
Conc. porewater	[mg.l-1]		7.368e-11
Conc. natural soil	[mg.kg-1]		2.757e-10
Conc. agricultural soil	[mg.kg-1]		1e-10
Conc. industrial soil	[mg.kg-1]		2.757e-10
LOCAL: CONCENTRATIONS IN HUMAN INTAKE MEDIA		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		0.03196
Conc. drinking water	[mg.l-1]		8.291e-06
Conc. fish	[mg.kg-1]		9.71e-05
Conc. stem of plants	[mg.kg-1]		0.003098
Conc. root of plants	[mg.kg-1]		0.004976
Conc. meat	[mg.kg-1]		1.3e-05
Conc. milk	[mg.kg-1]		4.111e-06
LOCAL: INTAKE BY PREDATORS		OVER-WRITE	CALCULATED
Conc. earthworms	[mg.kg-1]		0.07565
Conc. fish	[mg.kg-1]		9.71e-05
LOCAL: HUMAN INTAKE VIA INDIRECT EXPOSURE		OVER-WRITE	CALCULATED
Intake air	[mg.kg-1.d-1]		0.006849
Intake drinking water	[mg.kg-1.d-1]		2.369e-07
Intake fish	[mg.kg-1.d-1]		1.526e-08
Intake stem of plant	[mg.kg-1.d-1]		1.771e-05
Intake root of plant	[mg.kg-1.d-1]		8.815e-06
Intake meat	[mg.kg-1.d-1]		2.229e-08
Intake milk	[mg.kg-1.d-1]		2.22e-08
Total human dose	[mg.kg-1.d-1]		0.006876

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1			
REGIONAL: CONCENTRATIONS IN HUMAN INTAKE		OVER-WRITE	CALCULATED
Conc. air	[mg.m-3]		1.225e-06
Conc. drinking water	[mg.l-1]		2.487e-09
Conc. fish	[mg.kg-1]		2.912e-08
Conc. stem of plants	[mg.kg-1]		6.991e-09
Conc. root of plants	[mg.kg-1]		1.076e-09
Conc. meat	[mg.kg-1]		4.741e-10
Conc. milk	[mg.kg-1]		1.499e-10
Conc. earthworms	[mg.kg-1]		1.636e-08
REGIONAL: HUMAN INTAKE VIA INDIRECT EXPOSURE		OVER-WRITE	CALCULATED
Intake air	[mg.kg-1.d-1]		2.625e-07
Intake drinking water	[mg.kg-1.d-1]		7.105e-11
Intake fish	[mg.kg-1.d-1]		4.576e-12
Intake stem of plant	[mg.kg-1.d-1]		3.995e-11
Intake root of plant	[mg.kg-1.d-1]		1.907e-12
Intake meat	[mg.kg-1.d-1]		8.127e-13
Intake milk	[mg.kg-1.d-1]		8.095e-13
Total human dose	[mg.kg-1.d-1]		2.626e-07
NEC ECOSYSTEMS		OVER-WRITE	CALCULAT ED
NEC for micro-organisms	[mg.l-1]		115
NEC for aquatic species	[mg.l-1]		.0034
NEC terrestrial species	[mg.kg-1]		??
NEC predator in food	[mg.kg-1]		1
IF TOXICITY DATA ON TERRESTRIAL ORGANISMS ARE NOT AVAILABLE		OVER-WRITE	CALCULATED
NEC terrestrial species	(eq. part. [mg.kg-1]		0.004615
EXTRAPOLATION FACTORS		OVER-WRITE	CALCULATED
Extrapolation IC50micro to NECmicro	[-]		10
Extrapolation LC50 to NEC	[-]		1000
Extrapolation 3 LC50s to NEC	[-]		100
Extrapolation subchronic NOEC to NEC	[-]		10

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1			
FINAL RESULTS			
MICRO-ORGANISMS IN THE STP (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. micro-organisms	[-]	6.534e-06	0.01634
Distribution factor of the hazard quot.	[-]	43.72	43.72
Probability PEC/NEC > 1	[-]	0	0.01688
AQUATIC ECOSYSTEM (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. aquatic species	[-]	0.005934	14.83
Distribution factor for the hazard quot.	[-]	162.8	162.8
Probability PEC/NEC > 1	[-]	0.02454	0.8515
TERRESTRIAL ECOSYSTEM (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. terrestrial species	[-]	??	??
Hazard quot. terr. species (eq. part.)	[-]	0.7069	28.34
PREDATORS (LOCAL)		INTERMEDIATE	DIRECT
Hazard quot. fish-eating predators	[-]	9.71e-05	0.2427
Hazard quot. worm-eating predators	[-]	0.07565	3.033
MAN (LOCAL)		INTERMEDIATE	DIRECT
Margin of Safety for man	[-]	230	12.76
AQUATIC ECOSYSTEM (REGIONAL)		INTERMEDIATE	DIRECT
Hazard quot. aquatic species	[-]	1.463e-06	0.006102
TERRESTRIAL ECOSYSTEM (REGIONAL)		INTERMEDIATE	DIRECT
Hazard quot. terrestrial species	[-]	??	??
Hazard quot. terr. species (eq. part.)	[-]	1.529e-07	0.0007157
PREDATORS (REGIONAL)		INTERMEDIATE	DIRECT
Hazard quot. fish-eating predators	[-]	2.912e-08	0.0001215
Hazard quot. worm-eating predators	[-]	1.636e-08	7.659e-05
MAN (REGIONAL)		INTERMEDIATE	DIRECT
Margin of Safety for man	[-]	6.022e+06	8.928e+04

USES V1.0 SINGLE SUBSTANCE			
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1			
MODEL PARAMETERS			
DISTRIBUTION PARAMETERS FOR THE LOCAL MODEL	ACTUAL		DEFAULT
Size of the local STP [eq]	2.4e+05	S	1.2e+04
Dilution factor for STP effluent [-]	32	D	32
Distr. factor for dilution [-]	148	D	148
Distr. factor influent discharge [-]	41	D	41
Amount of sludge applied [kg.ha-1.yr-1]	2000	D	2000
DISTRIBUTION PARAMETERS FOR THE REGIONAL SYSTEM	ACTUAL		DEFAULT
Size of the regional STP [eq]	1e+07	D	1e+07
MAN	ACTUAL		DEFAULT
Daily intake of drinking water [m3.d-1]	0.002	D	0.002
Daily intake of fish [kg.d-1]	0.011	D	0.011
Daily intake of leaf crops [kg.d-1]	0.4	D	0.4
Daily intake of root crops [kg.d-1]	0.124	D	0.124
Daily intake of meat [kg.d-1]	0.12	D	0.12
Daily intake of dairy products [kg.d-1]	0.378	D	0.378
Bioavailability for inhalation [-]	0.75	D	0.75
Bioavailability for oral exposure [-]	1	D	1
Bioavailability for dermal exposure [-]	1	D	1
COUNTRY PARAMETERS			
EXTRAPOLATION FACTORS			ACTUAL
Extrapolation IC50micro to NECmicro [-]			10
Extrapolation LC50 to NEC [-]			1000
Extrapolation 3 LC50s to NEC [-]			100
Extrapolation subchronic NOEC to NEC [-]			10
METEO DATA			ACTUAL
Ave. temp. at the air-water interface [K]			285
Ave. wind speed 10m above surface [m.s-1]			5
DISTRIBUTION PARAMETERS FOR THE LOCAL MODEL			ACTUAL
Distribution factor for flushing factor [-]			2

USES V1.0 SINGLE SUBSTANCE		
Printed on: 22/12/1994 14:38 Country: NL Substance: allylchloride CAS-No: 107-05-1		
DISTRIBUTION PARAMETERS FOR THE REGIONAL SYSTEM		ACTUAL
Total area of the reg. system	[m2]	3.8e+10
Frac. of regional area that is water	[-]	0.125
Frac. of regional area that is nat. soil	[-]	0.415
Frac. of regional area that is agr. soil	[-]	0.45
Frac. of regional area that is ind. soil	[-]	0.01
Mixing depth of the reg. water comp	[m]	3
Sum disch. str. crossing sys. bound	[m3.s-1]	2600
DISTRIBUTION PARAMETERS FOR THE REGIONAL AND THE CONTINENTAL SYSTEM		ACTUAL
Atmospheric mixing height	[m]	1000
Mixing depth sediment compartment	[m]	0.03
Mixing depth compartment of natr. soil	[m]	0.05
Mixing depth compartment of agr. soil	[m]	0.2
Mixing depth compartment of ind. soil	[m]	0.05
Average annual precipitation	[m.s-1]	2.51e-08
Frac. rain water infiltrates soil	[-]	0.4
Frac. rain water that runs off soil	[-]	0.5
Dep. velocity aerosol particles	[m.s-1]	.001
Conc. of biota in surface water	[kg.m-3]	.001
Settling velocity susp. particles	[m.s-1]	2.98e-05
DISTRIBUTION PARAMETERS FOR THE STP MODEL (IN/OUT)		ACTUAL
Waste water per inhabitant	[m3.d-1]	0.15
Surplus sludge per inh. equiv.	[kg.d-1.eq-1]	0.0355
ORGANISMS		ACTUAL
Daily intake of soil by cattle	[kg.d-1]	0.41
Daily intake of grass by cattle	[kg.d-1]	16.9
Daily intake of air by cattle	[m.d-1]	122
Daily ventilation rate	[m3.d-1]	20
Average human bodyweight	[kg]	70

I U C L I D
D a t a S e t

Existing Chemical	ID: 107-05-1
CAS No.	107-05-1
EINECS Name	3-chloropropene
EC No.	203-457-6
TSCA Name	1-Propene, 3-chloro-
Molecular Formula	C3H5Cl

Producer Related Part

Company:	OECD
Creation date:	20-JAN-2003

Substance Related Part

Company:	OECD
Creation date:	20-JAN-2003

Memo:	OECD HPV Chemicals Programme, SIDS Dossier, approved at SIAM 4, May 1996
Printing date:	17-FEB-2003
Revision date:	
Date of last Update:	17-FEB-2003
Number of Pages:	93
Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 Applicant and Company Information

Name: DOW Deutschland Inc., Werk Stade
Street: Werkstade PO Box 1120
Town: 21677 Stade 5
Country: Germany

20-JAN-2003

Name: Shell Nederland Chemie B.V.
Street: P.O. Box 3030
Town: 3190 GH Hoogvliet-Rotterdam
Country: Netherlands
Phone: +31-10-2317005
Telefax: +31-10-2317125

20-JAN-2003

Name: Solvay Alkali GmbH
Street: Postfach 110270
Town: 42662 Solingen
Country: Germany

20-JAN-2003

Name: Solvay S.A.
Street: Rue du Prince Albert 33
Town: 1050 Bruxelles
Country: Belgium

20-JAN-2003

1.0.2 Location of Production Site, Importer or Formulator

1.0.3 Identity of Recipients

-

1.0.4 Details on Category/Template

1.1.0 Substance Identification

Smiles Code: C=CCCl
Mol. Formula: C3H5Cl

20-JAN-2003

1.1.1 General Substance Information

Purity type: typical for marketed substance
Substance type: organic
Physical status: liquid
Purity: > 97 - % w/w
Colour: colourless to straw
Odour: very pungent, garlic like

28-JAN-2003

1.1.2 Spectra

1.2 Synonyms and Tradenames

1-Chloro-2-propene

29-MAY-1994

1-Propene, 3-chloro-

29-MAY-1994

2-Propenyl chloride

29-MAY-1994

3-Chloroprene

29-MAY-1994

3-chloropropene (IUPAC name)

28-JAN-2003

3-Chloropropylene

29-MAY-1994

3-Chloror-1-propylene

29-MAY-1994

Allyl chloride

29-APR-1994

alpha-Chloroproylene

29-MAY-1994

CAL (usual abbreviation)

28-JAN-2003

Chlorallylene

29-MAY-1994

Chloroallylene

29-MAY-1994

chlorure d'allyle (usual French name)

28-JAN-2003

monochloropropylene

18-FEB-1994

Propene, 3-chloro-

20-JAN-2003

1.3 Impurities

Purity type: typical for marketed substance
CAS-No: 592-42-7
EC-No: 209-754-7
EINECS-Name: hexa-1,5-diene
Contents: .3 - % w/w

Source: Solvay S.A. Bruxelles
20-JAN-2003

Purity type: typical for marketed substance
CAS-No: 590-21-6
EC-No: 209-675-8
EINECS-Name: 1-chloropropene
Contents: .2 - % w/w

Source: Solvay S.A. Bruxelles
20-JAN-2003

Purity type: typical for marketed substance
CAS-No: 540-54-5
EC-No: 208-749-7
EINECS-Name: 1-chloropropane
Contents: .2 - % w/w

Source: Solvay S.A. Bruxelles
20-JAN-2003

1.4 Additives

Purity type: typical for marketed substance
CAS-No: 75-56-9
EC-No: 200-879-2
EINECS-Name: methyloxirane
Contents: < .1 - % w/w

Source: Solvay S.A. Bruxelles
20-JAN-2003

1.5 Total Quantity

Quantity: 100000 - 500000

20-JAN-2003

1.6.1 Labelling

Labelling:	as in Directive 67/548/EEC
Symbols:	(F) highly flammable (T+) very toxic (N) dangerous for the environment
Nota:	(D) Certain substances which are susceptible in spontaneous polymerisation or decomposition are generally placed on the market in a stabilized form. It is in this form that they are listed in Annex 1 to this Directive other RM: S
Specific limits:	no data
R-Phrases:	(11) Highly flammable (26) Very toxic by inhalation (50) Very toxic to aquatic organisms
S-Phrases:	(1/2) Keep locked up and out of reach of children (16) Keep away from sources of ignition - No smoking (29) Do not empty into drains (33) Take precautionary measures against static discharges (45) In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible) (61) Avoid release to the environment. Refer to special instructions/Safety data sets

20-JAN-2003

1.6.2 Classification

Classified:	as in Directive 67/548/EEC
Class of danger:	dangerous for the environment
R-Phrases:	(50) Very toxic to aquatic organisms

20-JAN-2003

Classified:	as in Directive 67/548/EEC
Class of danger:	highly flammable
R-Phrases:	(11) Highly flammable

20-JAN-2003

Classified:	as in Directive 67/548/EEC
Class of danger:	very toxic
R-Phrases:	(26) Very toxic by inhalation

20-JAN-2003

1.6.3 Packaging

-

1.7 Use Pattern

Type:	type
Category:	Non dispersive use

20-JAN-2003

Type:	type

Category: Use in closed system

20-JAN-2003

Type: industrial
Category: Chemical industry: used in synthesis

20-JAN-2003

Type: use
Category: Intermediates

Remark: Intermediate in the manufacture of epichlorhydrin, glycerol, allyl alcohol, diallyl phthalate, fine chemicals and pharmaceuticals.
20-JAN-2003

1.7.1 Detailed Use Pattern

1.7.2 Methods of Manufacture
-

1.8 Regulatory Measures

1.8.1 Occupational Exposure Limit Values

Type of limit: MAC (NL)
Limit value: 3 mg/m3

20-JAN-2003 (36)

Type of limit: MAK (DE)
Limit value: 3 mg/m3
Short term exposure
Limit value: 6 mg/m3
Schedule: 5 minute(s)
Frequency: 8 times

Country: Germany
Remark: Classified in carcinogenic group IIIB, i.e. it is justifiably expected of having carcinogenic potential.
20-JAN-2003 (32)

Type of limit: OES (UK)
Limit value: 3 mg/m3
Short term exposure
Limit value: 6 mg/m3
Schedule: 10 minute(s)

Country: United Kingdom
20-JAN-2003 (41)

Type of limit: TLV (US)
Limit value: 3 mg/m3
Short term exposure
Limit value: 6 mg/m3
Schedule: 15 minute(s)
Frequency: 4 times

Country: USA
Remark: Allyl chloride is identified by other sources as a suspected or confirmed human carcinogen.

