Euro Chlor Risk Assessment for the Marine Environment
OSPARCOM Region - North Sea

Vinyl Chloride

February 1999

Euro Chlor
representing the chlor-alkali industry

EURO CHLOR RISK ASSESSMENT FOR THE MARINE ENVIRONMENT

VINYL CHLORIDE

OSPARCOM Region - North Sea

EXECUTIVE SUMMARY

Euro Chlor has voluntarily agreed to carry out risk assessment of 25 chemicals related to the chlorine industry, specifically for the marine environment and according to the methodology laid down in the EU risk assessment Regulation (1488/94) and the Guidance Documents of the EU Existing Substances Regulation (793/93).
The study consists of the collection and evaluation of data on effects and environmental concentrations. Basically, the effect data are derived from laboratory toxicity tests and exposure data from analytical monitoring programmes. Finally the risk is indicated by comparing the “predicted environmental concentrations” (PEC) with the “predicted no effect concentrations” (PNEC), expressed as a hazard quotient for the marine aquatic environment.
To determine the PNEC value, three different trophic levels are considered: aquatic plants, invertebrates and fishes.

In the case of vinyl chloride, 6 data for fish, 3 data for invertebrates and 1 data for algae have been evaluated according to the quality criteria recommended by the European authorities. Only acute toxicity studies were available and an appropriate assessment factor has been used to define a final PNEC value of 210 µg/l.

The available monitoring data for vinyl chloride apply to river and estuary waters and were used to calculate PECs. The most recent data 1990-1993 support a typical PEC of < 0.008 µg/l and a worst case PEC of 0.15 µg/l. The calculated PEC/PNEC ratios give a safety margin of 500 to 250,000 between the predicted no effect concentration and the exposure concentration. Dilution within the sea would of course increase these safety margins.

Moreover, as the available data on persistence of vinyl chloride indicate a half-life in water of a few hours or days and as the bioaccumulation in marine organisms can be considered as negligible, it can be concluded that the present use of vinyl chloride does not represent a risk to the aquatic environment.

1. INTRODUCTION : PRINCIPLES AND PURPOSES OF EURO CHLOR RISK ASSESSMENT

Within the EU a programme is being carried out to assess the environmental and human health risks for "existing chemicals", which also include chlorinated chemicals. In due course the most important chlorinated chemicals that are presently in the market will be dealt with in this formal programme. In this activity Euro Chlor members are cooperating with member state rapporteurs. These risk assessment activities include human health risks as well as a broad range of environmental scenarios.

Additionally Euro Chlor has voluntarily agreed to carry out limited risk assessments for 25 prioritised chemicals related to the chlorine industry. These compounds are on lists of concern of European Nations participating in the North Sea Conference. The purpose of this activity is to explore if chlorinated chemicals presently pose a risk to the marine environment especially for the North Sea situation. This will indicate the necessity for further refinement of the risk assessments and eventually for additional risk reduction programmes.

These risk assessments are carried out specifically for the marine environment according to principles given in *Appendix 1*. The EU methodology is followed as laid down in the EU risk assessment Regulation (1488/94) and the Guidance Documents of the EU Existing Substances Regulation (793/93).

The exercise consists of the collection and evaluation of data on effects and on environmental concentrations. Basically, the effect data are derived from laboratory toxicity tests and exposure from analytical monitoring programmes.
Where necessary the exposure data are backed up with calculated concentrations based on emission models.

Finally the risk is indicated by comparing the "predicted environmental concentrations" (PEC) with the "predicted no effect concentrations" (PNEC), expressed as a hazard quotient for the marine aquatic environment.

2. DATA SOURCES

The data used in this risk assessment activity are primarily derived from the data given in the HEDSET (updated version of June 1995) for this compound. Where necessary additional sources have been used. The references of the HEDSET and additional sources will be given in chapter 10.

3. COMPOUND IDENTIFICATION

3.1 Description

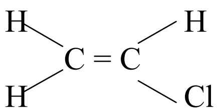
CAS number	:	75-01-4
EINECS number	:	200-831-0
EEC number	:	602-023-00-7
IUPAC name	:	chloroethene

Vinyl chloride is also known as chloroethylene and is commonly abbreviated to VC Other synonyms which are used include:

- chloroethylene
- monochloroethylene
- VC 1
- VCM

Vinyl chloride has the following formula :

C_2H_3Cl



3.2 EU labelling

According to Annex I of Directive 93/72/EEC (01.09.93 - 19th TPA), vinyl chloride is classified as extremely flammable (F+, R12) and toxic with carcinogenicity, category 1 (T, R45).

Vinyl chloride is not classified as dangerous for the environment.

4. PHYSICO-CHEMICAL PROPERTIES

Table 1 gives the major chemical and physical properties of the compound which were adopted for the purpose of this risk assessment.

