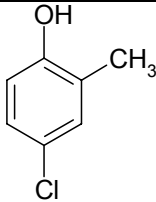


[FOREWORD](#)

[INTRODUCTION](#)

4-CHLORO-2-METHYLPHENOL
CAS N°: 1570-64-5

SIDS INITIAL ASSESSMENT PROFILE

CAS Nr.	1570-64-5
Chemical Name	Phenol, 4-chloro-2-methyl
Structural formula	

CONCLUSIONS AND RECOMMENDATIONSEnvironment

The chemical is very toxic to aquatic organisms. The chemical is considered as readily biodegradable and has a low bioaccumulative potential. The predicted environmental concentrations are lower than the predicted no effect levels for all environmental compartments. It is currently considered of low potential risk and low priority for further work.

Health

This chemical is corrosive and toxic by inhalation. Workers exposure is considered to be low because the substance is produced in a closed system as an intermediate for the manufacturing of phenoxyherbicides. Consumer exposure is considered to be negligible. It is currently considered of low potential risk and low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE CONCLUSIONS AND RECOMMENDATIONS

The EU tonnage of (4-chloro-2-methylphenol) for the year 1989 has been estimated as a total of 15000 tons per annum based on the production volumes presented by the manufacturers and supported by the production and consumption figures of the herbicides MCPA (4-chloro-2-methylphenoxy acetic acid), MCPB (4-chloro-2-methylphenoxy butyric acid) and MCPP (mecoprop 2-4chloro-2-methylphenoxy-propionic acid). The main points of emissions are at manufacturing sites of the substance where PCOC is used as an intermediate for manufacturing of the phenoxyherbicides (i.e. PCOC processing and phenoxyherbicides formulation sites) and where these herbicides are used in agriculture (PCOC occurs as an impurity in the phenoxyherbicides). The environmental distribution of PCOC (using a Mackay fugacity level 1 calculation (Mackay & Paterson 1990) is expected to be 33% in air, 56% in water, 6% in soil and 5% in sediment.

The environmental exposure assessment is primarily based on monitoring data from the two main manufacturing sites in EU where all production and all processing of PCOC takes place, and where approximately 60% of the production volume in EU is formulated. A worst case environmental exposure scenario for a separate, but hypothetical, formulation site has also been considered. PEC local water is calculated as 0.0038 mg/l and 0.0014 mg/l for specific site and formulation, respectively. For the exposure assessment of PCOC in sewerage treatment plants (STP), the dissolved concentration of PCOC is assumed to be equal to the effluent concentration. The predicted environment concentrations for the sewerage treatment plant are: 0.004 mg/l [specific

site], 0.0013 mg/l [formulation]. The predicted environmental concentration for soil is calculated as 0.00000088 - 0.000002 mg/kg.

PCOC is very toxic to aquatic organisms. The acute toxicity to fish LC_{50} (96h) was observed to be 2.3-6.6mg/l. The EC_{50} (48h) to daphnids was 0.29-1.0 mg/l and the EC_{50} (96h) to algae was 8.2 mg/l and EC_{10} to algae (96h) was 0.89 mg/l. The NOEC (28 days) for fish was 0.5 mg/l for histopathological changes in kidneys and liver. NOEC (21 days) for Daphnia reproduction was 0.55 mg/l. The presence of an algae EC_{10} , a long term NOEC for fish and a Daphnia reproduction test suggest that use of an assessment factor of 10 may be appropriate. The predicted no effect concentration (PNEC) is 0.05 mg/l. The PNEC $STP_{microorganisms}$ is obtained by using the EC_{50} for inhibition of respiration of activated sludge microorganisms and an assessment factor of 100 (0.55 mg/l). Since no ecotoxicological data are available for soil organisms the equilibrium partitioning method has been applied ($PNEC_{soil} = 0.36$ mg/kg).

A local risk for aquatic organisms is not anticipated as the predicted environment concentration is lower than the predicted no effect concentration (regardless of whether an assessment factor of 10 or 100 is employed). Similarly the risks for microorganisms in sewerage treatment plants and for soil organisms is not expected.

The most important sources of direct human exposure are assumed to be at production sites (with predicted exposures of up to 0.7 mg/kg/day) or in conjunction with the use of phenoxy herbicides where exposures of ca. 0.35 mg/kg/day is estimated. Indirect exposure is estimated as being several orders of magnitude lower than the above values at a regional level while consumer exposure to the substance as an impurity in lawn-treatment sprays may be as high as 0.07 mg PCOC /kg/event.

PCOC is corrosive and toxic by inhalation but is only moderately toxic in acute mammalian tests by other routes. The substance is not a skin sensitizer. In an OECD screening test 422, PCOC did not cause reproductive effects in rats. Tests for repeated dose toxicity suggest an NOAEL of 200 mg/kg and a LOAEL of 800/mg/kg (slight liver toxicity and decrease in haemoglobin concentration in the blood). PCOC was positive in an older mouse micronucleus test, but negative in a recent valid test performed according to the current OECD guideline. It did not give rise to genotoxicity in valid Ames tests. On the basis of current knowledge, the substance can not be considered a mutagen.

Repeat dose toxicity is not likely to present a major health problem. The margin of safety for workers based on a NOAEL of 200 mg/kg/day is $200/0.7 = 285$. For the end-points irritation/corrosivity the concentration is below the level of concern.

For consumers exposure may be in the order of 0.07 mg/kg for each event corresponding to a daily dose of 9.6×10^{-4} mg/kg/day. With a NOAEL for repeat dose toxicity of 200 mg/kg/day the margin of safety is at least 20,000 for each single event.

IF FURTHER WORK IS RECOMMENDED, SUMMARISE ITS NATURE

Danish Environmental Protection Agency

RISK ASSESSMENT

4-Chloro-2-methylphenol

CAS-No.: 1570-64-5

EINECS-No.: 216-381-3

June 29, 1998

FINAL

Information on the rapporteur

Rapporteur for the risk assessment report on 4-chloro-2-methylphenol is the Danish Environmental Protection Agency.

Responsible for the risk evaluation and subsequently for the contents of this report is the rapporteur.

Contact persons:

Jay Niemela & Henrik Tyle
Chemicals Division
Danish Environmental Protection Agency
Strandgade 29
DK-1401 Copenhagen K
DENMARK

Tel: +45 32 66 04 93 / +45 32 66 04 94

Fax: +45 32 66 02 61

E-mail: JRN@mst.dk / HTY@mst.dk

CONTENTS

0 OVERALL CONCLUSIONS/RESULTS OF THE RISK ASSESSMENT

1 GENERAL SUBSTANCE INFORMATION.

2 GENERAL INFORMATION ON EXPOSURE

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

- 3.1.1 General discussion
- 3.1.2 Environmental fate
- 3.1.3 Aquatic compartment
- 3.1.4 Atmosphere
- 3.1.5 Terrestrial compartment
- 3.1.6 Non compartment specific exposure relevant to the food chain

3.2 EFFECTS ASSESSMENT: HAZARD IDENTIFICATION AND DOSE (CONCENTRATION) - RESPONSE (EFFECT) ASSESSMENT

- 3.2.1 Aquatic compartment
- 3.2.2 Atmosphere
- 3.2.3 Terrestrial compartment
- 3.2.4 Non compartment specific effects relevant to the food chain

3.3 RISK CHARACTERISATION

- 3.3.1 Aquatic compartment
- 3.3.2 Atmosphere
- 3.3.3 Terrestrial compartment
- 3.3.4 Non compartment specific effects relevant to the food chain

4 HUMAN HEALTH

4.1 HUMAN HEALTH (TOXICITY)

- 4.1.1 Exposure assessment
- 4.1.2 Effects assessment: Hazard identification and Dose (concentration) - response (effect) assessment
- 4.1.3 Exposure assessment
- 4.1.4 Risk characterisation

5 CONCLUSIONS

6 REFERENCES

7 APPENDIX

7.1 PHOTOLYSIS OF PCOC IN SURFACE WATER.

7.2 QSAR ESTIMATIONS ON TOXICITY

7.3 TGD ESTIMATIONS ON EXPOSURE

- 7.3.1 PEC_{local, water} estimations
- 7.3.2 Atmospheric exposure estimations.
- 7.3.3 PEC_{local, soil} estimations

7.4 EUSES V. 1.0 ESTIMATIONS.

7.5 ESTIMATION OF INHALATION AND DERMAL EXPOSURE EASE-MODEL

0 OVERALL CONCLUSIONS/RESULTS OF THE RISK ASSESSMENT

CAS No.:	1570-64-5
EINECS No.:	216-381-3
Substance Name (IUPAC Name)	4-chloro-2-methylphenol
Trade Name	4-chloro-o-cresol
Synonyms	chlorocresol, PCOC
Annex I entry no.:	not available (not yet included in Annex I of Directive 67/548/EEC)
Proposed classification:	T; R23, C; R35; N; R50

- () i) There is a need for further information and/or testing.
- (X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those for which are being applied already.

With regards to the environment, the latest information from the manufacturers on release and monitoring data result in the conclusion that no further information and/or testing is needed as the endpoints do not give rise to concern beyond the need for classification and labelling..

With regard to effects on human health, an older positive *in vivo* mutagenicity assay was not confirmed by a test performed according to current guidelines. Other mammalian toxicity endpoints do not give rise to concern beyond the need for classification and labelling. While exposure can occur indirectly through the use of pesticides, PCOC itself appears to be used exclusively as an intermediate in the chemical industry.

Summary of conclusions**Environment:**

The environmental risk assessment was performed according to the "Technical Guidance Documents in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances" (TGD 1996). Calculations were made employing "Uniform System for the Evaluation of Substances", i.e. EUSES (ver. 1.0).

The documentation varies from original studies according to OECD test guidelines with GLP to literature references of varying quality. 4-Chloro-2-methylphenol (PCOC) is used in the industry as an intermediate in the synthesis of the phenoxy herbicides MCPA, MCPB, mecoprop (MCP) and mecoprop-p (MCP-P). From the industrial production, processing and formulation of phenoxy herbicides, PCOC is emitted to air and waste water. The release is estimated based on TGD and relevant information about environmental releases during production and formulation obtained from the manufacturers. The produced pesticides contain PCOC as impurity (normally < 1%). The use of the pesticides in the agriculture as herbicides results in exposure of soil to PCOC as an impurity and degradation product.

The emissions to surface water from production, processing and formulation sites are local and the number of sites are few. Sludge from the two major production sites are incinerated but one of the waste water receiving STPs does use sludge for field application. Therefore, the contribution from sludge application is considered local.

PCOC has been found in water, soil, air and groundwater. In water, PCOC was observed mainly around emission sources, in air near fields applied with MCPA or MCP, and in soil and biota after the application of the herbicides. The findings in groundwater are assumed to be the result of mobility and reduced degradation under anaerobic conditions.

As MCPA is transformed to PCOC and PCOC has a high vapour pressure, the atmosphere will receive a contribution from soil application of the above mentioned pesticides. PCOC has a low to medium adsorption to organic carbon and may be considered mobile in some soils.

According to an experiment, PCOC is primarily degradable by photolysis in clean water with a half-life of 4 days. However, a re-estimation of photolysis to typical EU surface water resulted in an estimated photolytic degradation half-life of 300-700 days and therefore photolysis is considered negligible. The available biodegradation data are somewhat conflicting but based on a judgement of the balance of evidence the "realistic worst case" aerobic biodegradation half-life of PCOC in soil is estimated to be 21 days, whereas no biodegradation has been found under anaerobic conditions. The aerobic biodegradation half-life in surface waters is also estimated to be 21 days. The estimated half-life in biological waste water treatment plants is 0.7 hour resulting in an estimated removal of 88%. The substance is therefore considered to be readily biodegradable (borderline).

PCOC has a bioaccumulation potential based on log Kow 3.09 but BCF found in fish was low (≤ 30). The risk characterisation of secondary poisoning is therefore not performed.

The exposure assessment is primarily based on monitoring data from the two main manufacturing sites where all production and all processing of PCOC takes place and where approximately 60% of the production volume is formulated. A worst case environmental exposure scenario for a separate formulation site is included in the risk assessment.

PCOC is very toxic to aquatic organisms. The acute toxicity to fish LC_{50} (96h) was observed to be 2.3-6.6 mg/l. The EC_{50} (48h) to daphnids was 0.29-1.0 mg/l and the EC_{50} (96h) to algae was 8.2 mg/l and EC_{10} to algae (96h) was 0.89 mg/l. The NOEC (28 days) for fish was 0.5 mg/l for histopathological changes in kidneys and liver. NOEC (21 days) for Daphnia reproduction was 0.55 mg/l.

The $PEC_{local, water} / PNEC_{aquatic\ organisms} < 1$.

The $PEC_{STP} / PNEC_{microorganisms} < 1$.

There are no data available on toxicity to soil organisms. Using the equilibrium partitioning method, it was possible to estimate a $PNEC_{soil}$ from $PNEC_{aquatic\ organisms}$. The resulting risk quotient indicated no potential risk to soil organisms, i.e. $PEC_{soil} / PNEC_{soil} < 1$. In all above cases the conclusion for the aquatic and soil compartment does not differ regardless of whether the substance is considered readily or inherently biodegradable or whether an assessment factor of 10 or 100 is employed

PEC_{air} : There are no effect data present and, therefore, no $PEC/PNEC$ ratio can be calculated.

Human health:

Information on mammalian toxicity includes both GLP studies done according to OECD guidelines, and older, unpublished citations of limited value. For most endpoints, there appears to be sufficient information to perform a preliminary risk assessment.

The most important sources of direct exposure are assumed to be during production (with predicted exposures of up to 0.7 mg/kg/day) or in conjunction with the use of phenoxy herbicides (containing PCOC as an impurity or breakdown product) where exposures of ca. 0.35 mg/kg/day may occur.

Indirect exposure is estimated as being several orders of magnitude lower than the above values at a regional level while consumer exposure to the substance as an impurity or breakdown product in lawn-treatment sprays may be as high as 0.07 mg/kg/event. Indirect human exposure (1.2×10^{-4} mg/kg/day) arising from production and formulation is unlikely to give rise to local concerns.

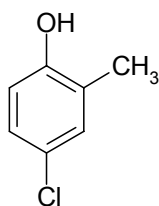
PCOC is corrosive and toxic by inhalation but is only moderately toxic in acute tests by other routes. The substance is not a sensitizer. According to OECD screening test 422, PCOC did not cause reproductive effects in rats. Tests for repeated dose toxicity suggest an NOAEL of 200 mg/kg and a LOAEL of 800/mg/kg (slight liver toxicity and effects on blood parameters) implying a worst case safety margin of about 285 at production sites.