ACGIH TLV and OSHA PEL are both 3 mg/m3 TWA and 6 mg/m3 STEL.
28-JAN-2003 (2)

Type of limit: other: NIOSH
Limit value: 3 mg/m3
Short term exposure
Limit value: 10 mg/m3
Schedule: 15 minute(s)

20-JAN-2003

Type of limit: other: OSHA (PEL)
Limit value: 3 mg/m3
Short term exposure
Limit value: 6 mg/m3

20-JAN-2003

1.8.2 Acceptable Residues Levels

1.8.3 Water Pollution

Classified by: KBwS (DE)
Class of danger: 1 (weakly water polluting)

20-JAN-2003 (81)

1.8.4 Major Accident Hazards

1.8.5 Air Pollution

1.8.6 Listings e.g. Chemical Inventories

1.9.1 Degradation/Transformation Products

1.9.2 Components

1.10 Source of Exposure

Remark: Professional exposures related to the use pattern are described in section 1.7

Emission of Solvay production plants to the atmosphere was less than 0.1 % of the production; no emission into water takes place (Solvay internal data, 1992-93).

No further sources are known.

Countries where Solvay production plants are located in EU:
- France
- Germany

Source: Solvay S.A. Bruxelles
28-JAN-2003

Remark: Production process:
Allyl chloride is manufactured by the hot chlorination (500 deg. C) of propylene in a closed system.

Exposure:
A 24-hour air-monitoring (GC) is used to ensure that levels of allyl chloride stay below the applicable workplace exposure limits.

Source: DOW Deutschland Inc., Werk Stade Stade 5
28-JAN-2003 (35)

1.11 Additional Remarks

Remark: DISPOSAL (WASTE OR PRODUCT)

Recover or recycle if possible. Otherwise incineration with residence time of 2 secs above 1200 C and wet scrubbing facilities.

CONTAINER DISPOSAL

Drain container thoroughly. Rinse three times with suitable solvent. Treat rinsings as for product disposal. After draining, vent in a safe place away from sparks and fire. Residues may cause an explosion hazard. Do not puncture, cut or weld uncleaned drums. Send to drum recoverer or metal reclaimer.

TRANSPORT INFORMATION

UN Number: 1100
Class: 3 (subsidiary 6.1)
Packing Group: I
Proper Shipping Name: Allyl chloride

Sea (IMO)
Class: 3.1 (subsidiary 6.1)
Packing Group: I
Symbol: Flammable liquid and Poison
Marine Pollutant (Y/N): Yes (Marine Pollution Mark required)
Proper Shipping Name: Allyl chloride, Marine Pollutant

Rail/Road (RID/ADR)
Class: 3 (subsidiary 6.1)
Item: 16(a)
Symbol: Flammable liquid and Poison
Kemler Plate: 336/1100
Air (IATA/ICAO)
Class: 3 (subsidiary 6.1)
Packing Group: I
Symbol: Flammable liquid and Poison

INDUSTRIAL ACTIVITY

The three European producers have produced a document entitled "Guidelines for the Distribution of Allyl Chloride". The document also includes an extensive safety visit scheme for the reception and storage facilities of Allyl Chloride, as well as driver training programs,design and construction aspects plus procedures for loading/unloading.

Source: Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
03-JUN-1994

Remark: IARC classification : group 3.
Unclassifiable as to carcinogenicity to humans based on the following evaluation :
- There is INADEQUATE EVIDENCE for the carcinogenicity of allyl chloride in experimental animals.
- In the absence of epidemiological data, no evaluation could be made of the carcinogenicity of allyl chloride to humans.

Source: Solvay S.A. Bruxelles
21-FEB-1994 (53)

Remark: CONVERSION FACTORS (20 deg C, 101 kPa):
1 mg/m3 = 0.31 ppm
1 ppm = 3.18 mg/m3

Source: Solvay S.A. Bruxelles
28-FEB-1994

1.12 Last Literature Search

1.13 Reviews

-

2.1 Melting Point

Value: -135 degree C

GLP: no

20-JAN-2003 (11) (73)

Value: = -134.5 degree C

GLP: no

30-MAY-1994 (1)

2.2 Boiling Point

Value: = 43 - 49 degree C at 1013 hPa

Method: other: ASTM D 1078
GLP: no

21-FEB-1994 (11)

Value: = 45 degree C at 1013 hPa

GLP: no

30-MAY-1994 (1) (73)

2.3 Density

Type: density
Value: = 939 kg/m3 at 20 degree C

GLP: no

Remark: Liquid density.
30-MAY-1994 (1) (11)

Type: relative density
Value: = 2.64

GLP: no

Remark: Vapour density (air=1).
21-FEB-1994 (11)

2.3.1 Granulometry

2.4 Vapour Pressure

Value: = 395 hPa at 20 degree C

GLP: no

21-FEB-1994 (73)

Value: = 491 hPa at 25 degree C

21-FEB-1994 (88)

Value: = 587 hPa at 30 degree C

21-FEB-1994 (88)

Value: = 393 hPa

GLP: no

20-JAN-2003 (11)

2.5 Partition Coefficient

Partition Coeff.: octanol-water
log Pow: = 1.45

Method: other (calculated): C log P
Year: 1994

20-JAN-2003

Partition Coeff.: octanol-water
log Pow: = 2.1

Method: OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year: 1989
GLP: yes

20-JAN-2003 (15)

2.6.1 Solubility in different media

Solubility in: Water
Value: = 3.6 g/l at 20 degree C

GLP: no

20-JAN-2003 (11)

2.6.2 Surface Tension

2.7 Flash Point

Value: = -32 degree C
Type: closed cup

Method: other: ASTM D 56
GLP: no

21-FEB-1994 (11)

2.8 Auto Flammability

Value: 290 degree C

GLP: no

20-JAN-2003 (73)

Value: = 391 degree C

Method: other: ASTM D 2155
GLP: no

21-FEB-1994 (11)

2.9 Flammability

Result: highly flammable

GLP: no

Remark: Flammability limits in air : lower : 3.3 %
upper : 11.2 %
21-FEB-1994 (11)

2.10 Explosive Properties

Result: explosive under influence of a flame

GLP: no

Remark: 3.2 - 11.2%.
21-FEB-1994 (73)

2.11 Oxidizing Properties

2.12 Dissociation Constant

2.13 Viscosity

2.14 Additional Remarks

Source: Solvay S.A. Bruxelles
Test substance: Specific heat :
- Liquid : 1.5 J/g.K.
- Vapour : 0.95 J/g.K at 100 degree C.
22-FEB-1994

Source: Solvay S.A. Bruxelles
Test substance: Latent heat of vaporisation at boiling point (45 degree C) : 380 kJ/kg.
22-FEB-1994

Test substance: Heat of combustion : -22.7 kJ/g.
22-FEB-1994 (100)

Test substance: Viscosity at 20 degree C : 0.336 mPa.s
Method : ASTM D 445
GLP : no.
22-FEB-1994 (11)

Test substance: Refractive index n 20,D : 1.4157.
30-MAY-1994 (1)

Source: Solvay S.A. Bruxelles
Test substance: Solubility with common organic substances :
- Soluble (aceton, benzene, methanol, carbon tetrachloride).
- Very soluble (diethylether, ethanol, chloroform).
11-JUN-1993

Source: Solvay S.A. Bruxelles
Test substance: Coefficient of volume expansion at 20 degree C : 0.0014 K exp -1.
22-FEB-1994

Test substance: Surface tension : 23.06 mN/m at 20 degree C.
GLP : no.
22-FEB-1994 (11)

Test substance: Critical temperature : 241 degree C.
Critical pressure : 4.8 MN/m2.
22-FEB-1994 (100)

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: NO3
Conc. of sens.: 241000000 molecule/cm³
Rate constant: = .00000601 cm³/(molecule * sec)
Degradation: = 100 % after 160 day(s)

Method: other (measured)
Year: 1987
GLP: no
Test substance: no data

21-JAN-2003 (101)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: O3
Conc. of sens.: 71000000000000 molecule/cm³
Rate constant: = .00000000000000000161 cm³/(molecule * sec)
Degradation: = 100 % after 10 day(s)

Method: other (measured)
Year: 1987
GLP: no
Test substance: no data

21-JAN-2003 (101)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: O3
Degradation: = 50 % after 9 hour(s)

Year: 1978
GLP: no data
Test substance: no data

21-JAN-2003 (80)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 10000000 molecule/cm³
Rate constant: = .0000000000171 cm³/(molecule * sec)
Degradation: = 50 % after 11 hour(s)

Method: other (measured)
Year: 1987
GLP: no
Test substance: no data

07-FEB-2003 (101)

3.1.2 Stability in Water

```
Type:             abiotic
t1/2  pH :        = 7 day(s)

Method:           other
  Year:           1978
   GLP:           no
Test substance:   other TS: allyl chloride, purity not specified

28-JAN-2003                                                          (80)

Type:             abiotic
t1/2  pH :        = 3.8 - 5.3 day(s) at 30 degree C

Method:           other
  Year:           1986
   GLP:           no data
Test substance:   other TS: allyl chloride, purity not specified

Remark:           Hydrolysis product : allyl alcohol
28-JAN-2003                                                          (64)

Type:             abiotic
t1/2  pH 8 :      = 296 hour(s) at 20 degree C

Method:           other
  Year:           1988
   GLP:           no
Test substance:   as prescribed by 1.1 - 1.4

21-JAN-2003                                                          (34)
```

3.1.3 Stability in Soil

3.2.1 Monitoring Data (Environment)

```
Type of measurement: background concentration
Medium:              air

Remark:           In USA :
                    < 16 ng/m3 at Denver (CO), Houston (TX), Riverside (CA)
                  and St Louis (MO)
                    = 64 ng/m3 at Pittsburg (PA)
                    not detected at Chicago (IL) and Staten Island (NY).

                  Year: 1982
07-FEB-2003                                                          (86)

Type of measurement: background concentration
Medium:              surface water

Result:           Allyl chloride concentration < 0.1 ug/l, Rhine, Coblenz,
                  1983.
21-JAN-2003                                                          (27)
```

Type of measurement: background concentration

Medium: surface water

Result: Allyl chloride concentration < 5 ug/l (6 samples), Japan, 1977.
21-JAN-2003 (42)

3.2.2 Field Studies

3.3.1 Transport between Environmental Compartments

Type: volatility
Media: water - air
Method: other
Year: 1977

Remark: The evaporation rate of a dilute aqueous solution of allyl chloride (about 1 ppm) was determined.
Conditions : 200 rpm stirring, 25 oC, still air, 6.5 cm depth.
Result: t1/2 = 27 min.
28-JAN-2003 (33)

Type: volatility
Media: water - air
Method: other: model river (1 m depth, current 1m/s, wind velocity 3 m/s)

Remark: Based on Henry's law constant t 1/2 = 2.6 hours
21-JAN-2003 (66)

3.3.2 Distribution

Media: air - biota - sediment(s) - soil - water
Method: Calculation according Mackay, Level I

Remark: Based on the following properties :
MW : 76.5 g/mol
Density : 939 kg/m3
Boiling point : 45 degree C
Melting point : -135 degree C
Aqueous solubility : 3600 g/m3
vapour pressure : 39 500 Pa
temp : 25 degree C

Partition coefficients :
H = 839 Pa m3/mol
log Pow : 2.10
Koc : 51.74 l/kg
Kd (2 %) : 1.03 l/kg
Ks (4 %) : 2.07 l/kg
BCF : 6.04

Concentrations in compartments :
air : 99.35 %

water : 0.59 %
soil 0.06 %

sediment : 0.00 %
susp. aq. mat. : 0.00 %
biota : 0.00 %

17-FEB-2003

3.4 Mode of Degradation in Actual Use

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 100 mg/l related to Test substance
Degradation: 55 - 69 % after 28 day(s)

Method: OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year: 1992
GLP: no data
Test substance: other TS: allylchloride, no information about purity

Remark: Concentration of inoculum: 30 mg/l
28-JAN-2003 (26)

3.6 BOD5, COD or BOD5/COD Ratio

B O D 5

Method: other: APHA "Standard Methods" No 219 at 20 +- 1 °C
Year: 1971
GLP: no
BOD5: = 230 mg/l

C O D

Method: other: ASTM D 1252-67
Year: 1974
GLP: no
COD: = 860 mg/g substance

R A T I O B O D 5 / C O D

BOD5/COD: = .27
Method:
Remark: BOD5* with adapted seed = 420 mg/g
thus BOD5*/COD = 0.48 and BOD5*/ThOD = 0.25.
Result: Theoretical Oxygen Demand (ThOD): ThOD = 1670 mg/g
thus COD/ThOD = 0.51 and BOD5/ThOD = 0.14.
Test condition: Type : aerobic, stirring applied.
Medium : water, seeded with 10 ml effluent from a biological sanitary waste treatment plant per 500 ml test solution.

Test substance: Allyl chloride, purity not specified.
21-JAN-2003 (19)

3.7 Bioaccumulation

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day(s) at 25 degree C
Concentration: .05 mg/l
BCF: < 1.3 - 5.6

Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year: 1992
GLP: no data
Test substance: other TS: allylchloride, purity not specified

Remark: At 0.5 mg/l, the BCF was < 0.14 - 0.88
Test condition: flow-through test
21-JAN-2003 (26)

