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.