PCOC was positive in an older mouse micronucleus test, but negative in a recent test performed according to current guidelines. It did not give rise to genotoxicity in the Ames test. On the basis of current knowledge, the substance can not be considered a mutagen.

1 GENERAL SUBSTANCE INFORMATION.

Identity of the substance

CAS-No.:	1570-64-5
EINECS-No.:	216-381-3
IUPAC Name:	4-chloro-2-methylphenol
Synonyms:	4-chloro-o-cresol para-chloro-ortho-cresol (PCOC)
Trade Name:	4-chloro-o-cresol
Synonym	Chlorocresol
Molecular formula:	C ₇ H ₇ Cl O
Structural formula:	



Molecular weight:	142.59
-------------------	--------

Purity/impurities, additives

Purity:	approx. 97% w/w	
Impurities:	2-chloro-6-methylphenol (OCOC, CAS: 87-64-9)	<1.0%
	2-methylphenol (OC, CAS: 95-48-7)	<1.0%
	2,4-dichloro-6-methylphenol (DCOC, CAS: 1570-65-6)	<2.0%
	4-chloro-2,6-dimethylphenol	<0.5%
	4-chlorophenol	<0.5%
	5-chloro-2-methylphenol	<0.2%

Additives: None

Physico-chemical properties

Physical state:	solid at 25°C, 1 atm	
Melting point:	46-50°C	(OECD 102, Qvist Lab. 1983)
Boiling point:	231°C	(OECD 103, Qvist Lab. 1983)
	150-155°C at 20-25 hPa	(BASF 1994)
Relative density:	0.4769 g/cm ³ at 20°C	(OECD 109, Qvist Lab. 1983)
	1.2 g/cm ³ at 50°C	(BASF 1994)
Vapour pressure:	26.66 Pa at 20°C	(OECD 104, Dantest 1983)
	160 Pa at 70°C	(BASF 1994)
Water solubility:	2300 mg/l (20°C),	(OECD 105, Qvist Lab. 1983)
Octanol/water (Kow):	log Kow = 3.09	(OECD 107, BASF 1994)
pK _a	9.71	(BASF 1994)
Explosivity	No information (unlikely, structural considerations)	
Flammability	Not flammable	(EF 3.10, Quist Lab. 1983)
Oxidizing potential	Non oxidizing	(PC II Annex V EEC/831/79, Dantest 1983)

Comments on physico-chemical data

The physico-chemical data are present but with variations that may be attributed to different test methods, temperatures, etc. The results from tests performed by OECD guidelines have been used instead of handbook values and literature references when the test method has not been mentioned.

The melting point 50°C was found in an OECD 102, capillary method. The boiling point of 231°C has been found in an OECD 103, Siwoloboff method. The vapour pressure of 26.66 Pa (0.2 mmHg) at 25°C was found in an OECD 104 method and is used instead of the 3.2 Pa at 25°C mentioned by Seiber *et al.* (1986) who only states that the result was found in a laboratory study.

The water solubility was found to be 2300 mg/l (0.23 w/w%) in an OECD 105 at 20°C. In a BASF study, a water solubility of 7600 mg/l at 25°C is found after solution in hot water, centrifugation and GC analysis without reference to test method. A water solubility of 1312 mg/l is mentioned by US-EPA (1996) without specifying the test method. A QSAR estimation by the EPIWIN model calculations (Meylan and Howard, Syracuse, 1995) results in an estimated water solubility of 1765 mg/l. The water solubility of 2300 mg/l which was observed in an OECD test is evaluated to be the most valid and is used in the risk assessment.

The octanol/water partition coefficient log Kow is stated to be 2.78 according to US-EPA (1996) without specifying the test method. Hansch *et al.* (1995) found an experimental value of 2.63. QSAR calculations by fragment analysis (KOWWIN, Syracuse 1995; ClogP) estimated the log Kow to be 2.70 and 3.13, respectively. However, a test performed according to the OECD guideline resulted in log Kow to be 3.09 which is used in the risk assessment.

The explosive properties of the substance has not been tested. However, no reports of explosive properties were found in the available literature, nor does the chemical structure contain elements associated with explosivity. According to methods EF 3.10 and EF 3.10 mod. the substance does not burn, nor is it flammable in contact with water (Quist Laboratory, 1983). The substance was classified as non oxidizing according to the test method from the working group PC II Annex V EEC/831/79, sixth amendment of Dir. 67/548/EEC (Dantest, 1983).

Classification:

According to Annex I: Not presently included in Annex I.

Proposed classification:

Human health:	T R23	Toxic by inhalation.
	C R35	Corrosive, Causes severe burns.
Environmental:	N	Dangerous for the environment
	R 50	Very toxic to aquatic organisms.

Comments on classification

The substance may be regarded as a borderline ready biodegradable substance but it is noticed that the data are somewhat conflicting (cf. section on biodegradability). The log Kow is greater than 3 but available BCFs in fish are below 100. (The closely related isomer 4-chloro-3-methylphenol recently has been classified as regarded the environment: N, R50 (EU classification)).

2 GENERAL INFORMATION ON EXPOSURE

PCOC is used as an industrial intermediate in the production of pesticides. The environmental exposure is due to release of the substance from the manufacturing of the substance itself and when using the substance for manufacturing and formulation of the phenoxy herbicides: MCPA (4-chloro-2-methylphenoxy acetic acid), MCPB (4-chloro-2-methylphenoxy butyric acid), and mecoprop (2-(4-chloro-2-methylphenoxy)-propionic acid (MCP)). Furthermore, environmental exposure is due to the agricultural use of the above mentioned pesticides. Mainly, because these pesticides are degraded in the environment to PCOC (main degradation product) but also because PCOC is an impurity in these pesticide formulations.

Production figure

In EU, PCOC has been produced in The United Kingdom (UK), in The Netherlands, and in Germany (BUA 1994). In 1996, the major production took place in UK by two major manufacturers. Other production sites in EU with a production below 1000 tons/year may exist but this data will first be available until 1998. In addition, PCOC may be produced as a non-isolated part of a continuous process which need not be reported under the Regulation. At least one such site has been identified in The Netherlands.

The current production of PCOC in EU takes place in UK by A.H.Marks and Nufarm. A part of the production volume of technical phenoxy acids are exported to be formulated elsewhere within and outside EU.

According to US-EPA, it is not known whether three different US manufacturers are still producing PCOC and using PCOC for manufacturing of MCPA, MCPB and MCP (US-EPA 1996).

The total production and consumption in EU, import and export etc. could not be obtained. Therefore, two methods have been used for the estimation.

Based on the information from the two manufacturers of PCOC (pers.comm., 1997), the total production of PCOC in EU is estimated to be approximately 15000 tons/year.

The latest figures from the ECDIN database (1995) indicate the value of production and consumption of the relevant pesticides to be approximately 22000 tons in 1989.

PCOC constitutes the main molecular fraction of the herbicides. Therefore, the total annual use of PCOC in EU is estimated using stoichiometric calculation to be approximately 15000 tons.

Recent data from manufacturers (confidential papers, October 1997) inform that the production of phenoxy acid herbicides in 1996 was 21000 tonnes of which 13000 was exported. This information supports the estimation of the *production PCOC to be approximately 15000 tonnes per year*. The import is unknown but assumed to be 0.

Summary

The tonnage of PCOC in EU has been estimated to a total of 15000 tons per annum based on the production volumes presented by the manufacturers and supported by the production and consumption figures of the herbicides MCPA, MCPB and MCPP in 1989. Main points of emissions are at manufacturing sites of the substance where PCOC is used as an intermediate for manufacturing of the phenoxyherbicides (i.e. PCOC processing and phenoxyherbicides formulation sites) and where these herbicides are used in agriculture.

3 ENVIRONMENT

3.1 Environmental exposure

The environmental exposure assessments considered combine the relevant exposure scenarios for the substance and apply recommended assessment methods for deriving PEC local and regional according to TGD (1996) and EUSES ver. 1.0 (1997). During 1997 monitoring studies have been performed by the two main manufacturers at their production sites which are both located in UK. The results are used in the exposure assessment but for confidentiality average values are used. The confidential report with the monitoring results has been submitted to the Competent Authorities.

The environmental exposure scenarios according to TGD would include:

- a) Production of PCOC.
- b) Processing: Manufacture of technical phenoxy acids (MCPA, MCPB and MCPP/MCPP-P).
- c) Formulation of the phenoxy herbicides.
- d) Agricultural use of herbicides.

In the TGD, "processing" covers all kinds of processes where the substance as such is applied or used, including application of use of preparations or articles containing the substance. In this risk assessment report, the term processing only covers the industrial transformation of PCOC into phenoxy acids. The term formulation covers the final stage in the manufacture of the plant protection products.

In this assessment report, the applied scenarios are based on the adoption of monitoring data from the two main manufacturers. The monitoring data covers the total emissions from the main production sites where production, processing and formulation takes place on the same manufacturing site. A part of the phenoxy acids are formulated elsewhere and therefore this scenario is included and the exposure estimations are based on TGD since monitoring data were not available.

Scenario:	Exposure estimation based on:	Compartment of primarily release:
a) Production of PCOC, processing and formulation of phenoxy herbicides at the same site	Monitoring data	Surface water
b) Formulation at another site	TGD/EUSES (generic)	Surface water
c) Agricultural use of herbicides	USES 1.0 (generic)	Agricultural soil

3.1.1 General discussion

3.1.1.1 Production

PCOC is produced and used in the production of pesticides and the exposure to the environment is related to the production of the pesticides and the degradation of the pesticides after application. The chlorophenols used in the production of MCPA, MCPB, MCPP and MCPP-P are obtained by chlorination of *o*-cresol, a starting material in abundant supply in Europe as a product of coal tar distillation. Although, chlorination occurs mostly at the 4-position, 6-chloro- and 4,6-dichloro-2-methylphenol are also produced when chlorine or alkali hypochlorites are used. Other cresol production ways are catalytic and thermal cracking of naphtha fractions during petroleum distillation, or direct production of *o*-cresols from methylation of phenol in the presence of catalysts (Fiege 1986).



The crude PCOC is purified by distillation.

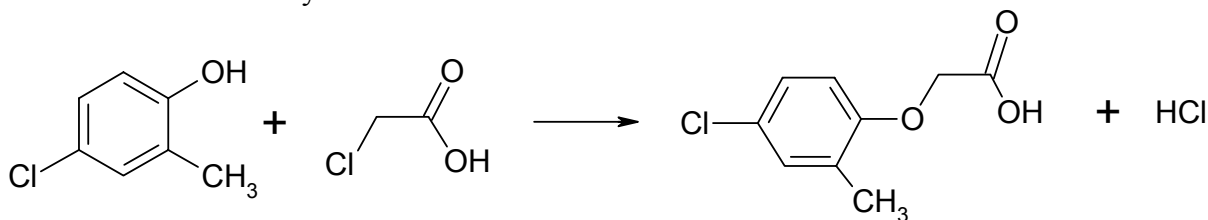
3.1.1.2 Processing

Most of the *o*-cresol manufactured in Europe is chlorinated to 4-chloro-*o*-cresol (PCOC) the starting material of the chlorophenoxyalkanoic acids; 4-chloro-2-methylphenoxy acetic acid (MCPA), 4-chloro-2-methylphenoxy butyric acid (MCPB), 2-(4-chloro-2-methylphenoxy)-propionic acid (mecoprop, MCPP) and its isomer mecoprop-p (MCP-P).

MCPA

CAS no.: 94-74-6. Molecular formula: C₉ H₉ Cl O₃. Molecular weight: 200.6.

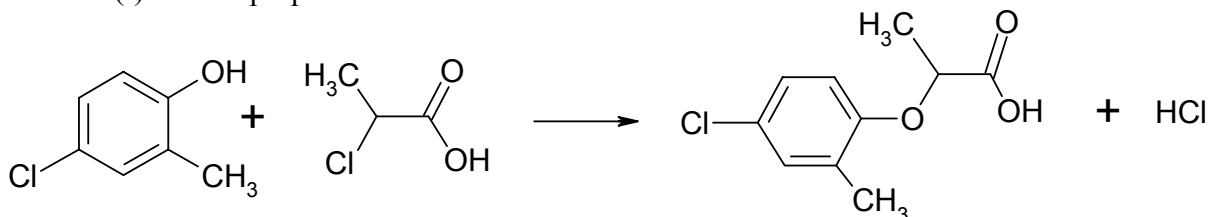
MCPA acid is formed by condensation of PCOC with monochloroacetic acid:



Mecoprop (MCP-P) / Mecoprop-P (MCP-P)

CAS no.: 7085-19-0 (racemate), 16484-77-8 (MCP-P). Molecular formula: C₁₀ H₁₁ Cl O₃. Molecular weight: 214.7.

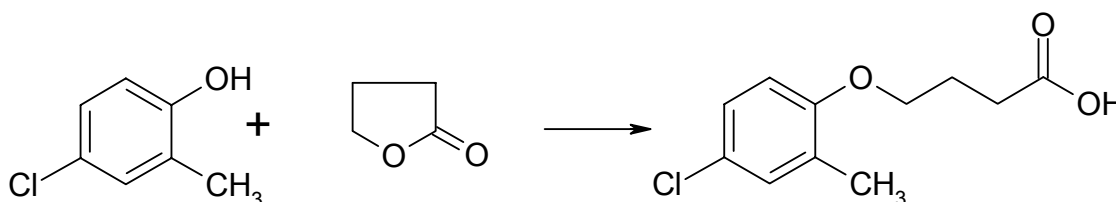
MCPP is formed by the condensation of PCOC with 2-chloropropionic acid. MCPB-P which is the biocidal active isomer is manufactured by a similar process in the same plant but by using the single isomer S(-)-2-chloropropionic acid.



MCPB

CAS no.: 94-81-5. Molecular formula: C₁₁ H₁₃ Cl O₃. Molecular weight: 228.6.

MCPB acid is manufactured by condensation of PCOC with gamma butyrolactone.



The phenoxy acids are produced as flaked solids, sold for further processing elsewhere or used on site for making fluids, aqueous salts or esters or formulations.

3.1.1.3 Formulation

MCPA, MCPB, and MCPB are formulated and sold as various kinds of phenoxy herbicides: acids, salts or esters. This takes place either at the manufacturer site or elsewhere.