Table 1 : Physical and chemical properties of vinyl chloride

Property	**Value**
Molecular weight	62.5
Aspect	gas
Melting point	- 153.8 °C
Boiling point	- 14 °C at 1013 hPa
Decomposition temperature	ca. 450 °C
Density	0.9 at 20 °C
Vapour pressure	3330 hPa at 20 °C
log octanol-water partition coefficient	1.58 at 22 °C (measured)
log Koc	1.75 - 2.1
Water solubility	1.1 g/l at 20 °C
Henry's Law constant	18,750 Pa.m^3/mol at 20 °C

5. COMPARTMENT OF CONCERN BY MACKAY LEVEL I MODEL

The risk assessment presented here focuses on the aquatic marine environment, with special attention for the North Sea conditions where appropriate. Although this risk assessment only focuses on one compartment, it should be borne in mind that all environmental compartments are inter-related.

An indication of the partitioning tendency of a compound can be defined using Mackay level I calculation obtained through the ENVCLASS software distributed by the "Nordic Council of Ministers". This model describes the ultimate distribution of the compound in the environment (Mackay & Patterson 1990 - Pedersen *et al.*, 1994).

The results are valuable particularly in describing the potency of a compound to partition between water, air or sediment. Practically, it is an indicator of the potential compartments of concern.

The results of such a calculation for vinyl chloride are given in Table 2.

Table 2 : Partition of Vinyl Chloride into different environmental compartments according to Mackay level I calculation (Mackay & Patterson, 1990)

Compartment	**%**
Air	99.99
Water	0.01
Soil	< 0.01
Sediment	< 0.01

(See Appendix 2 for details of calculation)

Due to the very low probability of partitioning to sediment, the risk assessment will focus on the water phase.

6. PRODUCTION, USES, EMISSIONS

6.1. Production and uses

Vinyl chloride is used primarily as monomer for the production of polyvinyl chloride (PVC) homopolymer and copolymer resins. In 1996, 22 million metric tonnes of PVC were produced worldwide. PVC represents 99% of the total vinyl chloride applications. 300,000 tonnes are estimated to be used in non PVC applications.

The production of Western Europe is estimated for 1996 to be 5,209 thousand tonnes with an annual growth of 2% compared to 4% in North America and 9.5% in Asia (ECVM, 1998).

The main manufacturing process of VCM is based on ethylene.

The ethylene process includes 3 steps:

- Direct chlorination of ethylene by chlorine to produce ethylene dichloride.
- Oxychlorination of ethylene by oxygen (or air) and hydrogen chloride to produce ethylene dichloride.
- Pyrolysis of ethylene dichloride to produce VCM, and HCl which is recycled in the second step.

Vinyl chloride is produced in Western Europe by 14 companies and 25 plants: in Belgium (3 plants), France (3 plants), Germany (8 plants), Italy (4 plants), Netherlands (1 plant), Norway (1 plant), Spain (2 plants), Sweden (1 plant), United Kingdom (2 plants) (ECVM, 1998).

PVC is used in a great number of user industries:

Building and construction	53%
Packaging	16%
Wire, cable, electrical	9%
Leisure	4%
Transport	3%
Furniture, office equipment	3%
Clothing and footwear	3%
Domestic appliances and	1%
Other uses of less than 1%	8%

(Source ECVM)

6.2. Applicable Regulation - Best Available Technique

The emissions of VCM from the PVC plants using the suspension technique (S.PVC) are governed by several national regulations in Germany (TA Luft), France (Arrêté intégré of March 1993), UK (Process Guidance Note IPR 4/6 under Environment Protection Act, 1990) etc. In all these national regulations, the air emission limit value for suspensions homopolymer is 100 g VCM per tonne of PVC production. Suspension polymerization represents about 86% of the total production of PVC.

The European Council of Vinyl Manufacturers has published in August 1994 a Best Available Technique document for VCM and S.PVC plants. For VCM emissions in the process water, the ECVM BAT gives a maximum of 1 mg/l for the process water of the S.PVC plants (or 5 g/t PVC).
This emission limit value is achieved in most plants in OSPARCOM countries, and a voluntary agreement made by ECVM requests compliance by 1998.

OSPARCOM has published in 1996 a Best Available Technique for the manufacture of VCM and S.PVC. For VCM plants, the BAT indicates for total chlorinated hydrocarbons in the process water – including VCM – a "reported achievable concentration" of 1 mg/l. For the S.PVC plants, a concentration of 1 mg/l VCM in the process water after stripper, and before biological treatment if any, is given by the draft PARCOM decision of December 1997 (see also national regulations), as well as an emission limit value of 80 g/t of S.PVC for emissions to the atmosphere (OSPARCOM/PRAM 98/15/1 Annex 15)

For emulsion-PVC plants (E.PVC) an industry charter based on BAT has been agreed (ECVM, November 1998). The environmental standards for VCM emissions have been fixed as a maximum of 1000 g/t E.PVC in the air and 1 mg/l in water effluent.

6.3. Emissions

The main route by which vinyl chloride enters the environment during manufacturing, processing and usage is the atmosphere. Emissions into air from the use of vinyl chloride can be estimated based on current national regulations and the BAT recommendations as 448 t/y for the S.PVC production in Europe. Emissions of vinyl chloride into water would be about 22 t/y for the S.PVC production.

6.4. Occupational exposure – Toxicity to human

The EU regulation requests a maximum level of 3 ppm VCM in annual average, in all plants handling VCM. It is recognised as a human genotoxic carcinogen.