3.8 Additional Remarks

Remark: Henry's law constant : 835 Pa.m3/mol at 20 degree C (calculated).
07-FEB-2003 (33)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

```
Type:              semistatic
Species:           Oryzias latipes  (Fish, fresh water)
Exposure period:   48 hour(s)
Unit:              mg/l                    Analytical monitoring: no
LC50:              6.9 -

Method:            other: Japanese standard JIS K 0102-1986-71
  Year:            1992
   GLP:            no data
Test substance:    other TS: allyl chloride, purity not specified

Test condition:    renewal of test medium every 8, 16 hours
                   fish, 28 days old, 10 fish/level, were exposed in 4 l tanks at
                   25 degree C
21-JAN-2003                                                                (26)

Type:              semistatic
Species:           Poecilia reticulata  (Fish, fresh water)
Exposure period:   14 day(s)
Unit:              mg/l                    Analytical monitoring: no
LC50:              = 1.2 -

Method:            other
  Year:            1985
   GLP:            no
Test substance:    other TS: allyl chloride, purity > 99%

Test condition:    Test solutions renewed every 24 h.
                   Nominal concentration.
28-JAN-2003                                                                (52)

Type:              static
Species:           Carassius auratus  (Fish, fresh water)
Exposure period:   96 hour(s)
Unit:              mg/l                    Analytical monitoring: no
LC50:              = 21 -

Method:            other: APHA Standard Methods
  Year:            1960
   GLP:            no
Test substance:    other TS: allyl chloride, boiling point = 45-45.5 degree C

Remark:            LC50 values calculated by moving average angle method.
Test condition:    Temperature : 25 degree C (soft water)
                   pH : 7.5
                   5 fish/10 l test solutions in duplicate
                   Nominal concentration.
28-JAN-2003                                                                (78)
```

```
Type:              static
Species:           Carassius auratus  (Fish, fresh water)
Exposure period:   24 hour(s)
Unit:              mg/l                    Analytical monitoring: yes
LC50:              = 10 -

Method:            other: APHA Standard methods No. 231
  Year:            1971
   GLP:            no
Test substance:    other TS: allyl chloride, purity not specified

Remark:            LC 50 value calculated by graphical interpolation (logarithm
                   of concentration versus %-age mortality).
Test condition:    Temperature : 20 +/- 1 degree C
                   pH : 6-8
                   6 fishes/25 l. test solution, no aeration
                   Measured concentration.
28-JAN-2003                                                              (18)

Type:              static
Species:           Lebistes reticulatus  (Fish, fresh water)
Exposure period:   96 hour(s)
Unit:              mg/l                    Analytical monitoring: no
LC50:              = 51 -

Method:            other: APHA Standard Methods
  Year:            1960
   GLP:            no
Test substance:    other TS: allyl chloride, boiling point = 45-45.5 degree C

Remark:            LC50 values calculated by moving average angle method.
Test condition:    Temperature : 25 degree C (soft water)
                   pH : 7.5
                   5 fish/2 l test solutions in duplicate
                   Nominal concentration.
28-JAN-2003                                                              (78)

Type:              static
Species:           Lepomis macrochirus  (Fish, fresh water)
Exposure period:   96 hour(s)
Unit:              mg/l                    Analytical monitoring: no
LC50:              = 42 -

Method:            other: APHA Standard Methods
  Year:            1960
   GLP:            no
Test substance:    other TS: allyl chloride, boiling point = 45-45.5 degree C

Remark:            LC50 values calculated by moving average angle method.
Test condition:    Temperature : 25 degree C (soft water)
                   pH : 7.5
                   5 fish/10 l test solutions in duplicate
                   Nominal concentration.
28-JAN-2003                                                              (78)
```

```
Type:             static
Species:          Leuciscus idus melanotus  (Fish, fresh water)
Exposure period:  48 hour(s)
Unit:             mg/l                    Analytical monitoring: no data
LC50:             = 70 -

Method:           other
  Year:           1978
   GLP:           no
Test substance:   no data

21-JAN-2003                                                          (55)

Type:             static
Species:          Pimephales promelas  (Fish, fresh water)
Exposure period:  96 hour(s)
Unit:             mg/l                    Analytical monitoring: no
LC50:             = 19.8 -

Method:           other: APHA Standard Methods
  Year:           1960
   GLP:           no
Test substance:   other TS: allyl chloride, boiling point = 45-45.5 degree C

Remark:           LC50 values calculated by moving average angle method.
Test condition:   Temperature : 25 degree C (soft water)
                  pH : 7.5
                  5 fish/10 l test solutions in duplicate
                  Nominal concentration.
28-JAN-2003                                                          (78)

Type:             static
Species:          Pimephales promelas  (Fish, fresh water)
Exposure period:  96 hour(s)
Unit:             mg/l                    Analytical monitoring: no
LC50:             = 24 -

Method:           other: APHA Standard Methods
  Year:           1960
   GLP:           no
Test substance:   other TS: allyl chloride, boiling point = 45-45.5 degree C

Remark:           LC50 values calculated by moving average angle method.
Test condition:   Temperature : 25 degree C (hard water)
                  pH : 8.2
                  5 fish/10 l test solutions in duplicate.
                  Nominal concentration.
28-JAN-2003                                                          (78)

Type:             static
Species:          other: Xenopus laevis (Clawed toad)
Exposure period:  48 hour(s)
Unit:             mg/l                    Analytical monitoring: no
LC50:             .34 -

  Year:           1987
   GLP:           no data
```

Test substance: other TS: allyl chloride, analytical grade

Test condition: organisms 3-4 weeks old, 10 animals/level, 5 concentration levels with a factoral difference of 1.5.
Test carried out in covered glass basins. No replicates.
21-JAN-2003 (30)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: = 250 -

Method: other
Year: 1977
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: EC 50 value calculated by graphical interpolation.
Test condition: Temperature : 20-22 degree C
pH : 7.6-7.7
No aeration.
Nominal concentration.
28-JAN-2003 (22)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Microcystis aeruginosa (Algae, blue, cyanobacteria)
Endpoint: biomass
Exposure period: 8 day(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 8.2 -

Method: other: cell multiplication inhibition test
Year: 1975
GLP: no
Test substance: other TS: allylchloride, purity not specified

Test condition: Test solution in bidistilled water.
pH : 7
Nominal concentration.
21-JAN-2003 (20)

Species: Scenedesmus quadricauda (Algae)
Endpoint: biomass
Exposure period: 8 day(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 6.3 -

Method: other: cell multiplication inhibition test
Year: 1975
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Test condition: Test solution in bidistilled water.
pH : 7

Nominal concentration.
21-JAN-2003 (23)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: Chilomonas paramaecium (Protozoa)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC : = 8.6 -

Method: other: cell multiplication inhibition test
Year: 1981
GLP: no
Test substance: other TS: allylchloride, purity not specified

Test condition: pH : 7
Nominal concentration.
21-JAN-2003 (24)

Type: aquatic
Species: Entosiphon sulcatum (Protozoa)
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC : = 8.4 -

Method: other: cell multiplication inhibition test
Year: 1981
GLP: no
Test substance: other TS: allylchloride, purity not specified

Test condition: pH : 7.
Nominal concentration.
21-JAN-2003 (24)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 16 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC : = 115 -

Method: other: cell multiplication inhibition test
Year: 1976
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Test condition: Total biomass.
28-JAN-2003 (21)

Type: aquatic
Species: Uronema parduzci (Protozoa)
Exposure period: 20 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC : > 240 -

Method: other: cell multiplication inhibition test
Year: 1981

GLP: no
Test substance: other TS: allylchloride, purity not specified

Test condition: pH : 7
Nominal concentration.
21-JAN-2003 (24)

Type: aquatic
Species: other bacteria: activated sludge mixed liquor
Unit: mg/l Analytical monitoring: no
EC75 : 180 -

Year: 1966
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Method: solutions of the test substance were inoculated with centrifuged liquid medium and incubated for 2-4 hours at 25 degree C. The effect of nitrification was determined by measurement of the nitrite and nitrate concentrations.
07-FEB-2003 (92)

Type: aquatic
Species: other bacteria: nitrifying return activated sludge/fresh settled sewage
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: >= 120 -

Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Method: solutions of the test substance were inoculated with filtered activated sludge mixed liquor and aerated for 2.5 hour at 20-25 degree C (pH 7.6). The effect of nitrification was determined by measurement of the ammonia, nitrite and nitrate concentrations.
07-FEB-2003 (102)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

4.5.2 Chronic Toxicity to Aquatic Invertebrates

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TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Sediment Dwelling Organisms

4.6.2 Toxicity to Terrestrial Plants

4.6.3 Toxicity to Soil Dwelling Organisms

4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

4.7 Biological Effects Monitoring

4.8 Biotransformation and Kinetics

4.9 Additional Remarks

Remark: Fish appeared to be the most sensitive species to allyl chloride and harmful effects were found with the lowest LC50 values varying from 10 to 20 mg/l. One prolonged toxicity test with poecilla reticulata showed a 14d LC50 of 1.2 mg/l. It has to be noted however that for most of the tests volatility was not taken into account and that tests results may have under-estimated the intrinsic toxicity of allyl chloride.
Source: Solvay S.A. Bruxelles
28-JAN-2003

5.0 Toxicokinetics, Metabolism and Distribution

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

```
Type:              LD50
Species:           rat
Sex:               male
Vehicle:           peanut oil
Value:             = 460 mg/kg bw

Method:            other
  Year:            1982
   GLP:            no
Test substance:    other TS: allyl chloride, pure grade > 99%

Method:            Gross and histological studies on representative animals (dead
                   or sacrificed) from each dose group.
                   - 14-day observation test.
                   - 6 animals per group
Result:            Toxic signs appeared 4-5 h. after dosing.
                   Irritation of mucous membranes, hypoactivity, drowsiness hind
                   limb paralysis, tremor and occasional convulsions.
                   Gastrointestinal congestion, kidney and tubular changes,
                   cloudy swelling of the liver, congestion and oedema of lung
                   at higher dose levels.
28-JAN-2003                                                                (65)

Type:              LD50
Species:           rat
Doses:             no data
Value:             = 700 mg/kg bw

Method:            other: range finding test
  Year:            1948
   GLP:            no
Test substance:    other TS: allyl chloride, purity not specified

Test condition:    6 animals per group
21-JAN-2003                                                                (87)

Type:              LD50
Species:           rat
Vehicle:           other: oil
Doses:             no data
Value:             = 450 mg/kg bw

  Year:            1966
   GLP:            no
Test substance:    other TS: allyl chloride, purity not specified

Result:            Histological examination of the animals revealed changes in
                   the liver, kidneys and myocardium.
28-JAN-2003                                                                (56)

Type:              LD50
```

Species: mouse
Sex: male
Vehicle: peanut oil
Doses: no data
Value: = 425 mg/kg bw

Method: other
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, pure grade > 99%

Method: Gross and histological studies on representative animals (dead or sacrificed) from each dose group.
- 14-day observation test.
- 10 animals per group
Result: Toxic signs appeared 4-5 h. after dosing.
Irritation of mucous membranes, hypoactivity, drowsiness hind limb paralysis, tremor and occasional convulsions.
Gastrointestinal congestion, kidney and tubular changes, cloudy swelling of the liver, congestion and oedema of lung at higher dose levels.
28-JAN-2003 (65)

Type: LD50
Species: mouse
Sex: male
Vehicle: peanut oil
Doses: no data
Value: = 550 mg/kg bw

Method: other
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, commercial grade about 90%

Method: Gross and histological studies on representative animals (dead or sacrificed) from each dose group.
- 14-day observation.
- 10 animals per dose
Result: Toxic signs appeared 4-5 h. after dosing.
Irritation of mucous membranes, hypoactivity, drowsiness hind limb paralysis, tremor and occasional convulsions.
28-JAN-2003 (65)

Type: LD50
Species: mouse
Vehicle: other: oil
Doses: no data
Value: = 500 mg/kg bw

Year: 1966
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Result: Histological examination of the animals revealed changes in the liver, kidneys and myocardium.
28-JAN-2003 (56)

Type: LD50
Species: rabbit
Vehicle: other: oil
Doses: no data
Value: = 300 mg/kg bw

Year: 1966
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Result: Histological examination of the animals revealed changes in the liver, kidneys and myocardium.
28-JAN-2003 (56)

5.1.2 Acute Inhalation Toxicity

Type: LC100
Species: rat
Strain: other: albino
Exposure time: 7 hour(s)
Value: = 1 mg/l

Method: other
Year: 1940
GLP: no
Test substance: other TS: allyl chloride, purity > 99.5%

Result: concentration: 1 mg/l; 2-9 hrs

LC50 after 7-8 hours exposure.
Drowsiness and unsteadiness at shorter exposure times proceeding to unconciousness (time scale unspecified). Eye irritation was observed after a few hours. All deaths occurred within 8 hrs.

concentration: 10 mg/l; 30 min - 4 hrs

LC50 after 2 hours approximately. No narcosis. Slight eye and nose irritation within a few minutes. All animals died after 3 hrs exposure.

concentration: 20 mg/l; 30 min - 2 hrs

LC50 after 1-2 hours exposure. Rapid onset of eye and nose irritation and drowsiness. No narcosis. All animals died within 2 hours.

concentration: 50 mg/l; 30 min - 2 hrs

LC50 after 1-2 hours exposure. Rapid onset of eye and nose irritation and drowsiness. Incomplete narcosis, drowsiness, weakness, instability and dyspnoea. All animals died within 1.25 hours.

concentration: 100 mg/l; 15 min - 1 hr

LC50 after 15-30 minutes exposure. Eye and nose irritation.

All animals died within 0.5 hour.

Histopathological examination of tissues from exposed animals revealed renal damage as the most characteristic lesion.

In animals which died, both glomeruli and tubules were distended with an albuminous exudate, epithelial lining cells were flattened and in the tubules, degenerative. There was moderate congestion throughout the kidney with intertubular haemorrhage.

Lung damage was also quite severe especially at higher exposure levels which were irritant. There was significant

congestion and haemorrhage into the alveolar spaces. Interstitial oedema was accompanied by exudation into the alveoli. Lung damage appeared to be the principle cause of death. The liver of most animals was normal and were there was damage, this was slight. The changes consisted of congestion of the central vein and adjacent sinusoids with some slight centrilobular parenchymatous degeneration and occasional fatty degeneration. Surviving animals examined 4 weeks after exposure were essentially normal, even following the highest exposures. Occasionally there was slight to moderate fibrosis in kidney and lungs with, in some cases, pneumonic consolidation.

Test condition: Method : dynamic airflow 30 l/min
5 animals per group
For exposures of 0.5 hrs or longe, 5 animals were placed in a monel wire cage within a glass-monel chamber of 154 l. Ventilation was assured by an adjustable airflow at rates between 15-30 l/min. allyl chloride vapour concentration was built up by spraying the required amount of liquid onto the chamber sides and further added to the airflow. For exposures of < 1 hr 2 animals were exposed in a 10 l glass jar.

07-FEB-2003 (3)

Type: LC50
Species: rat
Sex: male/female
Exposure time: 2 hour(s)
Value: = 3454 - 3705 ppm

Method: other: static inhalation chamber
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, pure (>99%) or commercial (about 90%)

Result: LC 50 males: 3454 ppm (11.0 mg/l)
LC 50 females: 3705 ppm (11.8 mg/l)

All animals showed eye and nose irritation, hypoactivity, hypopnoea, paralysis of the hind
limbs, drowsiness, narcosis, tremors and convulsions were all observed.
On autopsy there was marked congestion, swelling and haemorrhage of the lungs. This was confirmed histologically.

In all animals microscopic examination of the kidney revealed cloudy swelling and tubular degeneration with focal necrosis of the glomerular epithelium. In the liver there was cloudy swelling of hepatocytes and dilation of sinusoids.

Test condition: 6 animals per group

28-JAN-2003 (65)

Type: LC50
Species: rat
Exposure time: 4 hour(s)
Value: = 2100 ppm

Year: 1973
GLP: no
Test substance: no data

Remark: no further data available

21-JAN-2003 (83)

Type: LC50
Species: rat
Strain: Fischer 344
Sex: male/female
Doses: 200, 300, 500, 800, 1000, 1200, 2000 ppm
Exposure time: 6 hour(s)
Value: 1000 - 2000 ppm

Method: other
Year: 1982
GLP: yes
Test substance: other TS: allyl chloride, purity = 99.8%

Method: exposure conducted under dynamic air-flow conditions in a 160 liter glass and stainless steel chamber. Allyl chloride vapour was swept with filtered air into the main chamber airflow at a rate of approx. 30 l/min

10 M and 10 F animals per group
Result: LC50 male rats > 2000 ppm (6 hours)
LC50 female rats = 1000 - 2000 ppm (6 hours)

No mortality in either sex below 1000 ppm. All female rats at 2000 ppm died within 24 hours. Eye irritation from 200 ppm, nose irritation from 1000 ppm. Diarrhoea, decrease in usrine and faeces and lethargy were observed at 500 ppm and above. 24 hour body weight was reduced at all levels. BUM, SGPT, AP, SGOT and blood glucose were determined.

There was a dose related increase in 24 hour BUN at 500 ppm and above in females and at 1000 ppm and above in males. BUN remained elevated in top-dose males et 48 hours. There were other statistically significant changes in clinical chemistry parameters which were of a variable nature. These were considered by the authors to be the result of secondary effect associated with acute renal damage.

Kidney and/or kidney/body weight ratios were increased in both sexes at 500 ppm and above. Liver and/or liver/body weight ratios were increased from 800 ppm. The major pathological

findings both gross and microscopic were indicative of dose related acute renal tubular degeneration. This was evident in males at 500 ppm and above and in females at 300 ppm and

above.