3.1.1.4 Environmental release

Environmental release may take place from the production of PCOC, processing into phenoxy acids or from the formulation of the herbicides. All three processes may take place at the same site or the technical phenoxy acids is sold for the final formulation to take place at a separate site. According to manufacturers (pers. comm. 1997) no PCOC leaves the production sites.

3.1.1.4.1 Production, processing and formulation

According to TGD, the main category is Ib (intermediates stored on-site), the industrial category is 3 (chemical industry: chemicals used in synthesis) and the use category 33 (intermediates). The release from production, processing and formulation of PCOC is estimated based on monitoring data or by using the Emission Scenario Document (TGD, part IV, 1996) on intermediates and presented in the appendix 4 (EUSES v.1.0). For confidentiality, the average volumes are used.

Production

The local and regional values from production are based on the approximate production volume per production site according to the information given by the two main manufacturers covered by the Regulation (i.e. at each site 1/2 of the total EU production volume). All waste water from these two

industrial plants is treated in municipal biological Sewage Treatment Plants (STPs) before release to surface waters.

Processing

PCOC is used at the manufacturing site in the production of technical phenoxy acids and thus remains on-site. It has not been possible to obtain a precise figure for the number of plants producing and processing PCOC in EU. However based on information from the main manufacturers, the total number of processing plants in the EU covered by the Regulation is two which is used in this risk assessment.

Formulation

The technical phenoxy acids are formulated into phenoxy herbicides. It has not been possible to obtain a precise figure for the number of plants formulating phenoxy herbicides (based on PCOC) in EU. The two main manufacturers inform that they each formulate approximately 60% of the production volume of phenoxy acids on-site, that at least 30% of the production volume of phenoxy acids are exported out of EU and approximately 5% to 10% of the production volume is formulated outside the two main manufacturing sites but within EU. As *worst case*, therefore, *the approximate volume formulated elsewhere is estimated to be 10% of the total production volume and all formulated at one site.*

Summary of annual total production, processing and formulation volumes

Production: 15000 tonnes PCOC
 Processing: 15000 tonnes PCOC used to produce 21000 tonnes phenoxy acids,
 30% exported for formulation outside EU
 Formulation: 60% of production volume formulated on-site (9000 tonnes PCOC eqv.) and
 10% of the total phenoxy acid volume formulated elsewhere within EU (cf. below)

Regional release

For regional release, based on the information provided by the major manufacturers it is estimated that each production site is located in one region. Two main manufacturers are known, therefore, at the specific site ½ of the total EU PCOC production volume occurs and is processed into phenoxy acids and that 60% of this volume is formulated into the final product. The total volume released in the region is averaged over the year (365 days).

According to TGD the following default regional releases would occur:

Regional environmental release estimated according to TGD

Life-stage	Production of PCOC			Processing (manufacture of phenoxy acids)			Formulation of phenoxy herbicides			Total	
	No. of sites	2 (~7500 t/yr)			2 (~7500 t/yr)			2 (~4500 t/yr)			
Emission to:	Fraction	t/yr	kg/d	Fraction	t/yr	kg/d	Fraction	t/yr	kg/d	t/yr	kg/d
Air	0.00001	0.075	0.205	0.00001	0.075	0.205	0.001	4.5	12.33	4.65	12.7
Waste water	0.003	22.50	61.62	0.0005	3.75	10.3	0.003	13.5	36.99	39.75	108.9
Soil	0.00001	0.075	0.205	0.0001	0.75	2.05	0.0001	0.45	1.23	1.28	3.5

However, monitoring data from the two main manufacturers have been submitted. Because the monitoring data generally covers the total emissions from the specific production site, one scenario in

the risk assessment are based on the actual monitored values and identified "site specific" and where monitoring data are not present, values according to TGD are calculated. For confidentiality, average values are used.

A scenario on formulation was included in the risk assessment, because 10% of the production volume is formulated outside the two main manufacturers. The number of sites where formulation takes place is unknown and therefore, 10% of the total production volume of the phenoxyherbicide is estimated to be formulated at one other site (worst case) and release based on the default estimation procedures of the TGD. According to the manufacturers the content of PCOC as an impurity in the technical acids are below 1% (AHMarks 1997b, Nufarm 1997) and therefore 1 % is used in the assessment for formulation (cf. e.g. the footnote to the following table).

Emission to:	Specific site *		Formulation site **		
	t/yr	kg/d	Fraction	t/yr	kg/d
Air	0.2	0.6	0.001	0.021	0.058
Waste water	2.8	7.8	0.003	0.063	0.173
Soil	0	0	0.0001	0.002	0.006

*: Based on monitoring data from specific site including production, processing and formulation (cf. text above).

** : According to a worst case consideration (cf. above) the PCOC content in the phenoxy acids is max. 1%. Thus, a fraction of 0.001 of the total phenoxy acid production volume is used as the input volume to the release scenario.

3.1.1.5 Agricultural use

The following recommended application rates are taken from Pesticide Manual (9th ed., 1991):

MCPA:	0.3-2.25 kg /ha.
MCPP:	1.8-2.4 kg /ha.
MCPB:	1.7-3.4 kg /ha.

By considering these figures and the consumption volumes of these three different phenoxy herbicides "a realistic worst case" application rate of these herbicides of 2 kg/ha can be estimated.

PCOC is found as impurity in phenoxy herbicides: 0.2 to 0.5% in MCPA (HSDB, Seibert 1986, Technical product), 0.645-0.67% in MCPA-dimethylammonium, and 0.05-0.06% in MCPA -sodium-salt. Only Hattula (1978) reports on 4% PCOC as impurity in MCPA from Kemira Co, Finland, while A.H.Marks (1995) mentions < 1.0% impurity in a letter to Danish-EPA.

Considering these reported percentages of impurities in the herbicides and confidential information regarding the impurities in formulated phenoxy herbicides from the Danish EPA's Pesticides Division (pers. comm.), a general percentage of PCOC in these herbicides is today estimated to be 0.5 % according to "the realistic worst case concept".

3.1.2 Environmental fate

3.1.2.1 Degradation

PCOC is not expected to spontaneously *hydrolyse* (Lyman 1982) at environmental conditions as covalent bound substituents to a benzol ring normally is hydrolytically stable.

Formation of PCOC by photolysis of MCPA

PCOC is a photolysis degradation product of MCPA and a possible degradation product of MCPP. The major photodegradation product of MCPA was PCOC. The concentration was increasing with time (Clapes et al 1986, Benoit-Guyod *et al.* 1986). PCOC is further photodegraded to o-cresol and

methylhydroquinon (Clapes et al 1986). Photodecomposition is suggested by Clapes & Vicente (1986) by substitution of the chlorine by an hydroxyl group or by dehalogenation to 2-methylbenzene and 1,4-dihydroxy-2-methylphenol. Freiberg & Crosby (1988) suggest photodecomposition of PCOC to 5-chlorosalicylaldehyde and o-cresol or 2 methylphenol.

In sunlight (>300 nm) or under 40 W UV blacklight (Soderquist & Crosby 1975, Crosby & Bowers 1985), MCPA is degraded to PCOC, 4-chlorosalicyl-aldehyde, 4-chlorosalicylic acid and 2-methylphenol.

Crosby & Bowers (1985) found in a photoreactor using a spray solution of 200 mg/l MCPA that after 3.5 days of UV-irradiation 25% of the applied MCPA was degraded and PCOC increased to a maximum of about 12% of applied amount. Irradiation of droplets in an open dish gave noticeable odour of PCOC and chemical analysis confirmed PCOC to be the principal constituent. The low residues recovered may be the result of volatilization following the irradiation of MCPA/MCPP. In a field exposure, PCOC was removed by volatilization as it was formed. After 31 days outdoor exposure to sunlight in California, PCOC was 1.3% of original MCPA (Crosby & Bowers 1985).

In a simulated field study on photolysis using MCPA-dimethylammonium (MCPA-DMA), droplets containing 14.7 g MCPA/l were created at the tip of a 1.0 µl syringe and irradiated for 5 days. The evaporation residues contained 36% PCOC (Freiberg & Crosby 1986) and in the gas phase 92% PCOC. The degradation was 41% to 44% of the applied MCPA. After the application of a MCPA-DMA (480 µg/40 µl = 12 g/l) solution on a glass plate and irradiated for 6 days, it was found that 49% of the residues was PCOC.

A 71 hour irradiation of a 100 ppm MCPA solution with simulated sunlight ($\lambda > 290$ nm) resulted in the formation of 6% PCOC of the applied amount (Soderquist & Crosby 1975).

Photolysis of PCOC

The UV-spectrum of PCOC shows maximum absorption near 280 nm with an absorption tail reaching 300 nm. The effect of sunlight irradiation on aqueous solution of PCOC (100 mg/l = 0.7 mM) was studied (Soderquist & Crosby 1975). The PCOC solution was sealed in a flask to prevent volatilization. The exposure to "summer sunlight" (not further defined or specified) in California resulted in a stated photolytic half-life of 2.5 days (which from the presented graph rather seems to be 4 days) (Crosby & Bowers 1985).

In the Appendix "Photolytic degradation of PCOC in surface water" (cf. *appendix 1*), the estimation of the photolytic degradation in EU surface waters was performed by relating the sun light intensity in California (40° N) to EU (50°N) and according to TGD the dimensions of the "standard environment for EU" employed in the regional model for calculation of $PEC_{regional,water}$, i.e. a water depth of 3 m and a concentration of suspended solids of 15 mg/l. This results in a half-life for photolytic degradation in water of 301 days (annual mean) and 715 days (winter). Thus, the *photolytic degradation of PCOC in surface waters of EU is concluded to be negligible*.

Photolysis in the atmosphere

Experimental data on photochemical oxidation by OH-radicals are not available, however, using the model of Atkinson (1986), the degradation rate $k_{OH} = 1.3 \times 10^{-11} \text{ cm}^3/\text{mole} \cdot \text{sec}$ and the averaged OH-radical concentration $5 \times 10^5 \text{ molecules/cm}^3$, an *atmospheric half-life of 30 hours* can be calculated (BASF 1991).

3.1.2.2 Aerobic biodegradation in water

The toxicity to microorganisms of chlorophenols was studied as growth inhibition test on agar plates using bacterial isolates from a polluted and an unpolluted stream. PCOC in a volume of 0.01 ml and in the concentration 250 mM was observed to inhibit the growth of microorganisms (Milner and Goulder 1986).

PCOC is not readily degradable according to the modified MITI (I) test. In the MITI test 0% degradation was found at a test concentration of 100 mg/l (MITI 1992). As other studies at lower concentrations do find biodegradation the result is expected to be a consequence of toxicity to bacteria at the high test concentration. (e.g. bacterial toxicity was observed in the *Salmonella typhimurium* mutagenicity test at 500 µg PCOC/plate).

In a pilot plant study on activated sludge using sludge back-feeding and sludge from a municipal STP, the aerobic degradation on a mixture of chlorinated phenolics was studied (Buisson *et al.* 1988). The concentration of PCOC in the influent and effluent was in the order of 100 to 200 ng/l. The temperature was 17.5 °C. PCOC was found to be removed by adsorption and biodegradation but the relative importance of these processes was not investigated. The removal was found to depend on the sludge age. The reported removal and recovery percentages at sludge age of 4, 6 and 9 days were 10 and 88, -20 and 115, 36 and 63, respectively. A low removal of PCOC was thus observed under the study conditions. Biodegradation was probable under these conditions allowing adaptation of the microorganisms to PCOC but the data from the pilot plant study are not quantifiable in order to estimate a degradation rate in STPs. A biodegradation half-life of PCOC can therefore not be deducted from this study. The observed low removal of PCOC may be caused by transformation of other present chlorophenolics to PCOC. Another possible explanation may be that the other chlorophenolics inhibited the biodegradation of PCOC. This indicates that an assessment of the removal or degradation of chemical substances in studies performed on each individual substance may overestimate the actual biodegradation and thus, the total removal in STP where several substances are present at the same time.

In a shake flask die away test using DOC analysis at 15°C over 10 days, the degradation of PCOC in sea water from an initial concentration of 18 µg/l PCOC had a half-life of 3 days. In a mixture using 3.6 µg/l PCOC and waste water, the degradation was reduced and the half-life increased to 45 days, which like the study described above either suggests an inhibitive effect on the microorganisms active in the degradation of PCOC caused by the other organic compounds present in the mixture (0.1-0.5 mg/l) or that these other compounds were transformed to PCOC (Lindgaard-Jørgensen 1989).

3.1.2.3 Aerobic biodegradation in soil

Several degradation studies confirm PCOC to be the primarily metabolite of MCPA (e.g. Bollag *et al.* (1967), Paasivirta *et al.* (1983), Duah-Yentumi & Kuwatsuka (1980), Gaunt & Evans (1971), Gamar & Gant (1971) and Oh *et al.* (1995). In experimental studies, it is found that PCOC by biodegradation of MCPP and MCPA is a biodegradation product which will be further degraded (Smith 1985). The reported concentration of PCOC which is formed in the degradation process is mainly 2 to 5% of the applied amount of the phenoxy herbicide. In one study (Duah-Yentumi & Kuwatsuka 1980) in a fairly acid soil with pH 5.3, a maximum of 2% to 55% of the applied MCPA was reached after 25 days depending of the pH of the soil. "A realistic worst case" seems to be in the order of 5% of the applied pesticide dosage based on the majority of studies. In acid soils, however, considerably higher concentrations may occur.

The degradation half-lives of PCOC in aerobic soil are reported from few studies to be 14 to 21 days. For instance, Kinkannon and Lin (1985) found a half-life of 14 days in a bioreactor. The reactor was

filled with sandy loam covered with DAF sludge (not defined, 33 g/kg soil) and mixed into the top 20 cm soil. The sludge was spiked with 304 ppm PCOC and the degradation followed over 82 days.

The degradation of PCOC in loamy sand and sandy loam after application of 10, 200 and 2000 ppm PCOC was found to have a half-life of 14 days (Sattar 1981). The degradation rates in sandy clay were 0.0378 d^{-1} at the application of 10 mg/kg soil and 0.029 d^{-1} at 1000 mg/kg soil. The half-lives calculated as $T_{1/2} = 0.693/k$ were equivalent to 18 days and 24 days (Sattar 1989). An estimated half-life for degradation of PCOC in soil seems to be approximately 21 days ($k = 0.033 \text{ d}^{-1}$) according to the "realistic worst case" concept.