7. EFFECT ASSESSMENT

As a first approach, this chapter only considers the following three trophic levels: aquatic plants, invertebrates and fish. The effects on other organisms are only discussed when indicated.

The evaluation of the data was conducted according to the quality criteria recommended by the European authorities (Commission Regulation 1488/94/EEC). The evaluation criteria are given in *Appendix 1*.

Documented data from all available sources, including company data and data from the open literature, were collected and incorporated into the HEDSET for vinyl chloride, including their references (updated version of 6/95).

A summary of all data is given in *Appendix 3*. In total 6 data for fish, 3 data for invertebrates and 1 data for algae are given. Respectively 1, 0 and 0 data were considered valid for risk assessment purposes. For the respective taxonomic groups 0, 0 and 0 should be considered with care, and 5, 3 and 1 data respectively were judged as not valid for the risk assessment.

It is necessary to distinguish the acute studies (LC50/EC50) from chronic studies (NOEC/LOEC). In the tables presented in *Appendix 3*, the data are ranked based on class (fish, invertebrates, algae), criterion (acute, chronic), environment (freshwater, saltwater) and validity (1, 2, 3, 4) as required by the EU Risk Assessment process (TGD, 1996).

In the case of vinyl chloride, no data are available on marine species. However, evaluations from other chlorinated ethylenes showed a good correlation between freshwater and saltwater toxicity results. Therefore, data from freshwater organisms are regarded as relevant for a risk assessment for the marine compartment. Quantitative structure-activity relationship (QSAR) data were not considered. Due to its high vapour pressure, vinyl chloride should be tested under closed conditions (preferably with analytical measurements) to avoid losses by volatilization.

The different trophic levels are reviewed below. The reference cited in the Table of *Appendix 3* are given in *Appendix 6*.

7.1 Marine fish

No toxicity studies are reported for marine fish.

7.2 Freshwater fish

Six acute toxicity studies are reported for 5 freshwater fish species. Five studies were considered not valid (or validity was not assignable) for risk assessment purposes. Two with *Leuciscus idus* (Juhnke & Luedemann, 1978) were static exposures, without analysis of the test concentrations and without precautions to prevent volatile loss of the substance; a study with *Esox lucius* (Brown *et al.*, 1977) employed only one concentration, without analysis. However, the results for *Brachydanio rerio* (Groeneveld *et al.*, 1993) are considered valid without restriction. This was a semi-static test in closed vessels with analysis before and after renewal of the solutions. Solutions were prepared by bubbling the vinyl chloride through dilution water. Analyses were in good agreement with the nominal values and showed no significant loss of material from the test vessels. The study was conducted according to GLP.

The 96h LC50 for *Brachydanio rerio* was 210 mg/l (Groeneveld *et al.*, 1993) which is the lowest acute toxicity value for freshwater fish.

No long-term studies are reported for freshwater fish. The acute study (above) with *Brachydanio rerio* (Groeneveld *et al.*, 1993) provided a 96-hour NOEC for mortality of 128 mg/l but this short-term value cannot be used for calculation of a PNEC.

7.3 Marine invertebrates

No toxicity studies are reported for marine invertebrates.

7.4 Freshwater invertebrates

Three acute studies are reported, one for the freshwater protozoan, *Uronema parduczi* (Bringmann & Kuhn, 1980). The test used a non-standard procedure with the only reported result being a toxicity threshold, which is not a valid acute endpoint for this risk assessment. Also, insufficient information was available to validate the test procedure according to the criteria defined in *Appendix 1.*

Another static test with a protozoan, *Tetrahymena pyriformis*, employed an unconventional solvent (dimethyl acetamide) at unacceptably high levels (up to 1%), and was considered invalid (Sauvant *et al*., 1995).

A study with the nematode *Panagrellus redivivus* (Samoiloff *et al*., 1980) was a static test with no description of how the test concentrations were prepared or maintained, and showed no effect on survival at the maximum concentration tested (62.5 mg/l); it was considered invalid. The authors reported a significant (20%) effect on final larval molt at a concentration of 0.0006 mg/l. However, there was no concentration-related response, the reported effect at 62.5 mg/l being similar (27%); therefore, these results were not considered reliable.

No long-term studies are reported for freshwater invertebrates.

7.5 Marine algae

No toxicity studies are reported for marine algae.

7.6 Freshwater algae

Only one study is available for freshwater algae. Insufficient information is available to validate the test procedures, but the non-standard endpoint, toxicity threshold, is not equivalent to an acute EC50 and is not valid for the purposes of risk assessment. However, the result is approximately equivalent to a LOEC and is probably sufficient to indicate that algae are not more sensitive than fish to vinyl chloride.

No valid NOEC values are reported for freshwater algae.

7.7 PNEC for marine environment

There are insufficient data for vinyl chloride to compare the sensitivity of marine and freshwater organisms. However, from an evaluation of the available data for other chlorinated aliphatic compounds, it is reasonable to conclude that the sensitivity of marine and freshwater organisms is quite similar.

A summary of the valid data selected for the derivation of PNEC values at different levels is given in Table 3. This table summarises the PNEC values derived from acute studies. Although only one valid study is available, there is reasonable evidence that other trophic levels are of similar or lower sensitivity and that an assessment factor of 1000 is justified.