28-JAN-2003 (79)

Type: LC50
Species: rat
No. of Animals: 6
Doses: 2000 ppm
Exposure time: 4 hour(s)
Value: >= 2000 ppm

Method: other: range finding test
Year: 1948
GLP: no
Test substance: no data

28-JAN-2003 (87)

Type: other
Species: rat
Doses: 0.29, 0.1, 0.006 mg/l (approx. 92, 31, 2 ppm)
Exposure time: 4 hour(s)

Year: 1983
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Result: At the highest dose level a single exposure resulted in increased serum cholineesterase, increased respiration rate and a reduction in the so-called "cumulative threshold index" (CTI, indicative of CNS effects. Red and white cell counts, urinalysis, body weight and behavioural indices were unaffected. At 0.1 mg/l, the only parameter showing change was serum cholinesterase, which was increased. No deaths were reported.

22-JAN-2003 (45)

Type: LC50
Species: mouse
Doses: 24021, 48042, 72062 ppm (1, 2, 3 mM/l)
Exposure time: 10 minute(s)
Value: ca. 24000 ppm

Method: other
Year: 1938
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Method: 10 animals per concentration;
mice were exposed, 2 at a time, for 10 minute periods to given initial concentrations of volatilised allyl chloride in a 2.5

l glass bottle.
Result: Mortality 4/10, 9/10 and 10/10 respectively.
No narcosis at 1 mM/l. At 2 mM/l 9/10 mice were unconscious within 2-8 minutes. At 3 mM/l all mice were unconscious within

1-2 minutes. Pathological examination revealed severe pulmonary damage and unspecified effects on other organs.
22-JAN-2003 (85)

Type: LC50
Species: mouse
No. of Animals: 4
Doses: 1455 ppm
Exposure time: 1 hour(s)
Value: = 1455 ppm

Method: other: single exposure
Year: 1958
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Result: 2/4 died;
Pathological examination revealed pulmonary and pleural haemorrhages and enlarged kidneys in some animals.
22-JAN-2003 (84)

Type: LC50
Species: mouse
Exposure time: 2 hour(s)
Value: = 2600 ppm

GLP: no
Test substance: no data

Remark: no further data available
21-JAN-2003 (83)

Type: LC50
Species: mouse
Sex: male
Exposure time: 2 hour(s)
Value: = 3610 ppm

Method: other: Static inhalation chamber
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, pure (> 99%) or commercial (about 90%)

Result: LC 50 males: 3611 ppm (11.5 mg/l)

All animals showed eye and nose irritation, hypoactivity, hypopnoea, paralysis of the hind limbs, drowsiness, narcosis, tremors and convulsions were all observed.
On autopsy there was marked congestion, swelling and haemorrhage of the lungs. This was confirmed histologically.

In all animals microscopic examination of the kidney revealed

cloudy swelling and tubular degeneration with focal necrosis of the glomerular epithelium. In the liver there was cloudy swelling of hepatocytes and dilation of sinusoids.

Test condition: 10 animals per group
28-JAN-2003 (65)

Type: LC50
Species: mouse
Strain: B6C3F1
Sex: male/female
Doses: 500, 800, 1000, 1200, 2000 ppm
Exposure time: 6 hour(s)
Value: = 800 - 2000 ppm

Method: other
Year: 1982
GLP: yes
Test substance: other TS: allyl chloride, purity = 99.8%

Method: exposure conducted under dynamic air-flow conditions in a 160 liter glass and stainless steel chamber. Allyl chloride vapour was swept with filtered air into the main chamber airflow at a rate of approx. 30 l/min

10 M and 10 F animals per group
Result: LC50 males: 800 - 1000 ppm
LC50 females: 1200-2000 ppm

No mortality in either sex below 1000 ppm. At 2000 ppm all male and female animals died within 24 hours.
Eye irritation at all levels, nasal irritation at 200 ppm. Lethargy was evident from 1000 ppm. Body weight was reduced at 24 hours at 1000 and 1200 ppm. BUN was increased in male mice at both 24 and 72 hours following exposure to 1200 ppm. In females BUN was reduced at this level. There were other statistically significant changes in clinical chemistry parameters which were of a variable nature. These were considered by the authors to be the result of secondary effects associated with acute renal damage.

24 hour kidney and/or kidney/body weight ratios were increased at 1000 ppm and above in both sexes persisting in males to 72 hours.
24 hour liver weights and/or liver/body weight ratios were decreased in males at 1000 and 1200 ppm. The major pathological findings both gross and microscopic were indicative of dose related acute renal tubular degeneration. This was evident in males at 500 ppm and above and in females at 1000 ppm and above.
The changes observed in males at the two lower dose levels were minor.
28-JAN-2003 (79)

Type: other: sensory irritation test
Species: mouse
Strain: other: CF1
Sex: male

Doses: 1120, 1540, 2120, 3650 ppm
Exposure time: 10 minute(s)
Value: = 2330 ppm

Method: other
Year: 1985
GLP: no
Test substance: other TS: allyl chloride, purity = 99%

Method: Both normal mice and mice with tracheal cannulae were exposed and their respiratory rate monitored during exposure and for 20 min. afterwards.
Exposure duration 10-30 minutes
Result: The RD50 (50% reduction in respiration rate) within the first 10 minutes of exposure was 2330 ppm. This was due to sensory irritation as there was no reduction in respiration rate in cannuled animals.
28-JAN-2003 (74)

Type: LC50
Species: rabbit
Sex: male
Exposure time: 2 hour(s)
Value: = 7065 ppm

Method: other: static inhalation chamber
Year: 1982
GLP: no
Test substance: other TS: pure (> 99%) or commercial (about 90%)

Result: LC 50: 7065 ppm (22.5 mg/l)

All animals showed eye and nose irritation, hypoactivity, hypopnoea, paralysis of the hind
limbs, drowsiness, narcosis, tremors and convulsions were all observed.
On autopsy there was marked congestion, swelling and haemorrhage of the lungs. This was confirmed histologically.

In all animals microscopic examination of the kidney revealed cloudy swelling and tubular degeneration with focal necrosis of the glomerular epithelium. In the liver there was cloudy swelling of hepatocytes and dilation of sinusoids.
Test condition: 2 animals per group
28-JAN-2003 (65)

Type: LC50
Species: cat
Sex: male
Exposure time: 2 hour(s)
Value: = 3300 ppm

Method: other: static inhalation chamber
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, pure (> 99%) or commercial (about 90%)

Result: LC 50: 3300 ppm (10.5 mg/l)

All animals showed eye and nose irritation, hypoactivity, hypopnoea, paralysis of the hind limbs, drowsiness, narcosis,

tremors, convulsions, unsteady gait and ataxia were all observed.
On autopsy there was marked congestion, swelling and haemorrhage of the lungs. This was confirmed histologically.

In all animals microscopic examination of the kidney revealed cloudy swelling and tubular degeneration with focal necrosis of the glomerular epithelium. In the liver there was cloudy swelling of hepatocytes and dilation of sinusoids.

Test condition: 2 animals per group
28-JAN-2003 (65)

Type: LC100
Species: guinea pig
Exposure time: 3 hour(s)
Value: = 290 ppm

Method: other
Year: 1940
GLP: no
Test substance: other TS: allyl chloride, purity > 99.5%

Method: Method : dynamic airflow 30 l/min
4-5 animals per group
For exposures of 0.5 hrs or longe, 5 animals were placed in a monel wire cage within a glass-monel chamber of 154 l. Ventilation was assured by an adjustable airflow at rates between 15-30 l/min. allyl chloride vapour concentration was built up by spraying the required amount of liquid onto the chamber sides and further added to the airflow. For exposures of < 1 hr 2 animals were exposed in a 10 l glass jar.

Result: concentration 290 ppm, 1 mg/l; 1 - 9 hours

LC50 after 3-4 hours exposure.
Up to 4 hours exposure produced only drowsiness and unsteadyness. 6 hours produces eye irritation and narcosis. All death occurred within 6 hours.

concentration 2900 ppm, 10 mg/l; 30 min - 2 hours

LC50 after 1-2 hours exposure.
Eye and nose irritation within a few minutes. All animals died following a 2 hour exposure but there was no narcosis.

concentration: 14500 ppm, 50 mg/l; 10 min - 1 hour

LC50 after 30 minutes exposure.
Eye and nose irritation, drowsiness, weakness, instability and laboured breathing were observed without loss of consciousness. Deaths occurred within 30 minutes.

Histopathological examination was carried out with the same

lesions being described as for rats (see above). Guinea pigs were however more severely affected.
22-JAN-2003 (3)

Type: LC50
Species: guinea pig

Sex: male
Exposure time: 2 hour(s)
Value: = 1820 ppm

Method: other: Static inhalation chamber
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, pure (> 99%) or commercial (about 90%)

Result: LC 50: 1820 ppm (5.8 mg/l)

All animals showed eye and nose irritation, hypoactivity, hypopnoea, paralysis of the hind limbs, drowsiness, narcosis, tremors and convulsions were all observed.
On autopsy there was marked congestion, swelling and haemorrhage of the lungs. This was confirmed histologically.

In all animals microscopic examination of the kidney revealed cloudy swelling and tubular degeneration with focal necrosis of the glomerular epithelium. In the liver there was cloudy swelling of hepatocytes and dilation of sinusoids.
Test condition: 4 animals per group
28-JAN-2003 (65)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Value: = 2026 mg/kg bw

Method: other: range finding test
Year: 1948
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: no further data available
22-JAN-2003 (87)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain: ICR
Sex: male
Doses: 621 mg/kg bw
Route of admin.: s.c.
Value: 621 mg/kg bw

Method: other: no further data
Year: 1993

GLP: no data
Test substance: other TS: allyl chloride, purity not specified

Result: 16/25 mice died by the 7th day after injection and showed marked congestion with severe haemorrhage and oedema in the lung. Liver and kidney damage was also found (focal necrosis in the liver and necrosis of epithelium in tubules of the

kidneys).
The 9/25 mice that survived showed damages in the testes characterised by degeneration and exfoliation of germ cells, polynuclear giant cells in the seminiferous tubules, proliferation of Leydig cells in the interstitium, all type of cells in tubules including Sertoli cells, and necrotic Leydig cells.
22-JAN-2003 (77)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Exposure: no data
Result: slightly irritating

Method: other: range finding test
Year: 1948
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: The irritancy was equated with that of acetone, which is considered as slight.
Test substance: Concentration/dose : 0.1 ml undiluted.
22-JAN-2003 (87)

5.2.2 Eye Irritation

Species: rabbit
Dose: .01 ml
Result: slightly irritating

Method: other
Year: 1946
GLP: no
Test substance: other TS: allyl chloride, purity not specified

22-JAN-2003 (25)

Species: rabbit
Dose: .5 ml
Result: slightly irritating

Method: other: range finding test
Year: 1948
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Score 1-5 of a possible 20 after 18-24 hours.
22-JAN-2003 (87)

5.3 Sensitization

Type: other

Remark: No available data
22-JAN-2003

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: Fischer 344
Route of administration: inhalation
Exposure period: 90 d
Frequency of treatment: 6 h/d, 5 d/wk; interim kill at 1 month
Doses: 50, 100, 250 ppm; 25M, 25F/group
Control Group: yes, concurrent vehicle
NOAEL: = 50 ppm
LOAEL: = 100 ppm

Method: other: chamber of 14.5 m3 volume; air flow: 2200-2900 l/min
Year: 1982
GLP: yes
Test substance: other TS: allyl chloride, purity = 99.8%

Method: Test parameters: clinical observations, body weights, haematology, urinalysis, clinical chemistry, organ weights and gross microscopic pathology.
Result: In both male and female rats, effects were reported to occur in kidneys at the highest dose level only [250 ppm (795 mg/m3)].
However in rats exposed to 100 ppm (301 mg/m3) and 250 ppm (795 mg/m3) effects were observed. Rats exposed to 100 ppm exhibited a slight increase in the cytoplasmic granularity and oesonophilic staining of the cortica; epithelial cells when compared with the controls. These findings were also observed in the high dose animals as well as an increase in the number of tubules showing focal collapse and atrophy. The LOAEL in this study is 100 ppm (duration adjusted concentration 54 mg/m3). As NOAEL 50 ppm (duration adjusted concentration 27 mg/m3) can be established for this study.
28-JAN-2003 (79)

Species: rat Sex: male/female
Strain: Fischer 344
Route of administration: inhalation
Exposure period: 3 m
Frequency of treatment: 6 h/d, 5 d/wk; interim kill at 1 month
Doses: 1, 3, 10, and 20 ppm; 10M, 10F/group
Control Group: yes, concurrent vehicle
NOAEL: = 20 ppm

Method: other: chambers of 14.5 m3 volume; air flow: 2000-3500 l/min

```
  Year:           1982
   GLP:           yes
Test substance:   other TS: allyl chloride, purity = 99.8%

Result:           No adverse effects in any of the following test
                  parameters : clinical observations, body weights,
                  haematology, urinalysis, clinical chemistry, organ
                  weights, and gross and microscopic pathology.
28-JAN-2003                                                          (79)


Species:                 rat                              Sex: no data
Strain:                  no data
Route of administration: inhalation
Exposure period:         4 m
Frequency of treatment:  4 h/d, 5 d/wk
Post exposure period:    1 m
Doses:                   0.29, 1.1 and 3.1 mg/m3 (0.1, 0.3 and 1 ppm)
Control Group:           no data specified
NOAEL:                   = .1 ppm
LOAEL:                   = .3 ppm

Method:           other
  Year:           1983
   GLP:           no
Test substance:   other TS: allyl chloride, purity not specified

Remark:           Toxicological effects were  assessed at the end of each
                  month and following a 1-month recovery period
Result:           In a first study over 45 days (length of daily exposures not
                  reported, the results ere as follows:
                  0.1 and 0.3 ppm: No adverse effects observed
                  1 ppm: decreased CNS activity (increased CTI) changes in liver
                  (increased serum choline esterase) and kidney (anti-diuretic
                  effect with increased specific gravity of the urine)
                  functions.
                  At 0.1 ppm, no adverse effects observed
                  At 0.3 ppm, decreased CNS activity (reversible).
                  At 1.0 ppm, decreased CNS activity, increased bodyweight,
                   changes in liver (increased serum choline esterase) and
                  kidney (anti-diuretic effect with increased specific gravity
                  of the urine) functions. Changes in CNS activity and liver and
                  kidney function persisted through the recovery period.
22-JAN-2003                                                          (45)

Species:                 rat                              Sex: male/female
Strain:                  no data
Route of administration: inhalation
Exposure period:         35 d
Frequency of treatment:  7 h/d, 5 d/wk
Doses:                   25 mg/m3 (approx 8 ppm); 5M, 5F/group
Control Group:           yes, concurrent vehicle

Method:           other: glass walled chamber of 160 l
  Year:           1959
   GLP:           no
Test substance:   other TS: allyl chloride, purity not specified
```

Remark: Exposed to air or allyl chloride vapour in air, the animals were transferred daily and placed in the exposure chamber during the exposure period.
In view of the small number of test animals and poor reporting of the results as well as contradiction of these findings by better designed studies (e.g. Quast et al., 1982), this older study is considered to be not suitable for derivation of an overall NOAEL.