This latter biodegradation half-life in soil is based on considerably more experimental evidence than the above mentioned degradation half-life in surface waters. However, the half-lives for degradation in soil and surface water seem generally to be somewhat conflicting, because degradation half-lives are generally said to be of the same order of magnitude (Boethling *et al.* 1995) or twice as long in soil than in surface water for a substance with a $K_p < 100$ (TGD, 1996). Based on these considerations, a general approximate half-life for aerobic biodegradation in surface waters as well as in soil of 21 days seems justified according to "the realistic worst case concept".

Biodegradation half-life, conclusion

A *biodegradation half-life in soil and in surface water of about 21 days* would according to the TGD (cf. Chapter 3 table 5 & 6) indicate that the substance could be regarded as readily biodegradable in soil and surface water. By using this and the TGD concerning degradation rates for biodegradation in STPs (cf. TGD, Chapter 3, table 4), *an estimated degradation rate constant K_{STP} of 1 h^{-1} (half-life of 0.7 h)* can be estimated.

There is, however, quite some uncertainty as regards the biodegradability of PCOC, also because of the uncertainty as regards the extrapolation from degradation half-lives in soil and surface water to a degradation rate in STP. Based on the available information, it therefore seems to be justifiable to include for information the EUSES model estimations employing half-lives equivalent with inherent biodegradability (cf. *appendix 4B*).

3.1.2.4 Anaerobic degradation

Anaerobic degradation in sewage sludge treatment pilot plant has been studied by Buisson *et al.* (1986). PCOC was resistant to chemical or biologically mediated changes (no abiotic or biotic degradation) during anaerobic degradation at $10 \mu\text{g/l}$. PCOC was also resistant to anaerobic degradation in soil. Buisson *et al.* (1986, 1990) and Kirk & Lester (1988) found no anaerobic degradation within 32 days.

3.1.2.5 Adsorption

In an experimental adsorption/desorption study from New Zealand on an acid soil (pH 5.2 and 3.6% organic carbon), a low adsorption coefficient; K_d 0.008, was observed and the resultant K_{oc} 0.22 was calculated (Bhamidimarri & Petrie 1992). Buisson *et al.* (1986) observed some adsorption of PCOC to sludge from a municipal STP, but no K_d or K_{oc} was given nor could they be estimated based on the available information. Based on an estimated K_{oc} of 400, calculated from K_{ow} (TGD: $\log K_{oc} = 0.81 \log K_{ow} + 0.10$), PCOC may exert a medium adsorption in soil and may partition to sediments and particulate materials in water. PCOC has a pK_a of 9.71 (Weast *et al.* 1986) and the adsorption may be sensitive to pH. The adsorptive capability will increase and the leaching potential will decrease in increasingly alkaline soils due to a greater presence of the ionic form under alkaline conditions. Thus, in acid soils leaching may be expected.

Various QSAR estimations give a K_{oc} of 14 to 700. Analogue substances like chlorobenzenes have K_{oc} 's of 83 to 389, chlorophenols approximately 51 and cresols 22 to 49. Due to lack of an experimental K_{oc} in non-acidic soils which are more representative for most soil types in the EU, the calculated value of $K_{oc} = 400 \text{ l/kg}$ has therefore been used in the risk assessment.

The *adsorption to sediments* is unknown but based on an estimated K_{oc} of 400, PCOC is expected to adsorb to sediments and particulate materials in the water column depending of the pH.

3.1.2.6 Bioaccumulation

A log K_{ow} of about 3 indicates that bioaccumulation may occur.

However in a bioaccumulation test on orange red killifish, *Oryzias latipes*, during 42 days at 25°C after OECD 305C and a concentration of 2 µg/l, a BCF of 6.4 to 14 was found, and at 20 µg/l a BCF of 8.2 to 28 was found. The fish average lipid content was 4.9% (MITI 1992).

In a 28 days study on rainbow trout, *Salmo trutta*, Hattula (1979) found BCF 6.9 to 4.3 at concentrations 0.5 to 1.5 ppm (average 6.6 at 0.5 ppm, 4.7 at 1.0 ppm and 4.3 at 1.5 ppm). In a short term study (24 hours) the BCF was 8.2. Based on the log K_{ow} and the time to reach equilibrium in a BCF fish study : $t_{95} = 3.0/k_2 = 3.0/(-0.414 \log K_{ow} + 1.47)$ (cf. OECD Test Guideline 305, 1996), an estimated $t_{95} = 16$ hours is obtained, i.e. steady state in the above mentioned bioconcentration studies can be assumed and the measured BCF (fish) values therefore regarded as reliable.

Based on the above mentioned data, a "realistic worst case" *BCF for fish is 30*.

3.1.2.7 Environmental distribution

Volatilisation. PCOC may form rapidly from sun irradiated water solutions or irradiated deposits or volatilize from water. In a study (Seiber et al 1986) around flooded rice fields in California treated with MCPA at 0.87 kg ai/ha, it was observed that air samples contained more PCOC than MCPA. Several kilometres from the fields 30 ng/m³ PCOC was found. The highest normalised flux was found on the day of spraying and decreased with time. The daily averaged volatilisation flux for day 0, 1, 2 and 3 was 1.27, 0.43, 0.27 and 0.24 ng/cm²/h.

The volatilisation was evaluated by Henry's Constant, H . H was calculated to be 0.11 Pa m³/mol (VP 3.2 Pa, SOL 4 g/l at 25°C) by Seibert *et al.* (1986). However, using VP 26.66 Pa and SOL 2.3 g/l resulted in $H = 1.65 \text{ Pa m}^3/\text{mol}$. All results indicate that volatilisation may be expected from water and wet soil.

Performing a Mackay fugacity level I calculation (Mackay & Paterson 1990) based on physico-chemical properties results in an environmental compartment distribution of 33% in air, 56% in water, 6% in soil and 5% in sediment.

3.1.2.8 Summary

The environmental exposure assessments considered combine the relevant exposure scenarios for the substance and apply recommended assessment methods for deriving PEC local and regional, i.e. the applied environmental exposure scenarios are:

Scenario:	Compartment of primarily release
a) Production of PCOC, processing and formulation of phenoxy herbicides at the same site (monitoring data)	surface water
b) Formulation at another site (generic)	surface water
c) Agricultural use of herbicides (generic)	agricultural soil

Performing a Mackay fugacity level I calculation (Mackay & Paterson 1990) results in an environmental compartment distribution of 33% in air, 56% in water, 6% in soil and 5% in sediment.

4-Chloro-2-methylphenol (PCOC) may be released to the environment in waste water and air effluent from its production and its use as a chemical intermediate in the synthesis of phenoxy herbicides (MCPA, MCPB, MCPP). Environmental release is also present via degradation at points of herbicide application and sites of subsequent environmental transport.

Considering the reported percentages of impurities in the herbicides, a general impurity percentages in these herbicides according to the "realistic worst case" approach of 0.5 % is used.

Soil exposure to PCOC from degradation and impurities of the herbicides is estimated to be maximum 5 % of the herbicide application rate of 2 kg/ha. It is noted that there will be a prolonged exposure of PCOC after the application of herbicides which are continuously broken down via PCOC.

If released to the atmosphere, PCOC may be physically removed by settling or washing out in precipitation. Model calculations indicate that the photochemical degradation in the atmosphere is rapid with an estimated half-life rate of 1.25 days whereas photodegradation in surface water is negligible.

Available data suggest that PCOC is biodegradable in soil and surface waters under aerobic conditions with an approximate half-life of 21 days ($k = 0.03 \text{ d}^{-1}$) and resistant to anaerobic degradation. By using the estimation tables of the TGD concerning degradation rates for biodegradation in STPs, a degradation rate constant K_{STP} of 1 h^{-1} can be estimated. The available experimental data on biodegradation are somewhat conflicting and the estimated half-lives are quite uncertain.

The adsorption coefficient in soil (K_{oc}) is calculated to be 400 l/kg. Volatilisation is expected to be slow. Henry's Law constant is calculated to be $1.65 \text{ Pa m}^3/\text{mol}$.

The hydrolysis of PCOC in water is estimated to be negligible.

A "realistic worst case" BCF for fish is 30.

3.1.3 Aquatic compartment

3.1.3.1 Measured data

Historical data exist from a Danish production site of phenoxyherbicides which is no longer operating. The effluent from a municipal waste water treatment plant receiving waste water from the plant had PCOC as the dominant chlorophenol. The effluent from the manufacturer (600 m³/d) contained 2400 µg/l PCOC (1.4 kg PCOC/d). The effluent was diluted before entering a biological STP to 3% of the total waste water loading and the PCOC concentration in the influent was thus reduced to 72 µg/l. The effluent had a mean concentration of PCOC of 4 µg/l (64 g/d), resulting in a total removal of 94% of the inflow concentration (Folke & Lund 1983, Folke 1984). These values can, however, not be used in this risk assessment because no information about the representativeness of this single measured value is available. Furthermore, no information about the concentration of PCOC in the waste water nor of the dilution in the receiving river was present.

Monitoring results from the effluent from the two main manufacturing sites ranged from <1 mg/l to 45 mg PCOC/l in the raw effluent leaving the production sites including production, processing and formulation. The average concentration was 34 mg/l during a one year measuring period (1996 to 1997) of one manufacturing site but during a one-week period from both manufacturers in October 1997 values around 18 mg/l was measured.

The raw effluents from the manufacturing sites were diluted with municipal STP influent before STP treatment. Dry weather flow at the municipal STPs varied from 130,000 m³/day to 200,000 m³/day.

The measured concentrations in STP effluent varied from below detection level to 3.6 µg/l at one of the two main production sites. In the two STP effluents receiving waste water from the main production sites, the same variation in measured concentrations was observed. Because the detection limit is approximately 3.6 µg/l, the level before dilution in the receiving rivers is estimated to be <3.6 µg/l (A.H. Marks and Nufarm, October 1997).

Of more recent surface water monitoring data, a single sample from approximately 1.3 km downstream from a municipal STP discharge was sampled and analysed. The municipal STP received waste water from a PCOC production site. PCOC could not be measured above a detection limit of 0.2 µg/l, and therefore, it was concluded that PCOC concentration was below 0.2 µg/l. However, because this value can not be validated as regards representativeness according to the TGD, the figure can not be used directly in the assessment.

In a monitoring programme during September 1997, 2 km downstream in the receiving river during the production period, the measured concentrations ranged from <0.2 to 3.0 µg/l. The instrument detection limit was observed to be 0.2 µg/l. The limit of detection (LOD) was found to be 3.6 µg/l and the limit of quantitation (LOQ) 12 µg/l. During a factory "shut down" period, no PCOC was detected in the river. The analytical method was modified which reduced the LOD to 0.7 µg/l and LOQ to 2.4 µg/l. It was concluded considering the measure error that the concentration in surface water was less than 3.6 µg/l.

After the application of MCPA to a rice field in California, PCOC was measured in the water during 4 days. The concentrations found were relatively constant confirming the continuous transformation of MCPA to PCOC and the intermediate nature of PCOC. PCOC concentrations of 1.4, 1.3, 1.2 and 1.3 µg/l were measured on day 0, 1, 2, 3 after application, respectively (Seiber *et al.* 1986).

3.1.3.2 Aquatic exposure estimations

The local emissions and concentrations rely on the monitoring results from the two main manufacturers. For comparison, the local emission from production, processing and formulation is also estimated according to the TGD (cf. appendix 3 for TGD calculation methods and appendix 4 for the results of the model calculations employing EUSES v.1.0).

The observed removal in a Danish STP was 94% (including adsorption, evaporation and degradation) (Folke 1984). However, it is not known how representative this percentage of removal is for biological STP's of the EU in general, but the observed removal figure is in general accordance with calculated removal figures employing EUSES, i.e. the SIMPLETREAT model using the environmental fate data mentioned in section 3.1.0 (cf. also appendices with print out of results from EUSES model calculations). Thus in the estimations, the TGD based removal value of 88% (cf. TGD erratum, 19 february, 1997), is used.

The results from the manufacturer monitoring programmes are inconclusive regarding the removal in STP as the measured values are approximately at the detection level after the dilution into the municipal sewage flow (130000 to 200000 m³/day) (AHMarks 1997b, Nufarm UK 1997b). However, a rough estimate of the removal in the municipal STP can be calculated. The average emission to STP waste water is 7.8 kg/day (cf. below). The concentration in the STP effluent was measured below 3.6 µg/l and using the highest average dry weather STP flow rate of 200,000 m³/day then $3.6 \times 10^{-6} \text{ g/l} * 200 \times 10^6 \text{ l/d} = 720 \text{ g/day}$ leaves the STP (worst case). The estimated removal would then be: $1 - (720 * 100 / 7800) = 91\%$. The result support the above made estimation.

PEC_{regional,water}

As regards the calculation of the PEC_{regional,water}: cf. the appendices with the results of model calculations employing EUSES 1.0 (appendix 4).

When PCOC is released from production, processing and formulation of herbicides:

PEC_{regional,water}: $1.69 \times 10^{-4} \text{ mg/l}$.

PEC_{regional,water} is not estimated in the pesticide scenario.

3.1.3.3 Calculations of PEC_{local,water}

3.1.3.3.1 PCOC released from production, processing and formulation:

The site specific emissions and concentrations are based on average monitoring results from the two main manufacturers. The waste water effluents from the production sites including production of PCOC, processing into phenoxy acids and formulation to phenoxy herbicides together with water from air scrubber etc. are collected and chemically treated in a main effluent treatment plant on-site prior to disposal via tanker or drain to the effluent system. The measured concentrations in the raw effluent are shown in the table below.

PCOC concentration in on-site effluent before entering the STPs.

PCOC (mg/l)	Minimum	Average	95% percentile	Maximum
Specific site 1	<1	17	29	45

Specific site 2	16	18	34	45
-----------------	----	----	----	----

At the municipal STP the raw effluent is mixed with the incoming domestic sewage water and passed to biological treatment beds before being discharged to the river. The STP dry weather flows varied from 130000 to 200000 m³/day.

During 1 week in October 1997, the concentration in STP influent was measured to vary between 0.15 to 2.0 µg/l (n=6, detection limit (DL) 0.1 µg/l) (Nupharm, 1997b).

The concentration in one of the specific STP during 1 week in October 1997, the STP effluent varied 0.13 to 3.1 µg/l (n=6, DL 0.1 µg/l). During one month, September 1997 at the other STP, the measured concentration of PCOC in the STP effluent was <0.2 to 3.3 µg/l (n=13, instrument detection limit 0.2 µg/l).

In the risk assessment on specific sites where production, processing and formulation takes place, the average measured values where available are used (AHMarks 1997, Nufarm 1997, 1997b). For illustrative purposes appendix 3 shows a comparison of environmental exposure estimates from main manufacturing processes: production, processing and formulation, respectively, calculated according to TGD with the measured values.