<u>The final PNEC which is calculated for this risk assessment of vinyl chloride is 210 µg/l.</u>

Table 3: Summary of ecotoxicity data selected for the PNEC derivation, with the appropriate assessment factors, for vinyl chloride

Data set	Assigned Assessment Factor	Lowest toxicity values
Short-term LC50 – one trophic level (fish)	1000	*Brachydanio rerio*, LC50, 96h = 210 mg/l, Groeneveld *et al* (1993).
	PNEC = 210 μg/l	

7.8 Bioaccumulation

Bioaccumulation of vinyl chloride in aquatic species is unlikely in view of its physical and chemical properties. A measured log P_{ow} of 1.58 indicates a low bioaccumulation potency. The measured BCF ranges from less than 10 for fish (*Leuciscus idus*) to 15-30 for invertebrates and 40 for algae (*Chlorella spec.*) (Freitag *et al.*, 1985; Malle, 1984).

7.9 Persistence in water

As indicated by a high Henry's law constant (18,750 Pa.m^3/mol at 20 °C), vinyl chloride entering aquatic systems would be transferred to the atmosphere through volatilization; a calculated half-life of 0.8 hour was estimated for evaporation from a river 1 m deep with a current of 3 m/sec and with a wind velocity of 3 m/sec (Lyman *et al*, 1982).

The volatilization half-life of vinyl chloride from surface water ranges from several minutes to a few hours depending on water turbulence (Dilling *et al.,* Hill *et al.,* 1976; EPA, 1979).

Such values will involve a rapid disappearance in a few hours of vinyl chloride by volatilization to atmosphere from the water.

Hydrolysis will not be a significant loss process (Mabey *et al*, 1981).

7.10 Persistence in air

In the troposphere vinyl chloride is photochemically oxidized by hydroxyl radicals (8.10^5 rad/cm^3) abstracting H atoms. The reported degradation products are chloroacetaldehyde, HCl, chloroethylene epoxide, formaldehyde, formic acid and carbon monoxide (Muller *et al*, 1977). Final decomposition products are carbon dioxide and hydrogen chloride. Half-life has been reported to be about 1.5 days (Perry *et al*, 1977). In the presence of nitrogen oxides, e.g. photochemical smog situations, the reactivity is higher and leads to a half-life reduced to a few hours (3 to 7 hours) (Carassiti *et al*, 1978; Gay *et al*, 1976; Woldbaek *et al*, 1978).

7.11 Degradation in biological systems

In the aquatic environment, biodegradation will not be a significant sink due to the volatility of vinyl chloride.
Limited existing data indicates that vinyl chloride is resistant to biodegradation in aerobic systems (Callahan *et al*, 1979; Helfgott *et al*, 1977). Vinyl chloride was approximately 50 % and 100 % degraded in 4 and 11 weeks, respectively, in the presence of sand by methanogenic microorganisms under anaerobic conditions in laboratory scale experiments; the degradation level was reduced to 20 % and 55 %, respectively, in the absence of sand. (Brauch H J *et al*, 1987).

Vinyl chloride is also a degradation product resulting from the anaerobic dechlorination of tri- and perchloroethylene. The complete reduction process leads to the transformation of vinyl chloride into ethylene and further ethane. In some cases mineralisation to CO_2/CH_4 is observed. The chlorinated compounds act as electron acceptors (Van Dijk, 1995).

7.12 Conclusion

It can be deduced from the above information that vinyl chloride is not a "toxic, persistent and liable to bioaccumulate" substance as mentioned by the Oslo and Paris Conventions for the Prevention of Marine Pollution (OSPARCOM) according to the criteria currently under discussion and especially those defined by UN-ECE, Euro Chlor and CEFIC.

8. EXPOSURE ASSESSMENT

The exposure assessment is essentially based on exposure data from analytical monitoring programmes. Vinyl chloride has been measured in a number of water systems. These levels in surface waters (river water and marine waters) are detailed in *Appendix 4*. References of the available monitoring data can be found in HEDSET Data Sheet for vinyl chloride (updated version of June 1995). Additional sources have been also used. All the references are given in *Appendix 7*.

As it is generally not specified if the location of sampling is close to a source of emission (production or processing), it is assumed that the lower levels correspond to the background "regional" concentrations and the higher to contaminated areas, or "local" concentrations, considered as worst cases.

8.1 Marine waters

In coastal waters and estuaries, observed concentrations are in a range from below 0.15 µg/l. Typical recent monitoring data for vinyl chloride in coastal waters and estuaries which are part of the OSPARCOM region are given in *Appendix 4* and illustrated on the North Sea map in *Appendix 5*.

8.2 River waters

Background levels of vinyl chloride in typical river in non-industrialized areas are most probably lower than the detection level (0.008 µg/l).

In the Rhine river water and other adjacent industrialized rivers, up to 0.4 µg/l is measured recently near emission point (see *Appendix 4*).

9. RISK ASSESSMENT CONCLUSION

In the risk characterization of vinyl chloride for the aquatic organisms, the PNEC is compared to the PEC.

A PNEC of 210 µg/l was obtained for the aquatic species exposed to vinyl chloride.