Result: No effect on growth, behaviour, body weights or mortality. Reduced spleen weight in females only. Histopathologically no changes in the spleen, but all animals showed severe liver and kidney damage. In the liver dilation of sinusoids, cloudy swelling and focal necrosis and in the kidney, glomerular changes, tubular necrosis and proliferation of interstitial tissues.
23-JAN-2003 (93)

Species: rat Sex: male/female
Strain: no data
Route of administration: inhalation
Exposure period: 6 mo
Frequency of treatment: 7 h/d, 5 d/wk
Doses: 9 mg/m3 (approx 3 ppm); 24M, 24F/group
Control Group: yes, concurrent vehicle

Method: other: vault-type stainless steel chambers of 3700 l capacity
Year: 1959
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Exposed to air or allyl chloride vapour in air. The animals were transferred daily and placed in the exposure chamber during the exposure period.
Air flow : 340 l/min; even air distribution through the chambers was assured.
In view of the small number of test animals and poor reporting of the results as well as contradiction of these findings by better designed studies (e.g. Quast et al., 1982), this older study is considered to be not suitable for derivation of an overall NOAEL.
Result: No changes in growth, behaviour, mortality, body weight, gross appearance, haematological parameters, histopathology, BUN or blood non-protein nitrogen related to the compound. One female rat only showed slight reversible centrilobular degeneration of the liver.
23-JAN-2003 (93)

Species: rat Sex: male
Strain: no data
Route of administration: inhalation
Exposure period: 5 m
Frequency of treatment: 6 h/d; 6 d/w
Doses: 17.5 mg/m3 (5.5 ppm); 10 M/group
Control Group: yes, concurrent vehicle

Method: other: glass-walled hexagonal chamber (5 m3, 1500l/min)
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, purity > 99%

Result: No adverse effects. Parameters examined were the same as for the study in rabbits by the same author (see below). For the rats, the renal function was also determined by the dilution test.
28-JAN-2003 (65)

Species: rat Sex: no data
Strain: no data
Route of administration: inhalation
Exposure period: 1 m
Frequency of treatment: 4 h/d, 5 d/w
Doses: 400 mg/m3 (126 ppm)
Control Group: no data specified

Method: other: no data
Year: 1973
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Result: Reduced body weight, CNS effects and changes in renal function.
23-JAN-2003 (83)

Species: rat Sex: no data
Strain: other: Donryo
Route of administration: inhalation
Exposure period: 34 wk
Frequency of treatment: 8 h/d, 5 d/wk
Post exposure period: no
Doses: 10, 50 and 100 ppm (31, 156 and 313 mg/m3); 5 animals/conc.
Control Group: no data specified
NOAEL: = 10 ppm
LOAEL: = 50 ppm

Year: 1991
GLP: no data
Test substance: other TS: allyl chloride, purity not specified

Result: Significant reduction of motor and sensory nerve conduction velocities and nerve action potential at 100 ppm after 28 wk exposure; clinical signs included weakness of hindlimbs and extended landing foot-spreads. After 34 wk exposure motor distal latency was retarded at 100 ppm, and amplitude of nerve action potentials was depressed at 50 ppm. (only abstract in english)
07-FEB-2003 (69)

Species: rat Sex: no data
Strain: no data
Route of administration: drinking water
Exposure period: 6 m

Frequency of treatment: 5 d/w
Doses: 0.015 mg/kg; 6 animals
Control Group: yes, concurrent vehicle

Year: 1969
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Animals selected on the basis of their response to behavioural tests.
Result: When assessed by behavioural tests, no effects on conditioned reflex activity were observed.

23-JAN-2003 (57)

Species: rat Sex: no data
Strain: other: white
Route of administration: gavage
Exposure period: 10 d
Frequency of treatment: daily
Doses: 45 and 90 mg/kg; administration in sunflower oil
Control Group: no data specified
LOAEL: = 45 mg/kg

Year: 1969
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Result: On autopsy the organs were generally congested. Microscopic examination confirmed this observation and also revealed dystrophic change.
22-JAN-2003 (4)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of administration: inhalation
Exposure period: 3 m
Frequency of treatment: 6 h/d, 5 d/w; interim kill at 1 month
Doses: 1, 3, 10 and 20 ppm; 25M, 25F/group
Control Group: yes, concurrent vehicle
NOAEL: = 20 ppm

Method: other: chamber of 14.5 m3 volume; air flow: 2000-3500 l/min
Year: 1982
GLP: yes
Test substance: other TS: allyl chloride, purity = 99.8%

Result: No adverse effects in any of the following test parameters : clinical observations, body weights, haematology, urinalysis, clinical chemistry, organ weights, and gross and microscopic pathology.
28-JAN-2003 (79)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of administration: inhalation
Exposure period: 90 d
Frequency of treatment: 6 h/d, 5 d/wk; interim kill at 1 month

Doses: 50, 100, 250 ppm;
Control Group: yes, concurrent vehicle
NOAEL: = 250 ppm

Method: other: chamber of 14.5 m3 volume; air flow: 2200-2900 l/min
Year: 1982
GLP: yes
Test substance: other TS: allyl chloride, purity = 99.8%

Method: Test parameters: clinical observations, body weights, haematology, urinalysis, clinical chemistry, organ weights and gross microscopic pathology.
Result: No treatment related changes were observed.

There were statistically significant changes in various other parameters but for a variety of reasons were not considered of statistical relevance by the authors.
28-JAN-2003 (79)

Species: mouse Sex: male/female
Strain: other: TO albino
Route of administration: gavage
Exposure period: 2 to 17 wk
Frequency of treatment: 3 d/wk
Doses: 300 and 500 mg/kg; 20M, 20F in total
Control Group: yes
LOAEL: = 300 mg/kg

Method: other: development of neurotoxicity
Year: 1985
GLP: no

Result: The development of neurotoxicity in the progressively dosed mice was followed. Animals were killed after various periods of regular dosing.

Males were more severely affected than females, clinically signs were hunched back, sprawling gait, hind limb weakness and difficulty in crossing a horizontal grid.
The neuropathy was described as a central-peripheral distal type of axonopathy. Nerve fibre degeneration was found in many peripheral nerves and roots, being more marked distally and affecting more motor than sensory nerves. There was no neuronal death but occasional changes were seen in the anterior horn and dorsal root danglion cells. Tolerance developed following continuous dosing.
The only other change reported was focal kidney damage in 70 % of mice.
Test substance: Allyl chloride dilution : 0.93-0.94 g/ml at 20 degree C
23-JAN-2003 (50)

Species: rabbit Sex:
Route of administration: inhalation
Exposure period: 2 mo
Doses: 65 ppm

Result: Neurological changes, slight kidney and cardiac

pathological effect.
23-JAN-2003 (50)

Species: rabbit Sex: female
Strain: no data
Route of administration: inhalation
Exposure period: 35 d
Frequency of treatment: 7 h/d, 5 d/wk
Doses: 25 mg/m3 (approx 8 ppm); 1F/group
Control Group: yes, concurrent vehicle

Method: other: glass-walled chamber of 160 l
Year: 1959
GLP: no

Test substance: other TS: allyl chloride, purity not specified

Remark: Exposed to air or allyl chloride vapour in air, the animals were transferred daily and placed in the exposure chamber during the exposure period.
In view of the small number of test animals and poor reporting of the results as well as contradiction of these findings by better designed studies (e.g. Quast et al., 1982), this older study is considered to be not suitable for derivation of an overall NOAEL.
Result: No effect on growth, behaviour, body weights or mortality. Histopathologically no changes in the spleen, but all animals showed severe liver and kidney damage. In the liver dilation of sinusoids, cloudy swelling and focal necrosis and in the kidney, glomerular changes, tubular necrosis and proliferation of interstitial tissues.
23-JAN-2003 (93)

Species: rabbit Sex: male/female
Strain: no data
Route of administration: inhalation
Exposure period: 6 mo
Frequency of treatment: 7 h/d, 5 d/wk
Doses: 9 mg/m3 (approx. 3 ppm); 3M, 3F/group
Control Group: yes, concurrent vehicle

Method: other: vault-type stainless steel chambers of 3700 l capacity
Year: 1959
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Exposed to air or allyl chloride vapour, the animals were transferred daily and placed in the exposure chamber during the exposure period.
Air flow : 340 l/min; even air distribution through the chambers was assured.
In view of the small number of test animals and poor reporting of the results as well as contradiction of these findings by better designed studies (e.g. Quast et al., 1982), this older study is considered to be not suitable for derivation of an overall NOAEL.
Result: No ill effects.
23-JAN-2003 (93)

Species: rabbit Sex: male
Route of administration: inhalation
Exposure period: 3m
Frequency of treatment: 6h/d, 6d/w
Doses: 206 mg/m3 (64 ppm); 6M/group
Control Group: yes, concurrent vehicle

Method: other: glass-walled hexagonal chamber (5 m3, 1500l/min)
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, pure (> 99%) or commercial (about 90%)

Result: Clinical signs of peripheral polyneuropathy, confirmed by

electro-myography (EMG) and histopathology at the end of exposure. There was degeneration of the peripheral nerves more marked in distal positions. The severity of degeneration correlated with clinical symptoms and EMG findings.

Brain, spinal cord and roots were essentially normal except for slight changes in the spinal cord of one rabbit. Paralysis was observed in some animals. There were no changes in SGPT, serum SH or creatinine or urinalysis. Relative lung and liver weights were increased but not kidney weights. Histological examination of these tissues revealed dilation of sinusoids and vacuolar degeneration of the liver; congestion, cloudy swelling and tubular degeneration (fatty) in the kidney and thickening of the alveolar septa of the lungs.
28-JAN-2003 (65)

Species: rabbit Sex: male/female
Strain: no data
Route of administration: inhalation
Exposure period: 5 m
Frequency of treatment: 6 hours/day, 6 days/week
Doses: 17.5 mg/m3 (5.5 ppm)
Control Group: yes, concurrent no treatment

Method: other: glass-walled hexagonal chamber (5 m3, 1500l/min)
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, purity > 99%

Result: No adverse effects. Parameters examined were the same as for the other rabbit study by same author (see above).
28-JAN-2003 (65)

Species: rabbit Sex: no data
Strain: no data
Route of administration: gavage
Exposure period: 8 mo
Doses: 0.015 mg/kg; administration in sunflower oil
Control Group: no data specified

Year: 1969
GLP: no

Test substance: other TS: allyl chloride, purity not specified

Result: Histopathology only carried out. No significant changes.
22-JAN-2003 (4)

Species: rabbit Sex: no data
Strain: no data
Route of administration: s.c.
Exposure period: 1 wk (50 mg/kg) + 38-80 d (100 mg/kg)
Frequency of treatment: 3 d/wk
Doses: 50 mg/kg + 100 mg/kg
Control Group: yes

Year: 1980
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Method: Investigation of neuropathological aspects of chronic intoxication
6 treated animals, 3 controls
Result: Degeneration of peripheral nerve particularly in distal parts. EMG abnormalities correlating with the degree of functional disability were observed in all treated animals by week 5 - 6.
23-JAN-2003 (49)

Species: cat Sex: female
Route of administration: inhalation
Exposure period: 3m
Frequency of treatment: 6h/d, 6d/w
Doses: 206 mg/m3 (64 ppm); 1F/group
Control Group: yes, concurrent vehicle

Method: other: glass-walled hexagonal chamber (5 m3, 1500l/min)
Year: 1982
GLP: no
Test substance: other TS: pure (> 99%) or commercial (about 90%)

Result: The peripheral nerves of the cat appeared less susceptible to allyl chloride than those of the rabbit (see here above). The cat only showed muscle weakness and unsteady gait at the end of exposure.
23-JAN-2003 (65)

Species: dog Sex: male/female
Strain: Beagle
Route of administration: inhalation
Exposure period: 6 mo
Frequency of treatment: 7 h/d, 5 d/wk
Doses: 9 mg/m3 (approx 3 ppm); 1M, 1F/group
Control Group: yes, concurrent vehicle

Method: other: vault-type stainless steel chambers of 3700 l capacity
Year: 1959
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Exposed to air or allyl chloride vapour, the animals were transferred daily and placed in the exposure chamber during

the exposure period.
Air flow : 340 l/min; even air distribution through the chambers was assured.
In view of the small number of test animals and poor reporting of the results as well as contradiction of these findings by better designed studies (e.g. Quast et al., 1982), this older study is considered to be not suitable for derivation of an overall NOAEL.
Result: No ill effects.
23-JAN-2003 (93)

Species: guinea pig Sex: male
Strain: no data
Route of administration: inhalation
Exposure period: 35 d
Frequency of treatment: 7 h/d, 5 d/wk
Doses: 25 mg/m3 (approx 8 ppm); 4M/group

Control Group: yes, concurrent vehicle

Method: other: glass-walled chamber of 160 l capacity
Year: 1959
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Exposed to air or allyl chloride vapour in air, the animals were transferred daily and placed in the exposure chamber during the exposure period.
In view of the small number of test animals and poor reporting of the results as well as contradiction of these findings by better designed studies (e.g. Quast et al., 1982), this older study is considered to be not suitable for derivation of an overall NOAEL.
Result: No effect on growth, behaviour, body weights or mortality. Histopathologically no changes in the spleen, but all animals showed severe liver and kidney damage. In the liver dilation of sinusoids, cloudy swelling and focal necrosis and in the kidney, glomerular changes, tubular necrosis and proliferation of interstitial tissues.
23-JAN-2003 (93)

Species: guinea pig Sex: male/female
Strain: no data
Route of administration: inhalation
Exposure period: 6 mo
Frequency of treatment: 7 h/d, 5 d/wk
Doses: 9 mg/m3 (approx 3 ppm); 9M, 9F/group
Control Group: yes, concurrent vehicle

Method: other: vault-type stainless steel chambers of 3700 l capacity
Year: 1959
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Exposed to air or allyl chloride vapour, the animals were transferred daily and placed in the exposure chamber during the exposure period.
Air flow : 340 l/min; even air distribution through the

chambers was assured.
In view of the small number of test animals and poor reporting of the results as well as contradiction of these findings by better designed studies (e.g. Quast et al., 1982), this older study is considered to be not suitable for derivation of an overall NOAEL.
Result: No ill effects.
23-JAN-2003 (93)

5.5 Genetic Toxicity 'in vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA100, TA 1535, TA 1538
Concentration: 0, 0.2, 20, 500, 2000 microgram/plate
Metabolic activation: with and without
Result: negative

Method: OECD Guide-line 471
Year: 1983
GLP: no
Test substance: other TS: allyl chloride, purity = 98 %

Remark: S9 Rat liver arochlor induced
negative results were ascribed to volatility of test substance.
24-JAN-2003 (31)

Type: Escherichia coli reverse mutation assay
System of testing: WP2 and WP2 uvrA
Concentration: 20 microlitre
Metabolic activation: with and without
Result: positive

Method: other
Year: 1985
GLP: no
Test substance: other TS: allyl chloride, purity = 98 %

Remark: Spot test with undiluted material, rat liver arochlor induced, positive with and without metabolic activation.
24-JAN-2003 (31)

Type: Ames test
System of testing: Salmonella typhimurium TA 100, TA 1535, TA 1538
Concentration: 0, 0.1, 1, 10 microlitre
Metabolic activation: with and without
Result: positive

Method: other
Year: 1978
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Test material on filter discs in sealed bags, with and without S9 (arochlor induced).

TA 1538 numbers of revertants were decreased at all dose levels (toxicity). With TA 100 there was no dose related significant increase in reverse mutation rate. With TA 1535, significant dose-related increase in revertants only with S9.

(A separate test, plate incorporation assay with TA 1535 at 0, 1, 2, 5 or 10 microlitre/plate with or without S9 was negative)

24-JAN-2003 (67)

Type: Ames test
System of testing: Salmonella typhimurium TA 100, TA 1535
Concentration: 0, 2, 10, 40 microlitre/plate
Metabolic activation: with and without
Result: positive

Method: other
Year: 1980

GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Spot test with and without S9 (arochlor induced)

Result: at 10 and 40 ug dose-related increase in reverse mutation rate for TA 1535 with and without S9.

(In a separate test, plate incorporation assay with TA 100 and TA 1535, with and without S9 at 0, 1, 5, 10 microlitre/plate, a positive result was found for TA 1535 at 5 and 10 ul only in the presence of S9.)