The local emission during episode to the aquatic compartment, $E_{local,water}$, is calculated in EUSES by using the regional values in section 3.1.1.4 multiplied with the estimated release fractions. The release fraction for production was set to 0.5 due to two main manufacturers, 0.5 for processing as PCOC is not used elsewhere and 0.3 (0.5x60%) for formulation as this part of the life cycle was performed at another site. The site specific STP flow rate of 1.3×10^5 m³/d is included, because this is the lowest flow of the STPs receiving waste water from the two known manufacturers.

The release estimations from the formulation performed outside the specific sites are calculated according to TGD using 10% of total production and a PCOC content of the formulation of 1% (worst case). The default local waste water volume is according to TGD: 2000 m³/d, and number of days of emission is according to TGD: 300.

The average local on-site monitoring results and the estimated results on a generic formulation site (10% of total production volume) are shown below.

Concentration in waste water before treatment in municipal STP

Life cycle stage	Based on	Emission (t/y)	Emission (kg/d)	C _{site effluent} ** (mg/l)	C _{STP influent} (µg/l)
Specific site	monitoring	2.5 *	7.8 *	29 & 34	43 & 52***
Formulation (10% of total)	TGD defaults	0.063	0.21	-	110

*: Estimated by using measured effluent concentration at each of the two sites times the respective volumes of waste water at the sites. (At these sites production, processing and formulation occurred (cf. the text)).

** : Measured concentrations from each of the two sites' waste water (from production, processing and formulation) before dilution at STP, 95% percentile.

***: Average concentrations, estimated by using the average measured effluent concentration times the actual dry weather STP-dilution at each site. Measured concentration at one of the sites was one order of magnitude below the estimated concentrations but not much above the detection limit.

For the *site specific scenario* and in accordance with the principle of “realistic worst case”, a concentration (3.6 µg/l) from the upper range of the monitoring data of the STP effluents has been used (AHMarks 1997b, Nufarm 1997b). This concentration is in general accordance the estimated

“realistic worst case” concentrations in the STP effluents without any dilution in the receiving river. Measured concentrations approx. 2 km downstream one of the sites were fluctuating between a few µg/l and one order of magnitude below.

Local concentration during emission episode, PEC local_{river water}

	Clocal _{effluent} (mg/l)	Clocal _{river,water} (mg/l)	PEC local _{river water} *
Site specific (measurements)	0.0036	0.0036	0.0038
Formulation (estimations)	0.0126	0.0013	0.0014

*: Including PEC regional_{river water} 0.000169 mg/l.

The annual average concentration is estimated below to be:

Annual average concentration, PEC local_{river water, ann}

	PEClocal _{water, ann} *
Specific site **	0.0037
Formulation (TGD default)	0.0012

*: Including PEC regional_{water}.

** : Based on monitoring data

Calculation of PEClocal for sediment

The local concentration in sediments during emission episode is calculated according to TGD (cf. appendix 3).

Predicted environmental local concentration in sediments (PEClocal_{sed})

	PEC local _{water} (mg/l)	PEC local _{sed} (mg/kg)
Specific site **	0.0038	0.036
Formulation	0.0014	0.011

** : Estimated using monitoring data.

Calculation of STP concentration for evaluation of inhibition of microorganisms

For the risk characterisation of PCOC regarding microorganisms in STP, ideally the concentration in the aeration tank should be used. Because this value was not available, the dissolved concentration of PCOC is assumed to be equal to the effluent concentration according to the TGD:

$$PEC_{STP, microorganisms} = C_{effluent}$$

PEC_{STP, microorganisms}

Life cycle stage	PEC _{STP, microorganisms} (mg/l)
Specific site**	0.004
Formulation	0.013

** : Estimated using monitoring data.

3.1.3.3.2 Agricultural use of phenoxy herbicides

It is noted that the TGD does not include exposure scenarios for pesticides.

An initial exposure assessment for surface waters according to Annex VI of dir. 91/414/EEC, i.e. Directive 94/43/EC, is presented here. It is noted that the latter directive was annulled by an EU Court decision in 1996.

The aquatic environment close to areas where the herbicides are applied may receive direct exposure by overspraying (ponds, ditches, streams). It is assumed that direct application to a water body of 1 ha, 1/3 meter deep and density 1.0 takes place. The above described application would result in $10000 \times 0.333 = 3333 \times 10^3$ l. Using the application rate 2 kg/ha of e.g. MCPA, and assuming PCOC as 0.5% impurity and 4.5% as degradation product, the *initial* concentration would be: $100/3333 = 0.03$ mg/l. It is noted that the duration of exposure will be prolonged due to continuous degradation of MCPA to PCOC.

The concentration in surface water based on indirect exposure via spray drift from a nearby agricultural application (2 kg phenoxy herbicide/ha, resulting in 100 g PCOC/ha, 3% spray drift) is estimated to be 0.0009 mg/l.

USES ver 1.0 (employing the country code specifications for EU according to the TGD) (RIVM, 1994) which includes a pesticide scenario, calculates the initial concentration in a ditch to 0.0008 mg/l.

The PEC_{local, water} is calculated based on the yearly volume of PCOC which may be released to and within the environment whereas the estimations of PEC by direct application of the herbicides to water bodies are based on the steady state exposure where account of the continuous degradation from the herbicides is taken.

It is noted that surface waters besides exposure from STP receive contributions from possible incidences of direct application, spray drift, run off and atmospheric deposition.

3.1.4 Atmosphere

PCOC may enter the atmosphere from the production and processing. The use of MCPA, MCPB, and MCPP as agricultural herbicides results in the release of PCOC from evaporation and degradation to the atmosphere.

3.1.4.1 Measured data

Air from storage, handing and use of PCOC at the production sites are connected to a scrubber system to reduce emissions. Monitoring results of the process contribution from PCOC production combined at one of the manufacturing sites is estimated to be <0.027 mg/m³ based on the measured release 6.6×10^{-3} g/sec (0.57 kg/day). The concentration in air was below the detection level at

production site boundary. At the other manufacturing site the maximum quantities released from the plant main fume scrubber was 5 mg/m³ or 0.034 kg/hour (0.8 kg/d)

Measurements in air at local STP and at 112 m from STP

Based on the results a dispersion programme using a Gaussian dispersion model calculated short term concentrations directly downwind (wind speed 3.76 m) at approximately 100 m. The maximum ground level concentration ranged 27.0x10⁻⁸ to 10.4x10⁻⁵ mg/m³ with a time weighted average of 6.8x10⁻⁴ mg/m³.

3.1.4.2 Atmospheric exposure estimations

PCOC used in production, processing and formulation

The concentration in air is estimated according to TGD at a distance of 100 meters from the point source. In the calculation for PEC_{local} for air, both emissions from a point source as well as the emission from a STP are taken into account. The maximum from the two concentrations (direct and via STP) is used as the PEC_{local}.

The annual average predicted environmental concentration in air, PEC_{local air, ann}, is the local annual average added to the regional concentration in air.

PEC_{regional air} : 7.8x10⁻⁷ mg/m³ (EUSES)

PEC local_{air} calculations

	Emission (t/yr)	Elocal _{air} (kg/d)	Estp _{air} (kg/d)	Clocal _{air} (mg/m ³)	Clocal _{air, ann} (mg/m ³)	PEClocal _{air, ann} (mg/m ³)
Specific site**		0.57	0.047	0.000158	0.000130	0.000131
Formulation	0.021	0.07	0.0014	0.000020	0.000016	0.000016

Elocal_{air} : The local direct emission rate to air during emission episode.

Estp_{air} : The local indirect emission to air from STP during episode.

Clocal_{air} : The local concentration in air during emission episode.

Clocal_{air, ann} : The annual average concentration in air, 100 m from point source.

** : Estimated using monitoring data on total release to air and waste water and TGD estimation methods

Deposition from air

The deposition from air includes the emissions from the two sources (direct and STP). The total deposition from air during emission episode is calculated as:

$$DEP_{total} = (E_{local_{air}} + Estp_{air}) * [F_{ass_{aer}} * DEP_{std_{aer}} + (1 - F_{ass_{aer}}) * DEP_{std_{gas}}]$$

The annual average total deposition flux is defined as:

$$DEP_{total\ ann} = DEP_{total} * 300/365$$

Deposition from the atmosphere calculations

	Elocal _{air} (kg/d)	Estp _{air} (kg/d)	DEP _{total} (mg/m ² /d)	DEP _{total ann} (mg/m ² /d)
Site specific *	0.57	0.047	0.00025	0.00020
Formulation	0.07	0.0014	0.00003	0.00002

*: Estimations based on monitoring data

3.1.5 Terrestrial compartment

3.1.5.1 Measured data

During monitoring groundwater in Denmark and among 10 chlorophenols searched for, PCOC was found in 5 measurements out of 825 (5 filters in two wells) in the concentration 0.040 µg/l to 8.79 µg/l (Groundwater monitoring, DGU, 1994). The detailed information below is from W.Brüsch (pers.comm 1995);

Copenhagen county, 27 meter below terrain: 0.1 µg/l

Copenhagen county, same as above 1 year later: 0.04 µg/l

North Jutland county, 15 meter below terrain: 8.7 µg/l

North Jutland county, 26 meter below terrain: 0.84 µg/l

North Jutland county, 18 meter below terrain: 0.32 µg/l

A single finding of 0.13 µg/l is reported from 1992. No phenoxyacetic acids were found in the same measurements (Groundwater monitoring, DGU, 1994).

In a Danish study on leaching of pesticides from arable land, samples of stream water and soil water in the depth 80 cm below soil surface 1 m away from the stream bank were taken every 2nd week during 2 years. PCOC was found in the soil water at one location with clay soil at 0.03 to 0.08 µg/l in 6 out of 48 samples and in the stream water at 0.01 to 0.12 µg/l in 3 out of 47 samples. PCOC was observed to be present from April to October (Spliid & Mogensen 1995).

The findings confirm that PCOC is present in the environment but being an intermediate in a degradation sequence with a relatively fast degradation rate, the amount is expected to be temporarily under aerobic conditions. Under anaerobic conditions, PCOC is considered persistent.

The evaporation from MCPA and MCPP and photodegradation of MCPA (and MCPP though no records) to PCOC is also a route to be considered but the contribution is not quantifiable.

Thus PCOC is found to be a degradation product (from MCPA and MCPP) which is further degraded or transformed. The results from MCPA studies indicate 3% to 15% of applied amount found as PCOC after 20 to 25 days after application. In studies on MCPP, 2 to 3% of the applied amount of MCPP (1 mg MCPP/kg) was recovered after 20 days (Smith 1985). More recent studies on aerobic degradation indicated that PCOC was an intermediary degradation product from MCPA never present at more than 5% of the applied amount (Matt 1990 cited by AH Marks 1995). In a study on the degradation of MCPP, it was observed that one transient metabolite reached a maximum of 3.5% of applied. The metabolite was not identified (Saxena 1988 cited by AH Marks 1995).

3.1.5.2 Terrestrial exposure estimations

Regional concentration in soil, $PEC_{\text{regional, soil}}$

As regards the calculation of the $PEC_{\text{regional, soil}}$, cf. the appendices with the results of model calculations employing EUSES ver. 1.0.

PCOC released from production, processing and formulation

PEC regional in agricultural soil 2.7×10^{-5} mg/kg ww

PEC regional in natural soil 8.6×10^{-7} mg/kg ww

PCOC released from agricultural use

PEC_{regional, soil} (EU): not calculated

Local concentrations (PEC_{local, soil}) from production, processing and formulation

The estimated concentration of PCOC in soil may be a result of atmospheric deposition and sludge application.

Deposition from air

The contribution from atmospheric deposition, D_{air} is derived by converting the total deposition flux $DEP_{\text{total,ann}}$ into concentrations (cf. *appendix 3*).

The contribution from wet and dry deposition from the atmosphere is not quantifiable but in the section on air, a calculation of total deposition has been estimated.

Sludge application

Sludge from both main production sites are incinerated or landfilled. Sludge from the municipal STPs treating the waste water is incinerated at one STP and used for field application in the other STP. Therefore the estimations below has been performed to cover the sludge application scenario according to the realistic worst case concept.

Only few data on measured concentrations of PCOC in sludge exist e.g. Buisson *et al.* (1984) measured 0.09 mg/kg dry weight in sludge from a municipal STP in UK. During a week in October 1997, the sludge from the STP receiving effluent from a production site and where the sludge is used in field application has been analysed. The measured PCOC concentration varied between <1 to 2 µg/kg sludge (n=6, DL 1 µg/kg).

The concentration in soil will be high just after sludge application and reduced in time due to removal processes (degradation, volatilisation, leaching, etc.). Therefore, the concentration is averaged over a certain time period for different endpoints according to the TGD:

	Depth of soil (m)	Averaging time (days)	Sludge application (kg _{dw} /m ² /year)	Endpoint
PEC _{local,soil}	0.20	30	0.5	terrestrial ecosystem
PEC _{local,agr. soil}	0.20	180	0.5	crops
PEC _{local,grassland}	0.10	180	0.1	grass for cattle

The concentration in dry sewage sludge, C_{sludge} , is based on monitoring data for the specific site. For the formulation site, C_{sludge} is estimated from the emission rate to water, the fraction of emission sorbed to sludge and the rate of sewage sludge production according to TGD.

The initial concentration in sludge and in soil after the first sludge application is tabulated below.

Concentration in sludge and in soil just after sludge application

	C_{sludge} (mg/kg dw)	$C_{\text{sludge,local,agr. soil}}$ (mg/kg)	$C_{\text{sludge, local,grassland}}$ (mg/kg)

Site specific **	0.002	0.000003	0.000001
Formulation	0.161	0.000237	0.000095

** : Estimated using monitoring data from STP (C_{sludge})

The concentration in soil after sludge application for 10 consecutive years is assumed to be a “realistic worst case”. However based on the removal rates and the calculations in the *appendix 3* (calculation of PEC local soil), the estimated concentrations after 10 years of consecutive applications remain the same as after just one year.

Removal rates

The first order constant for removal from top soil, k , is derived by adding the biodegradation ($k_{\text{bio}_{\text{soil}}}$), volatilisation (k_{volat}) and leaching rate constant (k_{leach}) calculated for PCOC according to TGD.