In coastal waters and estuaries, vinyl chloride is observed up to 0.15 µg/l.

In non-industrialized areas, a typical river water concentration below 0.008 µg/l was derived from the measured levels; a worst case was also identified in industrialized zone with measured levels up to 0.4 µg/l.

These monitoring values allow to calculate the ratios PEC/PNEC which are summarized in Table 4.

Table 4 : Calculation of PEC/PNEC ratios for vinyl chloride

Type of water	Typical level	PEC/PNEC
Coastal waters/Estuaries		
• worst case	0.15 µg/l	0.0007
• typical water	-	-
River waters		
• worst case	0.4 µg/l	0.002
• typical water	< 0.008 µg/l	< 0.000004

These calculated ratios, **which do not take into account any dilution factor within the sea,** correspond to a safety margin of 500 to 250,000 between the aquatic effect and the exposure concentration so that the present use of vinyl chloride should not represent a risk to the aquatic environment.

10. REFERENCES

10.1 General references

Brauch H J; Kuehn W; Werner, P: Vinylchlorid in kontaminierten Grundwaessern. Vom Wasser 68, 23-32 (1987)

Callahan, M.A. *et al*. (1979): Water-related environmental fate of 129 priority pollutants, vol. II, P 49-10; USEPA-440/4-79-029b

Carassiti V (1978): Expressions pour la vitesse de formation des produits de photooxydation atmosphérique du VC; Annali di Chimia (ANCRA), IT 1977, V67, NR7-8, p. 499-512

Dilling, W.L., Tefertiller, N.B., Kallos, G.J. (1975): Evaporation rates of methylene chloride, chloroform, 1,1,1-trichloroethane, trichloroethylene, tetrachloroethylene and other chlorinated compounds in dilute aqueous solutions; Environ. Sci. Technol., 9(9): 833-838

ECVM: On the environmental impact of the manufacture of polyvinylchloride (PVC) – A description of Best Available Techniques – August 1994

ECVM: On the environmental impact of the manufacture of emulsion and microsuspension polyvinylchloride (PVC) – A description of Best Available Techniques – November 1998

EPA (1979): Water-related environmental fate of 129 priority pollutants; vol. II; USEPA, PB80-204381

Freitag, D., Ballhorn, L., Geyer, H., Korte, F. (1985): Environmental hazard profile of organic chemicals: an experimental method for the assessment of the behaviour of organic chemicals in the ecosphere by means of simple laboratory tests with 14C labelled chemicals. Chemosphere 14-1589-1616 (1985)

Gay B.W. (1976): Oxydation atmosphérique des chlorethylenes/VC, 1-1-dichlorethylene, 1-2-dichloroethylene, tri-perchloroethylenes; Environmental Science and Technology (ESTHA) US 1976, V 10, Jan, p. 58-67

Helfgott, T.B. *et al.* (1977): An index of refractory organics, p. 21; USEPA-600/2-77-174

Hill, J., Kollig, H.P., Paris, D.F., Wolfe, F.L., Zepp, R.G. (1976): Dynamic behaviour of vinyl chloride in aquatic ecosystems; USEPA-600/3-76-001

Lyman, W.J., Reehl, W.F., Rosenblatt, D.H. (1982) *Handbook of chemical property estimation methods*. Environmental behaviour of Organocompounds. New York McGraw-Hill Book Co. p. 960

Mabey, W.R. *et al.* (1981): Aquatic fate process data for organic priority pollutants, p. 156; USEPA-440/4-81-014

Mackay, D., Patterson, S. (1990); Fugacity models; in: Karcher, W., Devillers, J. (Eds); Practical applications of quantitative structure-activity relations in environmental chemistry and toxicology: 433-460.

Malle K.G. (1984): Priority list of 129 dangerous substances (occurrence in the Rhine, toxicology, open questions); Z Wasser Forsch. 17, 75

Muller J.P.H. (1977): Contributions à la chimie écologique – CXXXVI – Courte communication sur la photooxydation non sensibilisée des chloroethylenes; Chemosphere (CMSHA); GB 1977, V6, Jun, p. 341-346

OSPARCOM: Description of Best Available Technique for the Vinyl Chloride Sector (1996)

Pederson, F., Tyle, H., Niemelä, J.R., Guttmann, B., Lander, L., Wedebrand, A. (1994); Environmental Hazard Classification -Data collection and interpretation guide; TemaNord 1994:589.

Perry, R.A., Atkinson, R., Pitts, J.N. (1977): Rate constants for the reaction of OH radicals with CH2=CHF, CH2=CHCl, and CH2=CHBr over the temperature range 299-426°K; J. Chem. Phys., 67: 458-462

TGD (1996) – Technical Guidance Documents in support of the Commission Directive 93/67/EEC on Risk Assessment for new notified substances and the Commission Regulation (EC) 94/1488/EEC on risk assessment for existing substances (Parts I, II, III and IV) EC Catalogue numbers CR-48-96-001-EN-C, CR-48-96-002-EN-C, CR-48-96-003-EN-C, CR-48-96-004-EN-C

Van Dijk, N.R.M. (1995): Biodegradation of tetrachloroethylene (a literature survey); Solvay internal document) 56835/32/94

Woldbaek T. (1978): A molecular spectroscopy, Spectrochimica Acta, GB 1978, V34 A, Nr 5, p. 481-7

10.2 References for ecotoxicity data : see *Appendix 6*

Those references are used in *Appendix 3*.