28-JAN-2003 (16)

Type: other: gene mutation assay
System of testing: Streptomyces coelicolor A3, Aspergillus nidulans (Haploid strain 35)
Concentration: 0 to 40 microlitre/plate
Metabolic activation: without
Result: positive

Method: other
Year: 1980
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Two tests with Streptomyces coelicolor:

1) spot test: 0 and 10 ul/plate
2) plate incorporation assay 0, 10, 20 and 40 ul/plate

Two tests with Aspergillus nidulans

1) spot test: 0, 2 (sealed in a jar) and 20 ul/plate
2) plate incorporation assay 0, 10, 20 and 40 ul/plate

Result: Positive in S. coelicolor for both forward and reverse mutations either in the spot test or in the plate incorporation assay.

Negative in A. nidulans in both spot test and plate incorporation assay.

24-JAN-2003 (16)

Type: Ames test
System of testing: Salmonella typhimurium TA 100
Concentration: 0, 10, 20, 30 micromoles/assay
Metabolic activation: with and without
Result: positive

Method: other
Year: 1980
GLP: no
Test substance: other TS: allyl chloride, purity 100 %

Remark: Liquid suspension assay with and without S9 from arochlor and phenobarbitone induced rats and uninduced mice.
Result: positive without S9
negative with either S9 fraction

24-JAN-2003 (37)

Type: Ames test
System of testing: Salmonella typhimurium TA 100
Concentration: 0, 0.75, 1.5 microlitre/plate
Metabolic activation: with and without
Result: positive

Method: other
Year: 1985
GLP: no
Test substance: other TS: allyl chloride, purity = 100 %

Remark: - Incubation before plating of 0, 20, 60, 120, 180 minutes
- Arochlor induced S9 with a protein content of 4 or 12 mg/ml
Result: Weak mutagenic activity in the standard test (without pre-incubation) was enhanced by incubation, especially for 120 minutes. Enhanced mutagenicity after 180 was dueat least in part to bacterial growth. Increase in concentration of the S9 mix or addition of enzymatically inactive bovine serum decreased the mutagenicity.

24-JAN-2003 (72)

Type: Yeast gene mutation assay
System of testing: Saccharomyces cerevisiae JDI
Concentration: 0.1 ml of solution in DMSO
Metabolic activation: with and without
Result: positive

Method: other
Year: 1985
GLP: no
Test substance: other TS: allyl chloride, purity 98 %

Remark: Arochlor induced S9.
Positive with and without S9.

24-JAN-2003 (31)

```
Type:                    Yeast gene mutation assay
System of testing:       Saccharomyces. cerevisiae D4
Concentration:           6.1x10-5 to 30.7x10-7 molar
Cytotoxic Concentration: 30.7x10-7 molar
Metabolic activation:    without
Result:                  positive

Method:           other
  Year:           1978
   GLP:           no
Test substance:   other TS: allyl chloride, purity not specified

Remark:           Closed system, dose-relatesd increase in conversion
                  frequency up to 24.5 10-5 molar. Toxicity at top dose level.
24-JAN-2003                                                              (67)

Type:                    DNA damage and repair assay
System of testing:       Escherichia coli pol A+/pol A1
Concentration:           10 microlitre
Metabolic activation:    without

Result:                  positive

Method:           other
  Year:           1978
   GLP:           no
Test substance:   other TS: allyl chloride, purity not specified

Remark:           Closed system, test substance put on filter discs.
Result:           positive in pol A1
24-JAN-2003                                                              (67)

Type:                    other
System of testing:       Aspergillus nidulans (Diploid strain 35 x 17)
Concentration:           0, 0.6, 0.9 ml/20 l dessicator
Metabolic activation:    without
Result:                  positive

Method:           other: 24 h exposure
  Year:           1984
   GLP:           no
Test substance:   other TS: allyl chloride, purity = 99 %

Remark:           Significant increase in the frequency of haploid segregants
                  and diploid non disjunctional sectors.
24-JAN-2003                                                              (28)

Type:                    Cytogenetic assay
System of testing:       rat liver RL1
Concentration:           up. to 25 microgr/ml
Result:                  negative

Method:           other
  Year:           1985
   GLP:           no
Test substance:   other TS: allyl chloride, purity = 98 %
```

Remark: Sealed culture exposed to test material.
24-JAN-2003 (31)

Type: Unscheduled DNA synthesis
System of testing: Human HeLa S3
Concentration: 10-5 to 10-2 molar
Result: positive

Method: other
Year: 1983
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: exposure time 2.5 h
(H3)-thymidine incorporation assay
UDS was observed at 10-3 to 5x10-3 molar.
10-2 molar was lethal.
24-JAN-2003 (82)

Type: Unscheduled DNA synthesis
System of testing: Human embryonic intestinal cell (Flow 11000)
Concentration: 77-9900 microgr/ml

Cytotoxic Concentration: 9900 microgr/ml.
Metabolic activation: with and without
Result: negative

Method: other
Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity = 98 %

Remark: - 3 hours incubation at 37 degree
- solvent and positive control with and without S9 (rat, arochlor induced)
- C. Thymidine incorporation as an indicator of UDS was evaluated by autoradiography. 50 nuclei assessed/culture
Result: Cytotoxicity was 75-100% at 9900 ug/ml and 0% at 990 ug/ml. There was no increased incorporation of 6-[3H]-thymidine into the cell nucleus of cells treated with allyl chloride or the solvent control. Both positive controls gave evidence of increased UDS.
Test substance: Product diluted in DMSO.
24-JAN-2003 (68)

5.6 Genetic Toxicity 'in vivo'

Type: Cytogenetic assay
Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: inhalation
Exposure period: 1-5 exposure
Doses: 0, 1, 25 ppm

Method: other
Year: 1981
GLP: no

Test substance: other TS: allyl chloride, purity 98 %

Remark: 30 M and 30 F per group.
Rats were exposed 7 h/d in a 1.5 m3 exposure chamber. Either a single exposure or 5 daily exposures with sampling after 6, 24, 48 hours.
Cytogenetic analysis of 50 metaphase cells from bone (femur) marrow was carried out. Positive controls received EMS by gavage in a single dose of 100 or 250 mg/kg/day or for 5 days.

Result: Repeated exposure: There was no evidence of an increase in chromosome aberration rate in either test or positive control animals.
Singl exposure: There was no evidence of an increase in chromosome aberrations in rats exposed to allyl chloride. There were no signs of systemic toxicity attribuable to allyl chloride at either dose level. The positive controls showed an increase in total aberrations in all male groups and in females other than the 48 hour sampling.

24-JAN-2003 (68)

Type: Dominant lethal assay
Species: rat Sex: male
Strain: Sprague-Dawley

Route of admin.: inhalation
Exposure period: 5 d
Doses: 0, 1, 25 ppm

Method: other
Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity = 98 %

Remark: 10 M per group.
Males were exposed for 7 h/d for 5 consecutive days in a 1.5 m3 inhalation chamber. Immediately after cessation of exposure on day 5, males were caged afterwards with two virgin females for a week.
Females were killed 10 days after separation from the males and examined for pregnancy and dominant lethal effects. This mating procedure was repeated with fresh females for 9 consecutive weeks.
Positive controls received 100 mg/kg/d EMS by gavage for 5 consecutive days prior to mating.

Result: There was no signs of systemic toxicity in the allyl chloride treated animals. There were no effects on pregnancy frequency, numbers of corpora lutea graviditatis or implantations or the frequency of early death attributable to allyl chloride.
The positive control did show changes in these parameters.

24-JAN-2003 (68)

Type: Drosophila SLRL test
Species: Drosophila melanogaster Sex: male
Strain: other: 3 day old OrK males
Route of admin.: inhalation
Exposure period: 7 h

Doses: 150 ppm

Method: other
Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity = 98 %

Remark: Exposed males were mated with virgin Muller-5 females at 1, 3 and 8 days after exposure. Mating of brothers and sisters was continued to an F3 generation.
Positive controls received a solution of 0.4 % EMS in sucrose for a 5 hour exposure.
Result: No increased incidence of recessive lethals related to allyl chloride treatment.
Flies exposed to EMS gave 14 % lethals in the F2 generation.
24-JAN-2003 (68)

Type: other: sperm abnormality
Species: mouse Sex: male
Strain: B6C3F1
Route of admin.: inhalation
Exposure period: 7 h/d, 5 d
Doses: 0, 1, 25 ppm

Method: other
Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity = 98 %

Remark: Mice were sacrificed 5 weeks after dosing. Sperm suspension from the cauda epididymis was examined for abnormalities.
Positive controls received 100 mg/kg/d by gavage.
Result: No increase in the frequency of abnormal sperm.
EMS increased the frequency of aberrant sperm with amorphous head and folded tail.
24-JAN-2003 (68)

5.7 Carcinogenicity

Species: mouse Sex: female
Strain: other: Ha: IRC Swiss
Route of administration: dermal
Exposure period: 440,594 d
Frequency of treatment: 3 d/wk
Doses: 31, 94 mg/d
Control Group: yes

Method: other: topical application in acetone
Year: 1979
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: 30 F per group, age 6-8 weeks, 6 per cage
Result: No skin tumours and no increased incidence of other tumours compared to controls were observed following repeated topical

application of allyl chloride.
27-JAN-2003 (95)

Species: mouse Sex: female
Strain: other: Ha: IRC Swiss
Route of administration: dermal
Exposure period: life-span
Frequency of treatment: 3 d/wk
Doses: 94 mg
Control Group: yes, concurrent vehicle

Year: 1979
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Method: A single dose of 94 mg/mouse in acetone followed after 2 weeks by thrice weekly application of 5 ug phorbol myristate acetate (PMA) for life. A PMA control group was included.
Remark: Mice aged 6-8 weeks, 30F/group, 6/cage.
Result: 10 papillomas occured in 7/30 mice initiated with allyl chloride, the first tumour appearing after 197 days, compared to 7 papillomas in 6/90 PMA controls (1st tumour after 449 days).
27-JAN-2003 (95)

Species: rat Sex: male/female
Strain: Osborne-Mendel
Route of administration: gavage
Exposure period: 78 wk
Frequency of treatment: 5 d/wk
Post exposure period: 30-33 wk
Doses: 57, 77 (male) + 55, 73 (female) mg/kg/d
Control Group: yes, concurrent vehicle

Method: other: solution in corn oil
Year: 1978
GLP: no
Test substance: other TS: allyl chloride, purity 98-99%

Remark: - Rats aged 6 weeks individually caged.
- 50M + 50F on test, 20M + 20F vehicle and untreated controls.
- Initial doses : 70, 140 (M) and 55, 110 (F) mg/kg/d.
- Due to toxicity, doses were reduced on 2 separate occasions to give time weighted averages of 57 and 77 mg/kg for males and 55 and 73 mg/kg for females.
Result: Body weight gain reduced in both sexes relative to controls. In high dose males body weight was reduced from week 46 on-wards. Clinical signs were hunched appearance and abdominal urine stains. There was a statistically significant dose related increase in mortality. There was no obvious reason for this increase as neither neoplastic nor non-neoplastic lesions were increased relative to controls. Early mortality at the high dose level precluded meaningful statistical analysis of late developing tumours.
27-JAN-2003 (70)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of administration: gavage
Exposure period: 78 wk
Frequency of treatment: 5 d/wk
Post exposure period: 14 wk
Doses: 172, 199 (male) + 129, 258 (female) mg/kg/d
Control Group: yes, concurrent vehicle

Method: other: solution in corn oil
Year: 1977
GLP: no
Test substance: other TS: allyl chloride, purity 98-99%

Remark: - Mice aged 5 weeks
- 50M + 50F treated, 20M + 20F vehicle and untreated controls.
- Dosing regime and dose levels were adjusted during the study.

Result: Body weight gain was reduced in females only from week 10 at the high dose and week 20 at the low dose. The only clinical signs attributable to allyl chloride were loss of equilibrium and abdominal distention in high dose males surviving beyond 48 weeks. There was a statistically significant dose related increase in mortality. In males the high early mortality at the top dose level precluded meaningful statistical analysis of late developing tumours. The reason for this increased mortality is not obvious from the data given.
It was not attributed to tumour development and the only non-neoplastic, exposure related, changes were acanthosis and hyperkeratosis of the forestomach of both sexes at both dose levels. Treatment related tumours were squamous cell carcinomas and papillomas of the forestomach of both sexes. The incidence was not statistically significant in either sex when compared with concurrent controls but was higher than in historical controls. An increased incidence of hepatocellular carcinomas in low dose males (17% compared to 10% in vehicle controls and 2% in high dose males) was not in excess of the incidence occasionally seen in control groups.

27-JAN-2003 (99)

Species: mouse Sex: male/female
Strain: Strain A
Route of administration: i.p.
Exposure period: 8 wk
Frequency of treatment: 3 d/wk
Post exposure period: 16 wk
Doses: 50, 122, 245 mg/kg
Control Group: yes

Method: other: application in tricaprylin (mice killed at 24 wk)
Year: 1979
GLP: no
Test substance: other TS: allyl chloride, technical grade

Remark: Mice aged 6-8 weeks, 10M + 10F/group.
Animals killed after 24 weeks.
Result: The incidence of lung adenomas in the highest dose group increased from 0.19 in the controls to 0.6 which was significant using one of two tests applied to the data.
24-JAN-2003 (91)

Species: mouse Sex: female
Strain: other: Ha: IRC Swiss
Route of administration: s.c.
Exposure period: 549 d
Frequency of treatment: 1d/w
Doses: 1.5 mg
Control Group: no data specified

Method: other: application in trioctanoin
Year: 1979
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Mice aged 6-8 weeks, 30F/group, 6/cage.
Result: 1 local sarcoma developed.
24-JAN-2003 (95)

5.8.1 Toxicity to Fertility

Type: Fertility
Species: rat
Sex: male
Strain: other: white
Route of administration: inhalation
Exposure Period: 4 h
Frequency of treatment: 1 day
Duration of test: 24 h
Doses: 10.2, 58, 104, 294 mg/m3 (3.2, 18.2, 32.6, 92.3 ppm)
Control Group: yes

Method: other: acute study by inhalation with a dynamic method in 800 l chambers
Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Rats 10-15M/group.
Investigated 24 h. after exposure, the gonads were assessed histologically and sperm motility tests were carried out.
General toxicity was also observed.
Result: Decreased sperm motility time from 18.2 ppm. General toxic signs from 32.6 ppm (see also 5.4-3 and 5.10-6).
No morphological significant differences.
27-JAN-2003 (43)

Type: Fertility
Species: rat

Sex: male
Strain: other: white
Route of administration: inhalation
Exposure Period: 2.5 mo
Frequency of treatment: 4 h/d, 5 d/wk
Duration of test: 48-75d
Doses: 0.29, 1.06, 3.1 mg/m3 (0.1, 0.3, 1 ppm)
Control Group: yes

Method: other: subacute study by inhalation with the dynamic method in 800 l chambers
Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Rats 10-15M/group.
Investigated on the 48th and 75th day of exposure, the gonads were assessed histologically and sperm motility tests were carried out.
General toxicity was also observed.
Result: Signs of general toxicity were seen at the two highest dose levels, no signs of toxicity were seen at the lowest dose level. See also 5.4-3 and 5.10-6.

Sperm motility time was decreased and the testicular weight was increased at all dose levels, in addition the spermatogenic index was decreased at the highest two dose levels only.

27-JAN-2003 (43)

Type: Fertility
Species: rat
Sex: male

Strain: other: white
Route of administration: inhalation
Exposure Period: 4 mo
Frequency of treatment: 4 h/d, 5 d/wk
Duration of test: 4 mo
Doses: 0.29, 1.06, 3.1 mg/m3 (0.1, 0.3, 1 ppm)
Control Group: yes

Method: other: dynamic method in 800 l chambers
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Rats 12-15M/group.
The gonads were assessed histologically and sperm motility were carried out.
Result: There was no evidence of general toxicity at the lowest dose level and at this level the only effect on the male gonad was a reduction in sperm motility time.
At the two highest dose levels a number of parameters were

affected, sperm motility time was decreased as was the average number of normal spermatogonia and the number of tubules with desquamated spermatogenic epithelium. In addition at the top level, the testicular weight and spermatogenic index were reduced.