Removal rate constants

Soil depth	$K_{\text{bio}_{\text{soil}}} \text{ (d}^{-1}\text{)}$	$k_{\text{volat}} \text{ (d}^{-1}\text{)}$	$k_{\text{leach}} \text{ (d}^{-1}\text{)}$	$k \text{ (d}^{-1}\text{)}$
0.2 m	0.033007	0.000156	0.000197	0.033353
0.1 m	0.033007	0.000312	0.000393	0.033705
0.05 m	0.033007	0.000624	0.000785	0.034416

Local concentration in soil

The sum of both the concentration due to deposition and to the initial concentration from sludge application (cf. above) is used to estimate the local concentration in soil and averaged by the time periods in the table above. The results are tabulated below for the different endpoints.

For natural soil (soil depth 0.05 m), only the deposition from air is included because no sludge application is assumed.

$$\text{PEC}_{\text{local}_{\text{soil}}} = \text{C}_{\text{local}_{\text{soil}}} + \text{PEC}_{\text{regional}_{\text{natural soil}}}$$

PEC local_{soil}, however, in most situations are equal to C_{local_{soil}} because the regional contribution is estimated to be lower than the estimated values. Except for the site specific estimations which is estimated to be lower than the regional contribution.

Local concentration in soil

	PEC _{local_{soil}} (mg/kg)	PEC _{local_{agr. soil}} (mg/kg)	PEC _{local_{grassland}} (mg/kg)	PEC _{local_{natural soil}} (mg/kg)
Specific site **	0.000002	0.0000014	0.0000011	0.00000088
Formulation	0.000152	0.0000415	0.0000197	0.00000319

** : Estimated using monitoring data on C_{sludge} .

Concentration in pore water

The concentration in soil porewater is calculated in the *appendix 3*.

Local concentration in soil porewater

	Clocal _{soil, porewater} (mg/l)	Clocal _{agr. soil, porewater} (mg/l)	Clocal _{grassland, porewater} (mg/l)	Clocal _{natural soil, porewater} (mg/l)
Site specific *	0.0000003	0.0000002	0.00000015	0.00000012
Formulation	0.0000212	0.0000057	0.00000274	0.00000044

*: Estimated using monitoring data

Concentration in groundwater

The concentration in groundwater calculated for indirect exposure to humans through drinking water is initially assessed by the concentration in porewater in agricultural soil for a “realistic worst case” estimation according to TGD.

$$PEC_{local\ grw} = PEC_{local\ agr.\ soil,\ porew}$$

Sludge from the factory STP is either incinerated or disposed on landfill according to information from the main manufacturers (AHMarks 1997, Nufarm 1997). The basis for the estimation of $PEC_{local\ grw}$ is therefore the concentration in the influent to the municipal STP where sludge may be expected to be used on soil which is the situation at one municipal STP. If sludge is not applied, atmospheric deposition alone is considered relevant, except when phenoxy herbicides are used in agriculture. The atmospheric contribution is estimated to be insignificant.

Local concentration in groundwater

	PEC _{local_{grw}} (mg/l)
Site specific *	0.00000020
Formulation	0.00000577

*: Estimated using monitoring data

Agricultural use of phenoxy herbicides

The concentration in soil calculated according to TGD as an average concentration in agricultural soil using soil depth 0.2 meter^{*1} and density 1700 kg/m³ (wet soil) = 3400 ton soil/ha:

$$MCPA: 5\% \text{ of } 2 \text{ kg /ha} = 100 \text{ g PCOC/ha} = 0.029 \text{ mg PCOC /kg soil}$$

$$MCPP: 3.5\% \text{ of } 2 \text{ kg /ha} = 70 \text{ g PCOC/ha} = 0.021 \text{ mg PCOC /kg soil}$$

$$\begin{aligned} PEC_{soil,porewater} &= PEC_{soil} * RH_{soil} / (K_{soil-water} * 1000) \text{ (mg PCOC / l porewater)} \\ &= 0.029 * 1700 / (12.2 * 1000) \\ &= 0.004 \text{ mg PCOC/l porewater} \end{aligned}$$

Conclusion: The PEC_{soil} is calculated to be at maximum 0.029 mg PCOC /kg agricultural soil using the TGD setup (in this “pesticide scenario”).

¹In the TGD, a default soil depth of 0.2 m for the sludge application scenario is used. However, according to assessment schemes for agricultural pesticides such as those of EPPO, Germany, the Netherlands and Denmark, a default soil depth for pesticides which are applied as sprays, the soil default depth is four to eight times less. The present assessment has been conducted employing the soil depth recommended by the TGD. If the assessment was performed using the above mentioned soil depth, the PEC_{soil} would increase accordingly (i.e. four to eighth times).

By employing USES version 1.0 ("Pesticide scenario" by employing the country code file for EU according to the TGD; RIVM *et al.*, 1994), the initial concentration for PCOC in soil is 0.1143 mg PCOC / kg soil and the concentration over 28 days is 0.075 mg PCOC / kg soil.

For agricultural soils receiving atmospheric deposition, sludge application, and pesticides, the maximum $PEC_{total, local, soil}$ is estimated to be 0.03 mg PCOC / kg soil. The contribution from atmospheric and sludge application is negligible.

3.1.6 Non compartment specific exposure relevant to the food chain

In a specific monitoring study (Paasivirta *et al.*, 1983), the content of PCOC in plants from garden near a railroad site in Northern Finland were measured two weeks after MCPA spraying and the following concentrations were observed: 0.2 ppb PCOC (fresh weight) in potatoes, 2.9 ppb in carrots, 52.9 ppb in green salad and 593 ppb in onions.

3.2 EFFECTS ASSESSMENT: HAZARD IDENTIFICATION AND DOSE (CONCENTRATION) - RESPONSE (EFFECT) ASSESSMENT

3.2.1 AQUATIC COMPARTMENT

The following dose (concentration) - response (effect) results have been observed:

Fish, short term

Organism	Toxicity	Method	Reference
<i>Lepomis macrochirus</i>	LC ₅₀ (96h, static) 2.3 mg/l LC ₅₀ (24 h,static) 3.8 mg/l	USEPA 1975, nominal conc. #	Buccafusca <i>et al.</i> 1981
<i>Oryzias latipes</i>	LC ₅₀ (96h,static) 6.3 mg/l	JIS K0102-86-71, not specified*	MITI 1992
<i>Brachydanio rerio</i>	LC ₅₀ (96h,static) 3 to 6 mg/l	OECD TG 203, not specified*	VKI 1983
<i>Brachydanio rerio</i>	LC ₅₀ (96h,static) >3.2 (LC ₀) mg/l <4.2 (LC ₈₀) mg/l	OECD TG 203, nominal conc.	Bayer cit. in BUA 1994
<i>Salmo trutta</i>	LC ₅₀ (24 h, static) 2.12 mg/l	nominal conc.	Hattula <i>et al.</i> 1979

#: Precipitation and use of open system noted (- the actual effect concentration may have been lower ?).

*: Not specified whether measured or nominal concentrations (presumably nominal concentrations).

Crustaceans, short term

Organism	Toxicity	Method	Reference
<i>Daphnia magna</i>	EC ₅₀ (48h,static) 0.29 mg/l NOEC (48h,static): 0.028 mg/l	USEPA 1975, nominal concentration	LeBlanc 1980
<i>Daphnia magna</i>	EC ₅₀ (48h,static) 1.0 mg/l EC ₀ (48h,static) 0.32 mg/l	DIN34812 L11, not specified*	BASF cit. in BUA 1994
<i>Daphnia magna</i>	EC ₅₀ (48h,static) 0.63 mg/l	OECD TG 202.I, nominal concentration	VKI 1983
<i>Daphnia magna</i>	EC ₅₀ (48h, static) >0.56 mg/l EC ₁₀₀ (48h, static) ≤1.8 mg/l	OECD TG 202, ** nominal concentration	PCOC Task Force 1997 ***

*: Not specified whether measured or nominal concentrations (presumably nominal concentrations).

** : Range finding study for reproduction test. ***: full report submitted to CAs.

Algae

Organism	Toxicity	Method	Reference
<i>Scenedesmus subspicatus</i>	E _b C ₅₀ (72h,static) 15.0 mg/l EC ₁₀ : 0.97 mg/l	DIN38412 L9, not specified*	BASF 1994
	E _b C ₅₀ (96h,static) 8.2 mg/l EC ₁₀ : 0.89 mg/l	DIN38412 L9, not specified*	BASF 1994

*: Not specified whether measured or nominal concentrations (presumably nominal concentrations).

Higher plants, short term

Organism	Toxicity	Method	Reference
<i>Lemna minor</i>	EC ₅₀ (48 h, static) 93 mg/l	cf below ☐	Blackman <i>et al.</i> 1955

☐: Method: pH of test medium: 5.1; light intensity: 320± 20 ft.candles (approx. 3520 lux) ; effect endpoint chlorosis after 48 h exposure and 24 h in pure test medium; nominal concentration.

Microorganisms

Organism	Toxicity	Method	Reference
<i>Pseudomonas putida</i>	EC ₅₀ (17h): 110 mg/l	DIN 38412, part 8	BASF 1994
Activated sludge:	EC ₂₀ (30 min): 30 mg/l	Inhibition of oxygen consumption	BASF 1994
	EC ₅₀ (30 min): 70 mg/l		
	EC ₅₀ (30 min): 55 mg/l	(ISO 8192)	Bayer

Prolonged, fish

Organism	Toxicity	Method	Reference
<i>Salmo trutta</i>	NOEC (21 to 28d) 0.5 mg/l	daily renewal of test medium, nominal conc.	Hattula <i>et al.</i> 1979 **

** : At the exposure concentration of 0.5 mg/l an average BCF of 6.6. was observed, i.e. cf. section 3.1.2.6, time for reaching 95 % equilibrium concentration within the exposure time for the acute study

Long-term Daphnia, reproduction

Organism	Toxicity	Method	Reference
<i>Daphnia magna</i>	NOEC (21d) 0.55 mg/l	OECD TG 202-II, semi-static, measured concentrations	PCOC Task Force 1997 **

** : Full report submitted to the CAs. Generally there was good agreement between the nominal and measured concentrations.

Other effects:

In an *in vitro* assay with human breast cancer cells, PCOC was observed to have an estrogenic activity with a potency 1×10^{-6} of the potency of 17- β -estradiol (Körner *et al.* 1996, Körner *et al.* 1997).

Comments

The results from the above mentioned ecotoxicity tests are evaluated to be valid for use in this risk assessment. It was evaluated whether to exclude the studies of Bucafusco *et al.* (1981) and Blackman *et al.* (1955) but the former results are in general accordance with the other acute studies on fish and therefore accepted as valid whereas, the latter results are not considered important in this effects assessment context. When evaluating the validity of ecotoxicity test results, it was considered whether standardized test methods have been followed but also whether the effect concentrations are measured or nominal, from flow through, semi-static or static tests, from experiments with nominal

concentrations only but performed in closed systems or open systems, and whether or not solvent was used. When evaluating the test data validity information about the physical-chemical and environmental fate related properties of the substance was also considered.

Most of the mentioned test results are from methods performed according to standard methods / guidelines; US-EPA 1975 ("Methods for acute toxicity tests with fish, macro-invertebrates and amphibians"), OECD 1981, DIN 318412 and ISO 8192. The higher plant and algae study was performed in bright light and PCOC may have been subject to photodegradation which may have affected the result.

In a prolonged toxicity test, histopathological changes were found in livers and kidneys in fish exposed to 1 ppm PCOC or more (Hattula *et al.* 1979). The study was conducted before the adoption of test guidelines of OECD, DIN, ISO and US. However, the study seems well performed (cf. also US EPA AQUIRE data quality code 2) and also includes detailed histopathological examinations of various fish tissues using staining techniques.

In the *Daphnia magna* reproduction test, no significant effects were observed in mortality, length or reproduction at the highest concentration used. The study is performed according to OECD guideline 202-II 1984. The concentrations were measured and generally there was good agreement between the nominal and measured concentrations (88 to 106% of nominal in the two highest concentrations 0.32 and 0.56 mg/l). The study is valid and concludes that NOEC (21d) is 0.55 mg/l based on average measured concentrations.

The results from the long term-*Daphnia* reproduction test seems to be inconsistent with the acute results. One acute EC₅₀ and two NOECs (48h) are below the long term NOEC. This is rarely observed but may be caused by slight differences in the studies in medium, sensitivity of the *Daphnia* clone, etc. The observed EC₅₀-values from the three static tests based on nominal concentrations may not reflect the equivalent EC₅₀ if such had been based on measured concentrations. In range finding test of the *Daphnia* reproduction test only 5 *Daphnias* in 3 duplicate concentrations were used. The mortality was 0% after 48 h at 0 mg/l and 100% at 1.8 mg/l and 3.2 mg/l. EC₅₀ in the long term test was >0.56 mg/l after 48 hours. The conclusion was that EC₅₀ (48h) is estimated to be between 0.56 and 1.8 mg/l. This suggests that the acute study by LeBlanc (1980) might be invalid. Another explanation could be the presence of a steep concentration/effect curve and that the acute EC₁₀₀ is approximately 3 times the long-term NOEC. However, since the result from the long-term test is valid and therefore used in the risk assessment, a conclusion on the probable reasons for the discrepancy is not drawn but left open.

QSAR derived acute effect concentrations for polar narcotic substances according to the TGD for fish and daphnids compared to the experimental data suggest that for fish an acute polar narcotic toxic action seems plausible. This is supported by the evaluation of the acute mode of toxic action towards fathead minnow of the closely structurally related substance 4-chloro-3-methylphenol (Russom *et al.*, 1997). For daphnids, however, the difference between the experimental nominal and QSAR predicted EC₅₀-value is almost one order of magnitude (cf. *appendix 2*). However, the results from the acute preliminary *Daphnia* study and the *Daphnia* reproduction test employing measured concentrations indicate that the experimental EC₅₀-values based on nominal concentrations may be less correct (cf. above).

In a recent *in vitro* assay, PCOC was observed to have an oestrogenic activity with a potency 1×10^{-6} of the potency of 17 β -estradiol (Körner *et al.*, 1997). Oestrogenic effects have been observed e.g. in wild fish from UK rivers, especially downstream from STP discharges. The reason for the field observations in UK is, however, not fully elucidated and no hard evidence exists as regards whether PCOC in effluents may cause such effects *in situ*. A recent study in UK rivers indicates that other chemicals in this case may be responsible since chemicals with known oestrogenic effects were observed in the

rivers and the effects observed on caged fish (Harries *et al.* 1997). As the caged fish were placed upstream related to the location of the STP receiving PCOC discharge there was no indication of PCOC to be responsible for the observed effects.