10.3 References for monitoring data : see *Appendix 7*

Those references are used in *Appendix 4*.

APPENDIX 1

Environmental quality criteria for assessment of ecotoxicity data

The principal quality criteria for acceptance of data are that the test procedure should be well described (with reference to an official guideline) and that the toxicant concentrations must be measured with an adequate analytical method.

Four cases can be distinguished and are summarised in the following table according to criteria defined in IUCLID system).

Table: Quality criteria for acceptance of ecotoxicity data

Case	Detailed description of the test	Accordance with scientific guidelines	Measured concentration	Conclusion: reliability level
I	+	+	+	[1] : valid without restriction
II	±	±	±	[2] : valid with restrictions; to be considered with care
III	insufficient or -	-	-	[3] : invalid
IV	the information to give an adequate opinion is not available			[4] : not assignable

The selected validated data LC50, EC50 or NOEC are divided by an assessment factor to determine a PNEC (Predicted No Effect Concentration) for the aquatic environment.

This assessment factor takes into account the confidence with which a PNEC can be derived from the available data: interspecies- and interlaboratory variabilities, extrapolation from acute to chronic effects, etc.

Assessment factors will decrease as the available data are more relevant and refer to various trophic levels.

APPENDIX 2

Ultimate distribution in the environment according to Mackay level I model
(details of calculation)

Fugacity Level I calculation

Chemical: Vinyl Chloride

Temperature (C)	20
Molecular weight (g/mol)	62.50
Vapor pressure (Pa)	330000
Solubility (g/m3)	1100
Solubility (mol/m3)	17.60
Henry's law constant (PA.m3/mol)	18750
Log octanol water part. coefficient	1.58
Octanol water part. coefficient	38.02
Organic C-water part. coefficient	15.59
Air-water partition coefficient	7.69
Soil-water partition coefficient	0.47
Sediment-water partition coefficient	0.94
Amount of chemical (moles)	1
Fugacity (Pa)	.40614623E-6
Total VZ products	2462167.37

Phase properties and compositions:

Phase	Air	Water	Soil	Sediment
Volume (m3)	.6000E+10	.70000E+7	.45000E+5	.21000E+5
Density(kgm3)	.12056317E+2	.10000E+4	.15000E+4	.15000E+4
Frn org carb.	.00000E+0	.00000E+0	.20000000E-1	.40000000E-1
Z mol/m3.Pa	.41029864E-3	.53333333E-4	.24940424E-4	.49880848E-4
VZ mol/Pa	.24617918E+7	.37333333E+3	.11223190E+1	.10474978E+1
Fugacity	.40614623E-6	.40614623E-6	.40614623E-6	.40614623E-6
Conc mol/m3	.16664124E-9	.2166113E-10	.1012945E-10	.2025891E-10
Conc g/m3	.10415078E-7	.13538207E-8	.63309121E-9	.12661824E-8
Conc ug/g	.86386889E-6	.13538207E-8	.42206080E-9	.84412161E-9
Amount mol	.99984749E+0	.15162792E-3	.45582567E-6	.42543729E-6
Amount %	99.98	0.02	.45582567E-4	.42543729E-4

APPENDIX 3

SUMMARY TABLE OF ECOTOXICITY DATA ON VINYL CHLORIDE

1. FISH

Species	Duration h(hours)/d(days)	Type of Study	Criterion (LC50/EC50 NOEC)	Concentration (mg/l)	Validity	Comments	Reference
ACUTE STUDIES							
1. Freshwater							
Brachydanio rerio	96h	A,SS,C	LC50	210	1	OECD 203. Purity >99%. Performed to GLP. NOEC = 128 mg/l.	Groeneveld *et al.* (1993)
Leuciscus idus	48h	N,S	LC50	356	3	DIN38412.	Juhnke & Luedemann (1978)
Leuciscus idus	48h	N,S	LC50	406	3	DIN38412.	Juhnke & Luedemann (1978)
Esox lucius	10d	A,S	100% mortality	388	3	Single concentration. Non-standard test.	Brown *et al.* (1977)
Lepomis macrochirus	96 h		LC50	1220	4		Hann & Jensen, 1977
Micropterus salmoides	96 h		LC50	1060	4		Hann & Jensen, 1977
2. Saltwater							
No data available							
CHRONIC STUDIES							
1. Freshwater							
No data available							
2. Saltwater							
No data available							

Endpoints of the tests are based on survival/mortality. Other effects are explicitly mentioned in the table.