27-JAN-2003 (44)

5.8.2 Developmental Toxicity/Teratogenicity

Species:	rat	Sex: female
Strain:	Sprague-Dawley	
Route of administration:	inhalation	
Exposure period:	day 6 to 15 of gestation	
Frequency of treatment:	7 hours/day	
Duration of test:	until day 21	
Doses:	0, 30, 300 ppm	
Control Group:	yes	
NOAEL Maternal Toxity:	= 30 ppm	
NOAEL Teratogenicity:	= 30 ppm	

Method: other
Year: 1983
GLP: no
Test substance: other TS: allyl chloride, purity 98.6 %

Remark: controls 39F; treated 25F per group; caged singly between exposures
Result: Maternal weight gain reduced on first two days of exposure. Maternal liver weigths increased at both dose levels, kidney

weights increased only at 300 ppm.
At 300 ppm there was some evidence of an exposure related effect on the foetus with delayed ossification of vertebral centra and sternebrae. These are considered to be minor effects in this species which has a high background incidence of these anomalies. There were no significant adverse effects at 30 ppm.

27-JAN-2003 (54)

Species:	rat	Sex: female
Strain:	other: white	
Route of administration:	inhalation	
Exposure period:	through pregnancy	
Frequency of treatment:	4 hours/day	
Duration of test:	gestation lenght	
Doses:	0, 0.29, 3.1 mg/m3 (0, 0.1, 1 ppm)	
Control Group:	yes	
NOAEL Maternal Toxity:	= .1 ppm	

Method: other
Year: 1982
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: 34 pregnant F intotal were used
Result: At the higher dose level there was a non-significant reduction of live embryos/litter and a significant increase in resorption sites.

Foetal weight was also reduced. The increase in total embryo mortality was ascribed ot increased post-implantation loss but there was also a significant increase in pre-implantational loss. There was evidence of maternal toxicity at this dose level.

27-JAN-2003 (10)

Species: rabbit Sex: female
Strain: New Zealand white
Route of administration: inhalation
Exposure period: day 6 to 18 of gestation
Frequency of treatment: 7 hours/day
Duration of test: 29 days
Doses: 0, 30, 300 ppm
Control Group: yes
NOAEL Maternal Toxity: < 300 ppm
NOAEL Teratogenicity: = 300 ppm

Method: other
Year: 1983
GLP: no
Test substance: other TS: allyl chloride, purity 98.6 %

Remark: controls 25 F; treated 20 F per group; caged singly between exposures
Result: Maternal body weights were depressed from days 6 to 9 of gestation at 300 ppm. Liver weights and liver/bodyweight ratios were reduced at 300 ppm. There were 3 non-treatment related maternal deaths. Litter parameters were unaffected by

treatment other than an increased incidence of resorptiona at 300 ppm. However, this incidence was within historical control limits. There are no statistically significant increases in foetal anomalies.

27-JAN-2003 (54)

Species: mouse Sex: female
Strain: CD-1
Route of administration: gavage
Exposure period: day 6-13 of gestation
Frequency of treatment: once a day
Doses: 500 mg/kg/d
Control Group: yes, concurrent vehicle
NOAEL Maternal Toxity: < 500 mg/kg bw
NOAEL Teratogenicity: = 500 mg/kg bw

Method: Chernoff-Kavlok teratogenicity screening test
Year: 1987
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: Administered by gavage in corn oil at a volume of 10 ml/kg. The dose administered was the LD10 determined in range finding studies.
Result: There was 50 % mortality among the allyl chloride treated mice. There was a differential mortality between pregnant and non-pregnant animals with 21/28 pregnant and 4/22 non-pregnant

mice dying. 5/7 litters were viable. None of the litter variables was significantly different from controls. The percentage survival of newborn was reduced. 80% compared to 97.1% for controls but the standard deviation on the mean was

large (80% +/- 44.7) and the difference therefore not statistically significant. The number of liveborn/litter, birth weight and weight gain of pups were similar in control and treated groups.
Despite 50% maternal mortality, mostly among pregnant females, there was little evidence to suggest an adverse effect on foetal development. The significance of the results is much diminished by the small numbers of litters available from treated animals.

27-JAN-2003 (48)

Species: rat Sex: female
Strain: Sprague-Dawley
Route of administration: i.p.
Exposure period: day 1 to 15 of gestation
Frequency of treatment: once a day
Duration of test: 21 days
Doses: 0, 80 mg/kg
Control Group: yes
NOAEL Maternal Toxity: < 80 mg/kg bw
NOAEL Teratogenicity: < 80 mg/kg bw

Method: other
Year: 1981
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Remark: 15F per group; caged singly
Result: Increased maternal heart, liver, spleen and kidney weight with no histological changes. Increased fetal resorptions. Increased number of fetuses with oedema and short snout with protruding tongue. No visceral or skeletal malformations.

27-JAN-2003 (47)

5.8.3 Toxicity to Reproduction, Other Studies

-

5.9 Specific Investigations

Endpoint: other: ulcerogenic and adrenocorticolytic activity
Species: rat
Strain: Sprague-Dawley Sex: no data
Route of administration: subcutaneous

Year: 1982
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Method: Minimum of 3-5 rats/group
Dosing 3x daily for 4 or 5 days to give a total dose of 812 mM/kg subcutaneously. This dosage regimen aimed to result in 70-100% mortality.
The effect on the development of duodenal ulcers and

adrenocortical necrosis was determined by histopathological examination. The severity of the lesion was graded and together with the incidence was used to produce an index for relative comparison of ulcerogenic and adrenocorticolytic activity.
Result: weak uncerogenic and moderate adrenocorticolytic activity
27-JAN-2003 (90)

Endpoint: other: effect on lung defenses
Species: mouse
Strain: CD-1 Sex: no data
Route of administration: inhalation
Exposure Period: 3 hour(s)
Frequency of treatment: 5 x 3 hours
Doses: 0, 1 ppm
Control Group: yes

Year: 1986
GLP: no
Test substance: other TS: allyl chloride, purity not specified

Method: Mice aged 6-7 weeks
0 or 1 ppm allyl chlorde for a single 3 hour or multiple (5 x 3 hour) inhalation exposures. The effect on host lung defenses was evaluated by measuring the susceptibility (by increased mortality) to experimentally induced streptococcus aerosol infection and pulmonary bactericidal activity to inhaled Klebsiella pneumoniae.
Result: Increased susceptibility to streptococcal pneumonial infection was seen only after 5 daily 3 hour exposures, there being a 9% increase in mortality in the mice exposed to 1 ppm allyl chloride. Pulmonary bactericidl activity was increased

following both single and repeated exposure.
27-JAN-2003 (13)

5.10 Exposure Experience

Type of experience: other: Clinical observations

Remark: Irritating effect :

The most frequent observation following over-exposure to allyl chloride vapours is of eye irritation often with orbital pain which is usually delayed in onset by 2-6 hours.
Nose, throat and respiratory irritation have also been reported and sneezing and epistaxis have been observed.
Skin contact, particularly where the liquid is allowed to remain in contact with the skin, may result in chemical burns.
An associated deep-seated pain beneath the exposure site described as "bone-ache" has been reported following exposure to very small quantities (amount not specified) of allyl chloride.
24-JAN-2003 (12) (75) (84) (94)

Type of experience: other: Occupational exposure

Remark: Exposed group : 17 female workers; average age 42.
Concentration/dose : Air concentration described as high (actual concentration not given).
Period of exposure : 1970 - 1977

Observations:
All diagnosed as exhibiting toxic polyneuropathy due to allyl chloride over-exposure.
Symptoms: On initial exposure lacrimation and sneezing with symptoms gradually diminishing. Symptoms of polyneuropathy developed after 4 months to 5 years exposure. Major symptoms were weakness, tingling and numbness in the upper and lower extremities with cramping discomfort rather than pain together with coldness. Insomnia, dizziness and loss of appetite were rare. Neurological abnormalities were roughly symmetrical distal, sensory and motor disorders. Sensory deficits were more marked inthe distal part of the extremities. Muscle weakness was mild. Electromyographic (EMG) abnormalities consisting of fibrillation or positive sharp waves occurred in 8/13 cases with slowing of motor nerve conduction velocity (MCV) in tibial and peroneal nerves in 7. Of these, 5 showed prolonged motor distal latencies. Physical examination of heart, lungs, liver and spleen were normal as were liver function tests and other routine haematological and clinical chemical tests.
After 2-4 months treatment (including vitamin B supplements and traditional Chinese remedies) steady improvement was obtained. Recovery of sensory, reflex and EMG normality was not noted until the 9-11th month of treatment. 5 cases relapsed on return to the workshop following recovery.

Conclusion: Following excessive vapour exposure a number of workers were diagnosed as exhibiting toxic polyneuropathy. This improved slowly (over several months) following removal from exposure.

24-JAN-2003 (49)

Type of experience: other: Occupational exposure

Remark: .
Factory B

Exposed group : 27 workers (14 M, 13 F).

Exposure level : 0.2 to 25.13 mg/m3 (0.7-89 ppm).
Duration : 1 to 4.5 years.

Observations :
Symptoms were similar to those described above for Factory A but milder and without eye and upper respiratory tract irritation.
The cramping pain was reduced and few abnormal neurological signs were found. EMG investigation revealed an increase in

polyphasic potentials and increased duration of motor unit potentials without any denervation potentials in 13/27 workers examined. The degree of peripheral neuropathy was much less in this group of workers. No other changes attributable to allyl chloride exposure were found on physical, haematological or routine clinical chemical examination.
Factory A

Exposed group : 26 female workers.

Exposure level : 2.6 to 6650 mg/m3 (0.82-2088 ppm).
Mean concentration : 2966 mg/m3 (931 ppm).
Duration : 2.5 months to 6 years.
Observations :
Initial complaints of lacrymation and sneezing in all workers gradually diminishing. Most workers developed numbness, tingling, cramping pains and weakness in the distal part of the extremities. Shortest latent period 2 months.
2/3rds of thegroup showed symmetrical distal sensory deficits and there was decreased muscular strength in 57% of these. Ankle reflexes reduced in 42.3%. No muscular atrophy. EMG abnormalities of the type described above were observed in 10/19 subjects examined. Insomnia, dizziness and anorexia were rare.
Treatment and recovery as above (He et al, 1980), but in severe cases ankle relex loss and EMG abnormalities remained for years. No other changes attributable to allyl chloride exposure were found on physical, haematological or routine clinical chemical examination. The affected workers were diagnosed as exhibiting toxic polyneuropathy due to

allyl chloride overexposure.

Conclusion: The incidence of polyneuropathy in workers exposed to allyl chloride vapours was found to be dose related. The symptoms were persistent, some lasting for years in severe cases.

28-JAN-2003 (50) (51)

Type of experience: other: Occupational exposure

Remark: Exposed group : 60 manufacturing workers of which 15 F.
Concentration/dose : 1-113 ppm for 16 months

Observations:
Liver function was investigated and changes indicative of some impairment of liver function were observed. On cessation of exposure, those liver function parameters measured, rapidly returned to normal. The only other observation was of a smell of garlic emanating from the body and breath of exposed workers.

Conclusion :
Evidence is presented of reversible liver damage in workers occupationally exposed to allyl chloride vapours.

28-JAN-2003 (46)

Type of experience: other: Occupational exposure

Remark: Exposed group : 155 workers, 66.5 % males. Age range 20-45.
Concentration/dose : 6.4-140 mg/m3 (2-44 ppm).
Exposure periods: 1-5 years and > 5 years.

Observations:
Symptoms reported were headache, giddiness, darkness of vision, weakness, tiredness, irritability, poor sleep, cramps and tingling in the extremities, pain inthe heart region and palpitations, sweating and intolerance of manufacturing odours. These symptoms were more frequent with increasing length of exposure. Objective signs included finger tremor, stimulation of the periosteal and tendinous reflexes, unsteadiness in the Romberg test, skin hypothermia, cyanosis, capillary spasm and persistent dermography.
Also observed were increased urinary excretion of nor-adrenaline, increased blood acetylcholine with a decrease in true cholinesterase activity.

Conclusion :
Signs of intoxication reported are indicative of an adverse effect on the nervous system.

28-JAN-2003 (62)

Type of experience: other: Clinical symptoms

Remark: A literature search for the period 1976-1980 revealed a number of additional Russian papers describing various other
effects in exposed workers.
The types of disturbances described were cardiovascular,

respiratory, CNS, ocular, cerebral blood flow and thermoregulatory.
The papers were published in local journals.

28-JAN-2003 (6) (7) (8) (14) (58) (59) (60) (61)

Type of experience: other: Volunteer study

Remark: Exposed group : 13, sex unspecified.
Concentration/dose : 3 ppm for 1-3 minutes;
Observations: 10/13 reported a definite odour but no irritation.
Conclusion : An allyl chloride concentration of 3 ppm while detectable by odour was not irritant.

28-JAN-2003 (93)

Type of experience: other: Volunteer study

Remark: Exposed group : group size and sex unspecified.
Concentration/dose : 3-6 ppm, 25 ppm and 50-100 ppm

Observations :
3-6 ppm : Half the group detected the odour at this

level.

25 ppm : Odour threshold for the majority.
Nose irritation and pulmonary discomfort may be observed at lower levels.

50-100 ppm : Eye irritation.

Conclusion :
Some individuals detected the odour at 3-6 ppm, at 25 ppm there was nose irritation and pulmonary discomfort. Eye irritation was observed between 50 and 100 ppm.

28-JAN-2003 (84)

Type of experience: other: Volunteer study

Remark: Exposed group : group size and sex unspecified
Concentration/dose : 0.21 ppm and 0.5 ppm
Observations : 0.21 ppm : 50 % response to odour.
0.50 ppm : 100 % response to odour.

Conclusion : The odour was detectable by all individuals exposed to 0.5 ppm.

28-JAN-2003 (94)

Type of experience: Human - Epidemiology

Remark: Exposed group : 100 workers, 40 F, 60 M. All complaining of a bitter taste, dyspepsia and heaviness in the right thoracic and sub-costal area. An age matched Control group was included.

Concentration/dose : Exposure levels not given. Exposure periods 1-5 and 5-20 years.

Observations:

Liver function was evaluated using a number of tests. Increases were observed in levels of GPT, GOT, cholesterol, betalipoproteins. Bilirubinaemia, hypoalbumenia and hypergammaglubulinaemia were observed. Decreases were also noted in concentrations of bilirubin, cholesterol, and bile acids in the gall-bladder bile. These changes increased with length of service.

Conclusion :
Dose related changes in clinical chemical parameters indicative of liver damage were observed in workers exposed to allyl chloride vapours.

28-JAN-2003 (5)

Type of experience: Human - Epidemiology

Remark: Exposed group : Group of 120 workers. Control group 30. Age range 25-48.
Concentration/dose : Exposure concentrations were frequently
in excess of the MAC (1-3 mg/m3).

Exposure period 5-8 years.

Observations:
Renal function was assessed by a number of techniques. In exposed workers urea and creatinine clearance showed a 12% increase compared to controls. Chloride levels in the blood were up 26% while sodium and potassium were up 12%.

Conclusion :
Evidence of kidney damage attributable to occupational exposure to allyl chloride is reported.