PNEC-estimations

In the acute studies, the most sensitive aquatic organism was *Daphnia magna*. Based on three studies, a geometric mean EC₅₀ (48h) of 0.63 ppm in acute tests is calculated. Using the acute value and an assessment factor of 1000 would result in a PNEC_{aquatic organisms} of 0.00063 mg/l. However, the presence of an algae EC₁₀, a long term NOEC for fish and a *Daphnia* reproduction test justifies the use of an assessment factor of 10. Thus, the estimated PNEC-value according to the TGD is:

$$\text{PNEC}_{\text{aquatic organisms}}: 0.5/10 = 0.05 \text{ mg/l.}$$

The PNEC_{STP microorganisms} is obtained by using the EC₅₀ for inhibition of respiration of activated sludge microorganisms and an assessment factor of 100:

$$\text{PNEC}_{\text{microorganisms}}: 55/100 = 0.55 \text{ mg/l}$$

Because of the absence of experimental data for sediment-dwelling organisms and because log K_{ow} is less than 5, the PNEC_{sed} is not calculated. The reason is that employment of the equilibrium partition method and the PEC_{sed} - calculation method would result in the same PEC/PNEC-ratio for sediment dwelling organisms as for pelagic organisms.

3.2.2 Atmosphere

No results are available to support an effect assessment in the atmosphere. The atmospheric photochemical half-life is estimated to be 30 hours.

3.2.3 Terrestrial compartment

Since no ecotoxicological data are available for soil organisms the equilibrium partitioning method has been applied:

$$\text{PNEC}_{\text{soil}} = (\text{K}_{\text{soil-water}}/\text{RHO}_{\text{soil}}) * \text{PNEC}_{\text{aquatic organisms}} * 1000 = 0.36 \text{ mg/kg wet weight.}$$

3.2.4 Non compartment specific effects relevant to the food chain

The observed BCF's in fish were small (max. 30). Therefore, secondary poisoning is not likely.

3.3 RISK CHARACTERISATION

3.3.1 Aquatic compartment

Environmental risk related to production, processing and formulation

Aquatic organisms

Risk quotient by employing TGD and including connection to STP:

PEC/PNEC (local) for aquatic organisms

Life cycle stage	PEC _{local, water} (mg/l)	PNEC _{aquatic organisms}	PEC/PNEC
Site specific*	0.0038	0.05	0.08
Formulation	0.0014	0.05	0.03

*Based on monitoring data

The local PEC/PNEC is <1 and a local risk for aquatic organisms is not indicated. Considering formulation outside the two main manufacturing sites, the worst case approach using 10% of production volume at one formulation site did not indicate risk to aquatic organisms. The regional PEC/PNECs are clearly << 1 and therefore not presented here (cf. *appendix 4*).

Because PCOC ready biodegradability is considered a borderline case, the PEC/PNEC ratio is calculated considering PCOC as inherently biodegradable. This increases PEC/PNEC with a factor of 4. Thus, the PEC/PNEC ratios are <1 even when PCOC is considered inherently biodegradable (cf. *appendix 4B*).

Risk for microorganisms in STPs

Using the PNEC_{microorganisms} 0.55 mg/l and the estimated concentrations in STP effluent as the exposure concentration, the following ratios are found:

PEC/PNEC_{microorganisms}

Life cycle stage	PEC _{STP, microorganisms} (mg/l)	PNEC _{microorganisms} (mg/l)	PEC/PNEC
Specific site*	0.004	0.55	0.01
Formulation	0.013	0.55	0.03

* based on monitoring data

Based on these values, a local risk for effects on the microorganisms in STPs is not indicated.

Aquatic risk from agricultural use of phenoxy herbicides

The environmental risk assessment according to the pesticide scenario is not conducted based on a decision at EU Technical meeting on risk assessment of existing substances (TM III, Nov.1996) referring to this part of the risk assessment being conducted by DGVI working group on risk assessment of plant protection products.

Conclusion of the risk assessment of aquatic compartment

- (X) ii) There is at present no need for further information and/or testing and for risk reduction measures beyond those which are being applied already.

3.3.2 Atmosphere

Based on the calculated Henry's Law constant and the data on evaporation from rice fields, and other laboratory studies, it is concluded that PCOC will volatilize at significant rates from open water and wet soil.

In the air, the substance will be exposed to photochemical degradation at a half-life of 30 hours and based on the solubility, PCOC is expected to be washed out by rain to soil and water.

PEC_{air}: No effect data exist and therefore no PEC/PNEC ratio can be calculated.

Conclusion of the risk assessment of atmosphere compartment

- (X) ii) There is at present no need for further information and/or testing and for risk reduction measures beyond those which are being applied already.

3.3.3 Terrestrial compartment

No data are available on the terrestrial toxicity. Therefore, the equilibrium partitioning method described in the TGD is applied as a conservative approach, comparing PEC_{soil} to PNEC_{soil}.

$$PNEC_{soil} = 0.36 \text{ mg/l}$$

Risk to the terrestrial compartment from production, processing and formulation

PEC/PNEC local_{soil}

	local _{soil}	local _{agr. soil}	local _{grassland}
Specific site *	0.000006	0.000001	0.000006
Formulation	0.0004	0.0001	0.0005

* PEC specific site is estimated using monitoring data

Risk to the terrestrial compartment during agricultural use

The environmental risk assessment according to the pesticide scenario is not conducted based on a decision at a EU Technical meeting on risk assessment of existing substances (TM III, Nov.1996) referring to that this part of the risk assessment will be conducted by the DGVI working group on risk assessment of plant protection products.

Conclusion of the risk assessment of terrestrial compartment

- (X) ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

The risk ratios for the local risk is below 1 for the considered exposure scenarios (i.e. specific manufacturing site including production, processing and formulation of herbicides as well as the scenario employing a formulation of phenoxy acids. Based on the ratio PEC/PNEC soil estimated to be <1, no risk for terrestrial organisms is indicated.

3.3.4 Non compartment specific effects relevant to the food chain

The risk characterisation of secondary poisoning is not performed because the BCF for fish is max. 30, i.e. considerably below 100. Therefore, even though log Kow is above 3, there are no indications for a bioaccumulative potential of the substance and thus no concern for secondary poisoning.

Conclusion of the risk assessment of non compartment specific effects relevant to food chains

- (X) ii) There is at present no need for further information and/or testing and for risk reduction measures beyond those which are being applied already.

4 HUMAN HEALTH

4.1 HUMAN HEALTH (TOXICITY)

4.1.1 Exposure assessment

4.1.1.1 General discussion

P-chloro-o-cresol (PCOC) is used in the chemical industry as an intermediate in the synthesis of chlorophenoxy herbicides, e.g. MCPA (4-chloro-2-methylphenoxy acetic acid), MCPB (4-chloro-2-methylphenoxy butyric acid), and mecoprop (2-(4-chloro-2-methyl-phenoxy)-propionic acid, MCPP). PCOC is no longer produced in Denmark.

PCOC is found as an impurity in the herbicides MCPA, MCPB, and mecoprop. During production of PCOC and in the synthesis of other compounds (down stream uses) PCOC is released to the environment through emitted air and waste water. As a degradation product and as an impurity PCOC will also be found at the application sites of the herbicides mentioned above.

PCOC was detected upon branches sprayed with MCPA, 2 weeks post application, at concentrations of 8900 ppb; and upon potatoes, carrots, green lettuce and onions grown on fields adjacent to a treated railway bed in Northern Finland at concentrations of 0.2, 2.9, 52.9 and 593.0 ppb, respectively (Paasivirta *et al.*, 1983).

Concentrations in the environment are estimated in chapter 3.

The most important routes of direct exposure is by inhalation in occupational settings in the production of the substance itself or during use in the synthesis of other compounds (down stream uses). Oral or dermal exposure during production is assumed to be of relevance only in the case of accidents.

Exposure to PCOC as an impurity in herbicides such as MCPA can also occur during crop spraying.

In the Danish Product Register PCOC is only registered as a substance, but was formerly found in one product at a concentration of around 1% in a survey carried out in 1985. With reference to information from industry it is concluded, that no exposure takes place through use of ordinary (non-herbicidal) consumer products.

One potential source of indirect exposure is the consumption of food treated with the herbicides, of which PCOC is a degradation product or an impurity, and drinking of water contaminated by the substance.

4.1.1.2 Occupational exposure

Two companies in the U.K. are high volume producers of PCOC, which is also used as an intermediate for further synthesis at the same sites of the herbicides MCPA, mecoprop, and MCPB. In addition one Dutch high volume producer has been identified, producing PCOC as a non-isolated part of a continuous process which need not be reported under the Regulation. There are no data on occupational exposure available from this producer.

No occupational exposure limits for PCOC have been found but for related substances (cresols and chlorphenols) the values given below apply.

The occupational exposure limit (8-hour threshold limit value (TLV)) for cresols set by the UK and DK authorities (all isomers) is 22 mg/m³ (HSE 1994, AT, 1994). For chlorphenols (all isomers) the TLV in e.g. Denmark is 0.5 mg/m³ (AT, 1994).

Production: At one of the production sites, plant operators were monitored at the workplace and tank farm operators were monitored whilst offloading PCOC to the road tanker on four and three occasions, respectively (Road tanker is used to move the substance within the area). According to the manufacturer less than 20 people are involved in these operations (pers. communication, 1997). For the plant operators the monitoring period lasted from 183 to 238 minutes. For the tank farm operators the monitoring period lasted from 15 to 101 minutes. Concentrations for plant operation and offloading to road tankers ranged from below detection limit to about 5 mg/m³ (equivalent 8 hour TWA's max. ca. 5 mg/m³) (A.H. Marks, 1997b).

During cleaning operations, which were infrequent (twice per year) and where protective clothing and breathing apparatus was worn, a concentration of about 53.8 mg/m³ was recorded (8 hr. TWA 1.2 mg/m³). The monitoring was done at one occasion (A.H. Marks, 1997b). According to the manufacturer, less than 20 people are involved in this operation (pers. comm.). One of the main manufacturers has reported that the exposure actually only applies to one worker. (pers. comm., A.H. Marks, march 6 1998)

Beside the actual operator monitoring point location monitoring in working areas was performed showing TWA values of less than 5 mg/m³ for all instances (e.g. control room, by reactor, by holding vessels, process scrubber, and whilst offloading PCOC to road tanker) except cleaning of the equipment where a concentration of 1,274.8 mg/m³ was recorded (equivalent to 8 hr. TWA 18.6 mg/m³)(A.H. Marks, 1997b).

For production of phenoxy herbicides, which was done at the same plant, monitoring data (operator and point location monitoring) was of a similar order of magnitude, less than 5 mg/m³ at all occasions. Here cleaning of the equipment was not monitored (A.H. Marks, 1997b). PCOC is used in the molten state, which together with the corrosive nature of the substance, ensures that workers comply fully with PPE requirements (pers. Comm., A.H. Marks, march 6, 1998)

There are no monitoring data on PCOC available from the other U.K. production site. According to the producer the occupational exposure to PCOC is regarded as being minimal, because all vessels and sample points are enclosed and maintained under extraction with air being discharged via caustic scrubbing columns. In addition all employees are provided with appropriate Personal Protective Equipment which is laundered and maintained by the company (Nufarm, 1997b).

According to the producers most of the manufacture and use of PCOC do not require operator intervention. However, there are exceptions e.g. maintenance and tanker loading and unloading. For these operations as well as for emergency situations appropriate PPE are provided including suit (PVC or full body cotton overalls), full face mask, PVC gloves, boots (leather or PVC), safety helmet and glasses (A.H. Marks, 1997b; Nufarm, 1997b).

Assuming inhalation of 10 m³ of air during an eight hour work shift, for a 70 kg person, 5 mg/m³ would correspond to a realistic worst case dose for systemic toxicity of about 0.7 mg/kg/day. It can be noted that while this concentration is less than 0.25 of the TLV for cresols and thus meets U.K. regulatory standards, it is 10 times higher than the TLV for chlorphenols, which from a chemical-structural point of view are quite similar to PCOC.

The EASE estimation (app. 5) of inhalation exposure during production and further processing of PCOC assuming use pattern is closed system and the pattern of control is full containment resulted in exposures of 0 to 0.1 ppm corresponding to 0 to 0.6 mg/m³. This range is much lower than monitored data.

While some degree of dermal exposure may also occur, the EASE model predicts this as being of no consequence when compared with the inhalation route (app. 5). Direct contact with the skin would only happen in the case of accidents, where it could result in systemic toxicity as well as severe burns.

In conclusion the known corrosive nature of PCOC together with its use in the molten form ensures that routine transfer and equipment cleaning and maintenance operations are performed with strict adherence to PPE requirements, resulting in minimal exposure to workers via both dermal and inhalation routes.

Application²: In certain occupational settings such as municipal gardening, worst case exposures may be higher. Using a standard model for plant protection product use (Lundeher, 1992) which also incorporates exposure during mixing and loading, a geometric mean exposure of 0.047 mg/kg/day is calculated for hand-held (knapsack) spraying of 1 ha assuming application of 2 kg/ha MCPA with a 1% content of PCOC and 100 % absorption. The 90th percentile exposure using the same inputs results in a total of 0.35 mg/kg/day.

4.1.1.3 Consumer exposure

PCOC is not found in any ordinary consumer products. It can occur as an impurity or breakdown product in herbicides used for controlling weeds in lawns of private gardens. One such product available in the vegetable section of a Danish super market contains MCPA in concentrations of 5.20 g/l in a one-liter plastic bottle provided with a hand pump for aerosol generation. As this form of dispensation can lead to the highest exposures, a realistic worst case for combined inhalation and dermal exposure of 10% is assumed. If PCOC is present as an impurity at 0.5%, and a further 0.5% is generated by exposure of the aerosol to sunlight, a total exposure to PCOC of 5.2 mg/event, or 0.07 mg/kg/event for a 70 kg person could result.

It is difficult to assess the frequency with which such consumer exposure might occur, directions for use on the particular product only state that it can be used during the entire growth period, but is most effective during periods of rapid growth in May, June, July and August (Source, "Toxan" - Labelling information, Distribution: Bayer Denmark A/S, Gammelager 1, 2605 Brøndby. In addition to MCPA, one liter of this product is also stated to contain 1.50 g Dichloprop-p and 0.32 g Dicamba as active ingredients). Assuming a really worst case of five times application per year the total yearly dose of PCOC would be $5 \times 0.07 = 0.35$ mg/kg/year ($= 9.6 \times 10^{-4}$ mg/kg/day).