APPENDIX 3

SUMMARY TABLE OF ECOTOXICITY DATA ON VINYL CHLORIDE

2. INVERTEBRATES

Species	Duration h(hours)/d(days)	Type of Study	Criterion (LC50/EC50 NOEC)	Concentration (mg/l)	Validity	Comments	Reference
ACUTE STUDIES							
1. Freshwater							
Uronema parduczi	20h (?)	N,S	toxicity threshold	1050	3	Protozoan. Non-standard endpoint.	Bringmann & Kuhn (1980)
Tetrahymena pyriformis	9 h	N,S	IC50	540	3	50% inhibition of proliferation rate. Dimethyl acetamide solvent up to 1%.	Sauvant *et al.*, 1995
Panagrellus redivivus	96 h	N,S	LC50	> 62.5	3	No effect on survival at max. concentration	Samoïloff *et al.*, 1980
2. Saltwater							
No data available							
CHRONIC STUDIES							
1. Freshwater							
No data available							
2. Saltwater							
No data available							

APPENDIX 3

SUMMARY TABLE OF ECOTOXICITY DATA ON VINYL CHLORIDE

3. AQUATIC PLANTS

Species	Duration H(ours)/D(ays)	Type of Study	Criterion (LC50/EC50 NOEC)	Concentration (mg/l)	Validity	Comments	Reference
ACUTE STUDIES							
1. Freshwater							
Scenedesmus quadricauda	8d ?	N S	toxicity threshold	710	3	Growth threshold, not defined.	Bringmann & Kuhn (1978) Bringmann & Kuhn (1977)
2. Saltwater							
No data available							
CHRONIC STUDIES							
1. Freshwater							
No data available							
2. Saltwater							
No data available							

APPENDIX 3

ABBREVIATIONS

A	=	Analysis
C	=	Closed system or controlled evaporation
O	=	Open vessel
h	=	hour(s)
d	=	day(s)
MATC	=	Maximun acceptable toxicant concentration
N	=	nominal concentration
S	=	static
SS	=	semistatic
F-T	=	flow-through

Validity column:
1 = valid without restriction
2 = valid with restrictions: to be considered with care
3 = invalid
4 = not assignable

APPENDIX 4

Environmental monitoring levels of vinyl chloride in water

1. Coastal waters and estuaries

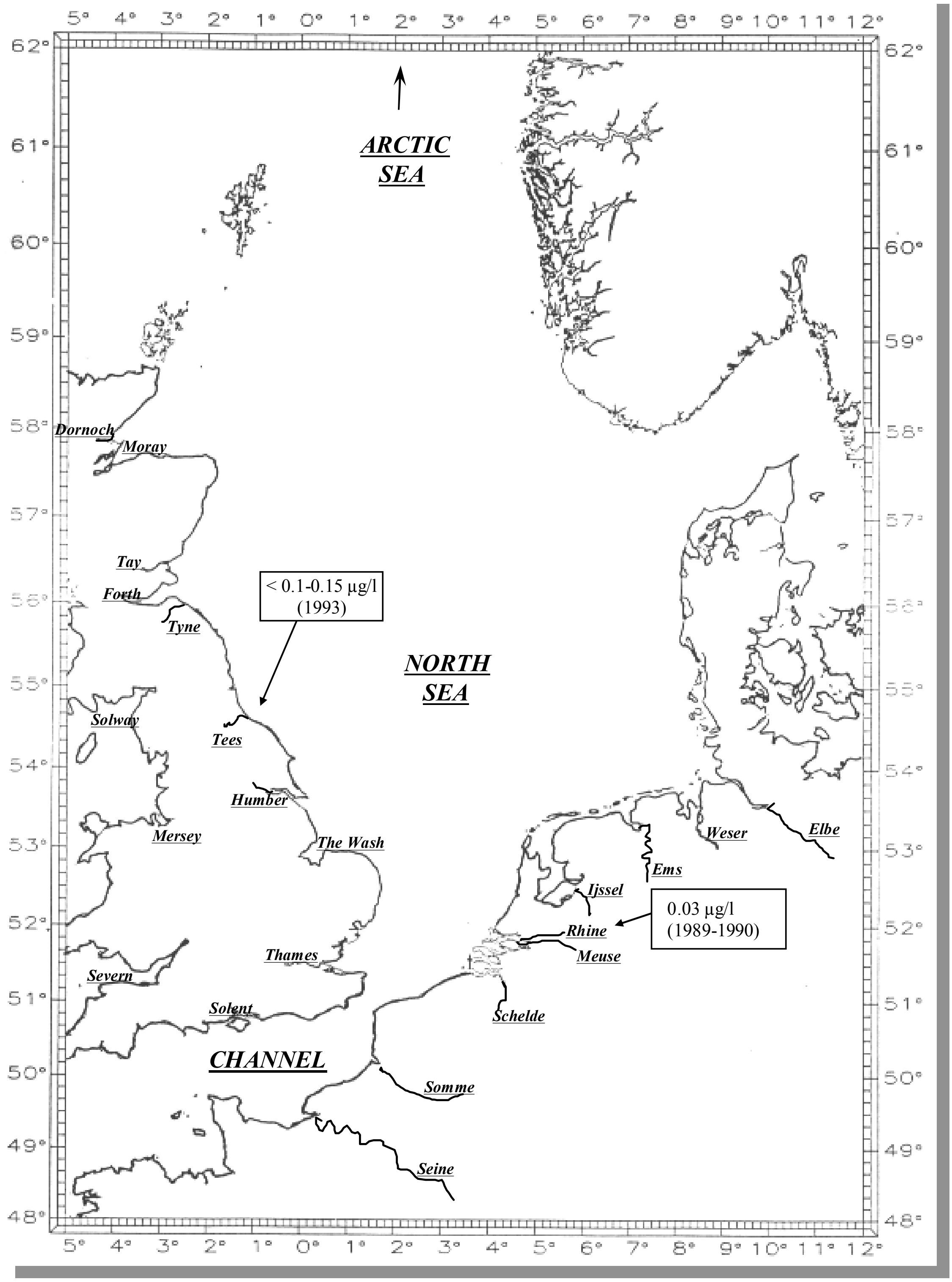
Location	Year of measurement	Mean concentration (µg/l)	Reference
USA :			
- San Francisco Bay	1987	< 0.3	Levaggi *et al.*, 1988
UK			
- Tees estuary	1993	< 0.1 – 0.15	UK Environmental Agency, 1997