28-JAN-2003 (9)

Type of experience: Human - Epidemiology

Remark: Exposed group :
44 men engaged in the production of various chlorinated hydrocarbons including epichlorhydrin (ECH) and allyl chloride.
6 different control groups were examined from 1976-1981 they were age and sex matched and matched for smoking habits. They comprised groups of non-exposed plant workers and administrative staff both on and off site.

Concentration/dose :
Exposure was for between 1 and 21 years. Allyl chloride exposure for 1978 averaged 4 mg/m3 (< 0.1-54) and ECH levels for 1977 averaged 6 mg/m3 (< 0.1-11) and for 1978 1 mg/m3 (< 0.1-3). Blood samples were collected for cytogenetic analysis of lymphocytes.

Observations:
When compared to the concurrent control group (other plant workers sampled in 1978), there was a atatistically significant increase in the frequencies of chromosome gaps, breaks and total aberrations. However when compared to a control group of manufacturing workers sampled in 1976-1977

there was no statistically significant differences. The incidence of chromosome aberrations in the concurrent control group was extremely low. There was a marked variability in the frequency of aberrant cells in control populations between 1976 and 1980. The difference in frequency of chromosome aberrations was not considered of biological significance.

Conclusion :
Occupational exposure to allyl chloride in combination with other chlorinated hydrocarbons did not result in a biologically significant increase in chromosome aberrations in human lymphocytes.

28-JAN-2003 (29)

Type of experience: Human - Epidemiology

Remark: Exposed group :
64 men (average age 40-63 years) working in the production of chlorinated 3-carbon compounds. Control group : 63 men

who had not worked in the production of industrial chemicals for at least 5 years. The groups were age matched. Alcohol consumption and smoking habits were taken into consideration. Only 64 % of the exposed population volunteered to participate in the study.

Concentration/dose :
Exposure levels (8 hr TWA) for the last 5 years were <= 1 ppm for allyl chloride, epichlorohydrin and 1,3-dichloropropene.
Within the overall group, 3 exposure subgroups were considered :

1. Allyl chloride with epichlorohydrin (ECH)
2. " with 1,3-dichloropropene (DCP), or
3. " with ECH + DCP.

Various indicators of fertility were investigated such as reproductive history, sperms counts and motility and levels of testosterone, FSH and LH.
In addition to investigating overall effects, the 3 different exposure groups were also investigated and the effect of duration of exposure (> 5 years or <= 5 years)

and
strength of exposure (actual levels not given) was assessed.
Observations:
Overall the results indicate that there was no detrimental effect on fertility attributable to exposure to 3-carbon chlorinated hydrocarbons. In subgroup 3 (10 individuals) there was a lower sperm count although the difference was not significant. Further examination of this group which contained 5 distribution workers and 5 glycerine workers revealed a statistically significant reduction in sperm count in the distribution workers. However, 4 of these workers were classified as low exposure workers, so that no real conclusion could be drawn. The actual values are given below.

.	Sperm count (MM/cc)	% normal forms	Group size
Group 1 mean	143.31	80.78	9
. (SD)	(109.24)	(11.54)	
Group 2 mean	126.36	74.92	25
. (SD)	(100.07)	(9.79)	
Group 3 mean	74.35	77.90	10
. (SD)	(71.41)	(13.16)	
Distribution Group mean + (SD)	31.60 (17.98)	Not given	5
Combined exposed mean + (SD)	134.24 (118.60)	76.94 (10.53)	64
Control mean	113.53	75.78	63
. (SD)	(95.64)	(11.15)	

Conclusion :
No adverse effects on male fertility could be attributed to

exposure to allyl chloride in combination with other 3-carbon chlorinated hydrocarbons.

28-JAN-2003 (96)

Type of experience: Human - Epidemiology

Remark: Olsen et al (1994) described an epidemiology study of 1064 male workers who had a minimum of 1 month work experience between 1957 and 1986 in the production or use of epichlorohydrin and allyl chloride. Vital status follow-up occurred through 1989. There were no significantly elevated SMRs for all malignant neoplasms, lung cancer, circulatory system disease or artheriosclerotic heart disease when compared to external or internal control populations. There were no apparent mortality trends with cumulative exposure analyses of potential epichlorohydrin exposure with and without allyl chloride exposure.

The study results are limited by the cohort's size, duration of follow-up, few numbers of observed and expected

deaths and the level of potential epichlorohydrin exposure experience.
Only abstract available, Exposure is not estimated quantitatively.

28-JAN-2003 (76)

Type of experience: Human - Epidemiology

Remark: An assessment has been made of biochemical alterations in kidney and liver functions of 73 male operators employed for an average of 8.2 yr (0.5 - 23 yr) in the organochlorine plant of Shell Pernis producing several chlorinated hydrocarbons, among which allylchloride. Exposure to allylchloride has regularly been determined by personal air monitoring since 1980. During 1980-1991 arithmetic mean allylchloride concentrations for normal operations ranged from 0.2 to 2.89 mg/m3. These sometimes relatively high exposures occasionally exceed the current

MAC of 3 mg/m3. It was concluded that mean exposures to allylchloride may still occur during maintenance and shut down activities (see table below). The results of the tests were compared with a control group of 35 men employed at the materials division and not occupationally exposed to chemicals.
Personal air sampling: allyl chloride (mg/m3)

Period	No	n	GM	GSD	AM	(95% CI)
May 1980	11	56	1.91	2.51	2.89	(2.25-3.70)
Aug 1980	13	45	0.25	3.32	0.50	(0.35-0.72)
Oct 1980	6	88	0.11	3.13	0.21	(0.16-0.27)
Feb 1981	5	14	2.11	2.21	2.81	(1.75-4.52)
Jun 1981	7	20	0.56	2.04	0.71	(0.50-1.00)
Sep 1981	9	28	0.23	2.17	0.31	(0.23-0.42)
Dec 1981	5	19	0.16	5.31	0.56	(0.24-1.27)
Mar 1982	8	32	0.99	3.16	1.86	(1.22-2.83)

Jan 1982	-	15	1.24	3.32	2.37	(1.19-4.71)
Sep 1982	7	20	0.77	3.94	1.82	(0.94-3.51)
Dec 1982	5	14	0.29	1.24	0.30	(0.26-0.34)
Mar 1983	18	18	0.28	2.13	0.37	(0.25-0.54)
Mar 1984	14	14	0.81	4.22	2.01	(0.85-4.76)
Aug 1987	44	44	0.37	4.66	1.14	(0.71-1.84)
Apr 1990	2	8	2.04	2.05	2.54	(1.34-4.81)
Apr 1991*	11	45	0.46	3.27	0.91	(0.63-1.30)

Period	P95	x(%)	Plant status
May 1980	8.68	31.2	Normal operation
Aug 1980	1.80	1.92	Normal operation
Oct 1980	0.72	0.19	Normal operation
Feb 1981	7.78	32.9	Normal operation
Jun 1981	1.81	0.93	Normal operation
Sep 1981	0.82	0.05	Normal operation
Dec 1981	2.49	3.96	Normal operation
Mar 1982	6.57	16.8	Normal operation
Jan 1982	8.93	23.1	Maintenance
Sep 1982	7.35	16.1	Normal operation
Dec 1982	0.41	<0.01	Normal operation
Mar 1983	0.97	0.09	Normal operation
Mar 1984	8.65	18.2	Maintenance
Aug 1987	4.65	8.69	Normal operation
Apr 1990	6.62	29.4	Shut down
Apr 1991*	3.24	5.72	Shut down

No = numbers of workers monitored
n = number of air measurements
GM (GSD) = geometric mean and standard deviation (log normal distribution)
AM = arithmetic mean
95% CI = 95% confidence interval of AM
x = compliance probability (probability that MAC value will be exceeded)
* Respiratory protective devices were worn; values reflect breathing zone air concentrations

Result: No differences in liver function parameters between the exposed group and a control group were found. Renal function tests were comparable in both groups, except for a significantly higher urinary albumin concentration in the exposed group for which no exposure duration relationship could be found.

28-JAN-2003 (17)

5.11 Additional Remarks

Type: Biochemical or cellular interactions

Remark: Method : no data
GLP: no.
Results : At the highest dose level a single exposure resulted in increased serum cholinesterase, increased respiration rate and a reduction in the so-called "cumulative threshold index"

(CTI) indicative of CNS effects.
Red and white cell counts, urinalysis, body weight and behavioural indices were unaffected.
At 0.1 mg/l the only parameter showing change was serum cholinesterase which was increased.
No deaths were reported.
Species : Rat.
Route : inhalation.
Substance : no data.
0.006, 0.1, 0.29 mg/l (2, 31, 92 ppm).
Exposure period : 4 h.

28-JAN-2003 (45)

Type: Neurotoxicity

Method: The effect of allyl chloride on peripheral nerve fibres and motor end places in the rat has been published by a group of Chines workers in a number of papers. Abstracts only were available, the papers not having been translated. The route of exposure was not reported in the abstract.

Result: It appears that allyl chloride decreases first the numbers of neurofilaments in myelinated nerve fibres and then the microtubules. There was slight mitochondrial degeneration but no degeneration of the myelinsheath.
In motor endplates there was again mitochondrial degeneration and a decrease in synaptic vesicles. Motor endplates of type II muscles were more affected, with wrinkled postsynaptic membrane.
Histochemical examination of the nerve fibres revealed a slight decrease in ATP-ase activity and a significant decrease in cholinesterase.
Histochemical examination of the spinal cord revealed a reduction of cholinesterase activity in the cytoplasm of the neurocytes, particularly in the lumbar region.
The results suggest that allyl chloride directly affects peripheral nerve fibres, causing degeneration of microtubules and neurofilaments with impairment of communication with the neurocyte which in turn affects cholinesterase synthesis.

30-MAY-1994 (89)

Type: Toxicokinetics

Remark: Species : Rat CFE; 137 M, housed individually in metabolism cages.
Route : s.c.
Dose : 1 ml of 10% solution in arachid oil.
Method : urine and bile collected for 24 hours.
GLP : no.

Result: Allyl mercapturic acid, its sulfoxide and 3-hydroxypropyl mercapturic acid detected in urine. S-Allyl glutathione and S-allyl-cysteine detected in the bile.

Test substance: Redistilled allyl chloride

23-FEB-1994 (63)

Type: Toxicokinetics

Method: Species : Rat Fisher 344, 6M + 6F.
Females with in-dwelling cannulae, housed in Roth metabolism cages.
2 males with bile duct cannulae.
Route : oral.
Dose : 1, 100 mg/kg.
Method : Urine, faeces and expired air collected for up to 48 hours. Bile samples were taken from callulated M. Blood was collected from F up to 48 h.
GLP : no

Result: Radioactivity was mainly excreted in urine and expired air. Radioactivity in the air was eliminated either as (C14)-CO2 or (C14)-allyl chloride, the amount of the latter dependant on dose, increasing from 1.5% at 1 mg/kg to 18.1% at 100 mg/kg. After the 1 mg/kg dose, 22.7% of the dose was excreted in the urine in the first 8 hours after administration. After 100 mg/kg, 14.6 % of the dose was excreted in the urine in the 0 - 8 hours interval and 19.0% in the 8 - 16 hours interval. Peak blood levels were achieved after 1 hour following 1 mg/kg and 4 hours after 100 mg/kg. An enterohepatic circulation has been demonstrated by the difference in radioactivity in the bile (12 %) and faeces (less than 5 %). No unchanged allyl chloride was excreted in the urine.

Test substance: C14-1,3-allyl chloride in corn oil.
Composition : Allyl chloride : 72 +/- 12%
Diethyl ether : 15 +/- 3%

Conclusion: The radioactivity assocuated with orally administered 14C-labelled allyl chloride was mainly excreted in expired air and urine. There was evidence of enterohepatic circulation. Unchanged allyl chloride is excreted in a dose-dependant manner in expired air. Unchanged allyl chloride is not excreted in the urine.

28-JAN-2003 (97)

Type: Toxicokinetics

Method: Species : rat Fischer 344; male rats fitted with in-dwelling jugular cannulae.

Route : oral.
Dose : 100 mg/kg.
Method : Urine and blood collected for 48 hours.
GLP : no.

Result: Bimodal absorption curve. No unchanged allyl chloride detected in the urine.
t 1/2 = 2.58 h.
Total clearance time about 13 h.

Test substance: Allyl chloride: purity : 97.7%.

23-FEB-1994 (97)

Type: Toxicokinetics

Method: Species : Rat Fischer 344; male rats fitted with in-dwelling jugular cannulae.

Route : i.v.
Dose: 100 mg/kg.
Method : Single dose; blood samples taken up to 180 min.
GLP : no.
Result: t 1/2 = 23.5 min.
Blood levels minimal after 150 min.
Test substance: Allyl chloride: purity : 97.7%.

17-FEB-1994 (97)

Type: Toxicokinetics

Method: Species : Rat Fischer 344, male rats fitted with in-dwelling jugular cannulae.
Route : inhalation.
Substance : 10, 100, 1000, 2000 ppm.
Duration : Exposure : 6h (head only exposure).
Post exposure : 12 h.
Method : Head only exposure.
Blood samples were taken from 10 min. for up to 12 h. post exposure.
GLP : no.
Remark: There was no linear dose response relationship for blood levels of allyl chloride.
Non-protein sulphydryl levels were reduced in the liver, lung and kidneys at 1000 and 2000 ppm, and in the blood at 2000 ppm.
Histopathological changes in the liver and kidneys at 1000 and 2000 ppm (kidney: degenerative epithelial changes in proximal convoluted tubules; liver: marked decrease in hepatic glycogen, as a result eosinophilic hepatocytes).
t 1/2 <= 30 min at 10, 100 ppm.
Test substance: Allyl chloride: purity : 97.7%.

28-JAN-2003 (97)

Type: other: Alkylation

Remark: Alkylating properties of allyl chloride were demonstrated using the non-biological NBP test and were found to correlate with observed bacterial mutagenicity.

In-vitro binding of allyl chloride to DNA from salmon sperm has been demonstrated, but was found to be weak.

27-JAN-2003 (37) (40)

Type: other: in-vitro effects on male gonads

Method: Foetal rat testes maintained in culture with hCG stimulation were exposed to 1 or 2 mM of allyl chloride (purity not specified) for 24 hours.
Result: Testosterone production was not different from that observed in controls.

27-JAN-2003 (98)

Type: other: metabolism and genotoxicity

Remark: Work has been carried out on the role of biotransformation on the genotoxicity of allyl chloride, using the Salmonella /mammalian microsome assay as an indicator and various enzyme inhibitors to delineate different metabolic pathways. Allyl chloride possesses both direct and indirect metabolic activity. The indirect activity increases with the lenght of the incubation period. It appears that this indirect mutagenicity is mediated by acrolein, as the use of aldehyde dehydrogenase blocker increased mutagenic activity, while microsomal oxidase and epoxide hydrolase inhibitors had no effect, suggesting that an intermediate epoxide is not important. In addition, no metabolites formed via epoxides have yet been identified but S-carboxyethyl mercapturic acid as the main metabolite of acrolein has been found, demonstrating that acrolein is an intermediate of the metabolism of allylchloride.
The addition of glutathione to the test system always leads to a decrease in mutagenic activity lending additional support to the hypothesis that acrolein may be the active genotoxic intermediate.

27-JAN-2003 (38) (39) (40) (71)

6.1 Analytical Methods

6.2 Detection and Identification

-

7.1 Function

7.2 Effects on Organisms to be Controlled

7.3 Organisms to be Protected

7.4 User

7.5 Resistance

8.1 Methods Handling and Storing
-

8.2 Fire Guidance
-

8.3 Emergency Measures
-

8.4 Possib. of Rendering Subst. Harmless

8.5 Waste Management
-

8.6 Side-effects Detection
-

8.7 Substance Registered as Dangerous for Ground Water
-

8.8 Reactivity Towards Container Material
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