2. Surface freshwaters

Location	Year of measurement	Mean concentration (µg/l)	Reference
Germany :			
- Rhine	< 1978	max. 1	Anna *et al.*, 1978
- Rhine tributaries in Nordrhein - Westfalen	< 1978	< 1 - 5	Anna *et al.*, 1978
- Rhine	1989 - 90	0.031	Wittsiepe, 1990
- Main	1989 - 90	0.008	Wittsiepe, 1990
- Lippe	1989 - 90	0.4 (near emission point)	Wittsiepe, 1990
- Ruhr	1989 - 90	0.06	Wittsiepe, 1990
- Wupper	1989 - 90	0.069	Wittsiepe, 1990
- Saale (ex DDR)	1989 - 90	69	Wittsiepe, 1990
- Rhine, G/NL borderline, km 865	1982	< 0.2	Malle, 1984

APPENDIX 5

NORTH SEA MONITORING DATA ON VINYL CHLORIDE



APPENDIX 6

REFERENCES TO ECOTOXICITY DATA

Bringmann G. and Kuhn R. (1980)
Bestimmung der biologischen Scahwirkung wasserfahrdender Stoffe gegen Protozoen II: Bakterienfressende Ciliaten.
Z. Wasser Abwasser Forsch. **1,** 26-31.

Bringmann G. and Kuhn R. (1978)
Grenzwerte der Schadwirkung wasserfahrdender Stoffe gegen Blaualgen *(Microcystis aeruginosa)* und Grunalgen *(Scenedesmus quadricauda)* im Zellvermehrungshemmtest.
Vom Wasser **50,** 45-60.

Brown E. R., Sinclair T., Keith L., Beamer P., Hazdra J. J., Nair V. and Callaghan O. (1977)
Chemical Pollutants in Relation to Diseases in Fish.
Ann. N. Y. Acad. Sci. **298** , 535-546.

Groeneveld A.H.C., Zijlstra A.G., Feenstra A.F.M. and Berends A.G. (1993)
The Acute Toxicity of Vinyl Chloride to the Zebra Fish.
Solvay-Duphar report 56635/64/92.

Hann R.W. & Jensen P.A. (1977): Water quality characteristics of hazardous materials, Texas A&M University, College Station Environmental Engineering Div., Report NOAA-780 13001, PB-285946

Juhnke I. and Luedemann D. (1978)
Results of the Study of 200 Chemical Compounds on Acute Fish Toxicity Using the Golden Orfe Test (paper in German.)
Z. Wasser Abwasser Forsch **11,** *5* , 161-164.

Samoïloff, M.R., Schulz, S., Jordan, Y., -Denich, K., Arnott, E. (1980)/ A rapid simple long-term toxicity assay for aquatic contaminants using the nematode *Panagrellus redivivus*; Can. J. Fish. Aquat. Sci., 37/ 1167-1174

Sauvant M.P., Pepin D., Bohatier J., Gr, C A (1995): Comparison of six bioassays for assessing in vitro acute toxicity and structure-activity relationships for vinyl chloride monomer, its main metabolites and derivates; Sci. Total Environ., 172: 79-92

APPENDIX 7

REFERENCES TO THE MONITORING DATA

Anna, K., Alberti, J. (1978); Herkunft und Verwendung von Organohalogenverbindungen und ihre Verbreitung in Wasser und Abwasser; Colloquium Verlag Berlin 1: 154-158; In: Datenbank für Wassergefährdende Stoffe (DABAWAS), S. 10252 (1986).

Levaggi, D.A., Siu, W., Zerrudo, R.V., LaVoie, J.W. (1988); Experiences in gaseous toxic monitoring in the San Francisco Bay area; Proceedings APCA annual meeting, Jun 19-24, 81 (5), (88-95A.3): 1-19.

Malle, K.G. (1987); Der Rhein muβ leben! wlb - Wasser, Luft und Betrieb 11-12/1987, 22/23.

Staples, C.A., Werner, A.F., Hoogheem, T.J. (1985); Assessment of priority pollutant concentrations in the United States using STORET database; Environmental Toxicology and Chemistry, 4: 131-142.

UK Environmental Agency (1997) : Personal Communication to ICI

Wittsiepe, J. (1990); Occurence of vinyl chloride and other halogenated C1 and C2 hydrocarbons in German surface water; Dioxin 90, Bayreuth 1990.