2

During spraying, including mixing of pesticides, using sprayers on tractors the exposure is generally estimated to be around 0.00005% of the amount sprayed in a concentration of 15 g/ha using the best available technology. Using standard spraying equipment the exposure is 0.0002% of the amount sprayed (Lund & Kirknel, 1995).

Using a standard model for plant protection product use (Lundeher, 1992) which also incorporates exposure during mixing and loading, and assuming 2 kg MCPA per ha, with a 1% content of PCOC, a geometric mean exposure of 0.02 mg/kg body weight/day is derived, or for the 90th percentile, 0.28 mg/kg body weight/day for 20 ha of downward vehicle-mounted spraying.

4.1.1.4 Indirect exposure via the environment

Exposure of the environment can take place during the production of PCOC itself, as well as from the production and use of phenoxy herbicides.

At the production site the potential exposure would be through waste water and air effluent.

At sites of MCPA or other phenoxy herbicide applications, indirect exposure may occur, since PCOC is an impurity in the herbicide and has been identified as a degradation product of MCPA.

According to USES1.0 calculations involving local indirect exposure due to use of herbicides the following daily doses can be expected:

Intake air:	1.63×10^{-9} mg/kg/day
Intake drinking water:	8.95×10^{-8} mg/kg/day
Intake fish:	4.04×10^{-9} mg/kg/day
Intake stem of plant:	7.97×10^{-10} mg/kg/day
Intake root of plant:	3.38×10^{-12} mg/kg/day
Intake meat:	5.49×10^{-13} mg/kg/day
Intake milk:	5.47×10^{-13} mg/kg/day

Amounting to a total human dose of 9.60×10^{-8} mg PCOC/kg/day

The EUSES calculations (November 1997) for local indirect exposure resulting from production of PCOC are as follows:

	Ready degradability	Inherent biodegradability
Specific site*:	1.18×10^{-4} mg/kg/day	2.52×10^{-4} mg/kg/day
Formulation site**:	1.25×10^{-4} mg/kg/day	4.30×10^{-4} mg/kg/day

*: Specific site incl. production, processing and formulation. The values are based on average monitoring data on emissions from the two main manufacturers.

** : Formulation site is a generic site where it is assumed that 10 % of the total PCOC production is formulated (worst case).

We assume PCOC being readily biodegradable. However, knowing the substance may be a borderline case, the calculations for inherent biodegradability are included for comparison purposes only.

EUSES calculations (November 1997) for regional indirect exposure assuming ready or inherent (worst case) biodegradability. Again, inherent biodegradability has been included for comparison purposes only:

Daily human dose through:	Ready biodegradability	Inherent biodegradability
Intake air:	1.60×10^{-7} mg/kg/day	2.17×10^{-7} mg/kg/day
Intake drinking water:	4.49×10^{-6} mg/kg/day	8.05×10^{-6} mg/kg/day
Intake fish:	7.74×10^{-6} mg/kg/day	1.39×10^{-5} mg/kg/day
Intake from leaf crops:	2.44×10^{-7} mg/kg/day	3.31×10^{-7} mg/kg/day
Intake root of crops:	2.56×10^{-7} mg/kg/day	3.01×10^{-7} mg/kg/day

Intake meat:	1.29x10 ⁻⁹ mg/kg/day	2.25x10 ⁻⁷ mg/kg/day
Intake milk:	7.60x10 ⁻¹⁰ mg/kg/day	1.33x10 ⁻⁷ mg/kg/day
Regional total daily intake:	1.29x10 ⁻⁵ mg/kg/day	2.28x10 ⁻⁵ mg/kg/day

4.1.1.5 Combined exposure

Some parts of a population are exposed to PCOC both during work and during indirect exposure via the environment.

A person working at a production site for PCOC and/or phenoxy herbicides or a person spraying phenoxy herbicides on a field might apart from the occupational exposure also be exposed via the environment. However, the potential routes of exposure differs and as can be seen from 4.1.1.1., 4.1.1.2., and 4.1.1.3. the magnitude of the exposure varies greatly. In table 1 the calculated exposure data are given.

Table 1. Calculated exposure data excl. agricultural spraying³

Exposure	mg PCOC/kg/day
Occupational exposure during production	0.7
Spraying (municipal - hand spraying)	0.35
Consumer exposure	9.5x10 ⁻⁴
Indirect regional exposure via the environment	1.3x10 ⁻⁵
Local indirect exposure*	1.2x10 ⁻⁴
Combined exposure, total	1.05 PCOC mg/kg/day

*: Local indirect exposure resulting from production, formulation or processing is estimated assuming ready biodegradability.

4.1.2 Effects assessment: hazard identification and dose (concentration) - response (effect) assessment

All the PCOC studies below that were performed by Scantox, Denmark and Teknologisk Institute were conducted in accordance with the OECD guidelines for testing of chemicals and GLP. The identity of the substance was as described in chapter 1 i.e. 97.09% 4-chloro-2-methylphenol, 1.21 % 6-chloro-2-methylphenol, 0.92% 2-methylphenol, and 0.78% 2,4-dichloro-6-methylphenol. The study by the Institute of Toxicology in Denmark (Hansen, 1996) used a 97% pure Aldrich PCOC batch no. C5.520-8. The study by Hattula *et al.* (1979) used 100% pure PCOC.

4.1.2.1 Toxicokinetics, metabolism and distribution

Very little is known about the toxicokinetics, metabolism, distribution, and excretion of PCOC in humans and experimental animals. However, from the acute toxicity studies it can be inferred that PCOC can be taken up in the body through the gastro-intestinal tract, the skin, and via inhalation. There is no information on the metabolism and excretion of PCOC.

³ Table 1a. Calculated exposure data for agricultural spraying for comparison purposes only.

Exposure	mg PCOC/kg/day
Spraying (agricultural)	0.28

The concentrations of PCOC in liver, kidney, spleen, and muscle was studied in an acute and a repeat dose study (Hattula *et al.*, 1979). After 28 days of dosing by gavage with 100, 250, or 500 mg PCOC/kg, PCOC was found in the highest concentration 2.81 mg/kg in the spleen, and in the lowest concentration 0.27 mg/kg in muscle tissue in the high dose group. In the low dose group only traces of PCOC were found.

PCOC was found in concentrations of 47-31 µg/g in the liver of rats receiving 2-3 g/l MCPA in the drinking water for three months (Hattula *et al.*, 1977). A recent rat metabolism study with MCPA performed at Hazleton Lab. showed that PCOC was not a metabolite. It is therefore possible that the PCOC in the Hattula - study was a contaminant of MCPA (Jahanshahi J., 1995).

Acute toxicity

Animal data: Acute oral toxicity

In a guideline (401) study using five male and five female rats per group and dosing by gavage with the doses 1728, 2488, 3583 and 5160 mg/kg with oleum arachidis as vehicle, an LD₅₀ of 3195 mg PCOC/kg (range 2698 - 3834 mg/kg) was found.

In the 5160 mg/kg group all animals died within one hour after dosing, in the 3583 mg/kg group 5 deaths occurred up to 6 hours after dosing, in the 2488 mg/kg group three deaths occurred within one day after dosing, and in the 1728 mg/kg group no deaths occurred. Symptoms observed just after dosing at all dose levels were paresis and depressions. On the second day, ruffled fur, which lasted to day five in the 3583 mg/kg group, was seen. Animals that died during the observation period showed bleeding in the mucous membrane of the stomach at autopsy. Animals sacrificed after the 14 days observation period showed no dose related macroscopic changes. However, two of the animals from the 2488 mg/kg group, sacrificed after the 14 days observation period, showed infiltrations between the oesophagus area of the ventricle and the diaphragm. In one animal from the high dose group, infiltrations between the oesophagus area of the ventricle and the liver were seen (Scantox, 1982b).

Groups of ten male Wistar rats, 2-3 months of age, were given 1000, 1100, or 1200 mg PCOC/kg with the substance dissolved in olive oil. The animals were all killed 24 hours after dosing. A LD₅₀ of 1190 mg/kg was derived (Hattula *et al.*, 1979). At the histopathological examination the following observations were made: At 1000 and 1100 mg/kg inflammatory mononuclear infiltration was seen in many glomeruli in the kidney. Inflammatory infiltrations were also seen in other parts of the kidney mostly around distal tubules. At 1200 mg/kg also histopathological alterations in the liver and spleen were seen. In the liver numerous pycnotic nuclei and hydropic degeneration of cytoplasm were observed. In the spleen the reaction centres were unusually large (Hattula *et al.*, 1979).

Further studies on the acute oral toxicity of PCOC to rats include BASF (1978) and Hazleton (1977). These test reports have not been available, but their results (see table 1) are in accordance with the results of the only guideline study available (Scantox, 1982b). It can be concluded that PCOC not only shows corrosive properties but also properties resulting in systemic effects i.e. effects on liver and kidney.

In rats the oral LD₅₀ of PCOC is above 2.000 mg/kg in the most reliable study.

In mice, Schrötter *et al.* (1977) report the oral LD₅₀ of PCOC as being 1330 mg/kg, but few experimental details are provided.

In range finding studies of PCOC in aqueous gum tragacanth emulsion, mice died consistently at lower doses (4/4 at 1200 mg/kg and 3/4 at 576 mg/kg) suggesting that the vehicle may play an important role in determining absorption following oral administration (Huntingdon, 1997).

Animal data: acute inhalation toxicity

Groups of five male and five female rats were exposed to an aerosol containing 0, 5.79, 8.33, 9.11, or 10% PCOC in 50% alcohol for 4 hours following OECD Guideline 403. All deaths during the study occurred during exposure or within the first hour after exposure. The deaths were distributed as follows between the groups: control 0 deaths, 5.79% 0 deaths, 8.33% two deaths, 9.11% four deaths, 10% 7 deaths. The LC_{50} was calculated as 900 mg/m³ (0.9 mg/l range 0.83 - 1.08 mg/l) (Scantox, 1983a). The alcohol aerosol was used as it was not possible to generate a dust aerosol, as the test substance clumped. The LC_{50} -value is based on the nominal concentration in the experiment. The symptoms observed during and after exposure were respiration difficulties, depressions, ruffled fur and bleeding from the nose. These symptoms occurred in a dose related manner. Petechiae of the lungs were also observed.

At macroscopic examination of the animals that died up to the first hour after dosing bleeding of the lungs and a thin, mucous, yellowish content of the small intestine were found.

Another study was performed by Hazleton Lab in 1977 is cited from BUA (1994): The original report is not available and the study was carried out before guidelines were in general use. By inhalation of 2000 - 30.000 mg PCOC/m³ (average particle size of 0.6 µm) for 4 hours no deaths occurred but swelling red noses and lips were seen. In one animal blood was found in the urine.

Animals sacrificed immediately after the exposure period or after 14 days of observation period showed no alterations in the lung or essential organs.

Animal data: acute dermal toxicity

Groups of five male and five female rats were dermally dosed with 1667, 2000, 2400, or 2880 mg PCOC in oleum arachidis in a guideline study (402). A LD_{50} of 2240 mg/kg (range 2023 -2484) was calculated from the observed deaths (Scantox, 1982c).

In the 2880 mg/kg group 9 animals died within 6 hours after dosing, in the 2400 mg/kg group six animals died within one day after dosing, in the 2000 mg/kg group four animals died within one day after dosing, and in the 1667 mg/kg group no animals died. At necropsy bleeding of the lungs, a mucous, red-yellow content of the jejunum, enlarged kidneys and blood or blood coagulum in the bladder plus bleeding of the bladder wall were observed.

During the first 24 hours after treatment blood was observed in the urine of all rats. From the day after treatment erythema and oedema at the application sites were seen. Paresis occurred in nearly all animals 1 to 6 hours after treatment. Depressions occurred up to 2 days after treatment, and ruffled fur up to 3 days after treatment. In animals sacrificed on day 14 weak bleeding of the intestine (jejunum) was observed in five of the rats (dose levels not stated).

In table 1 the acute toxicity data found for PCOC are given without any comments on quality of the studies.

Table 1. Data on acute toxicity of PCOC

species	application	dose	effect	literature
---------	-------------	------	--------	------------

rat	oral	3.195 mg/kg	LD ₅₀	Scantox, 1982b
rat	oral	1.190 mg/kg	LD ₅₀	Hattula et al, 1979
rat	oral	2.650 mg/kg	LD ₅₀	Hazleton Lab, 1977
rat	oral	2.700 mg/kg	LD ₅₀	BASF AG, 1978 *
mouse	oral	1.330 mg/kg	LD ₅₀	Schrötter et al, 1977
rat	i.p.	794 mg/kg	LD ₅₀	Hattula et al, 1979
mouse	i.p.	570 mg/kg	LD ₅₀	BASF AG, 1978 *
rat	inhal, 4h.	900 mg/m ³	LC ₅₀	Scantox, 1983a
rat	inhal, 4h.	>30.000 mg/m ³	LC ₅₀	Hazleton Lab., 1977
rat	dermal	2.240 mg/kg	LD ₅₀	Scantox, 1982c
rat	dermal	>5.000 mg/kg	LD ₅₀	Hazleton Lab, 1977*

*: unpublished results sited in a BUA report (BUA, 1994).

In relation to acute oral, dermal and inhalation acute toxicity the Scantox Reports (1982b,c, 1983a) are found to be most reliable. For the acute oral toxicity the Hazleton and BASF studies support the oral LD₅₀ found by Scantox. Poor reporting of the Hattula study makes its interpretation difficult. No details are available which would allow further interpretation of the Hazleton inhalation study.

The overall conclusion for acute toxicity is:

LD _{50 oral, rat} =	2650 - 3195 mg/kg
LC _{50 inh, rat} =	0.9 mg/l (as an EtOH aerosol)
LD _{50 dermal, rat} =	2240 mg/kg

4.1.2.2 Irritation

&

4.1.2.3 Corrosivity

Animal data: skin irritation

In a guideline (404) study 6 female rabbits were dermally exposed to 0.5 g PCOC in 0.1 ml oleum arachidis. A primary irritation index of 8.0, the maximum value obtainable, was calculated. Immediately after removal of the test substance the skin was white as a sign of initial necrosis (Scantox, 1982d).

BUA (1994) reports a study of Hazleton labs (1977), where rabbits received 500 mg PCOC on the shaved back in a semi-occlusive bandage. It is not stated if a vehicle was applied, and what time of exposure was used. After 12 hours necroses were observed and after 24 hours pronounced erythema with light oedema was observed

BUA (1994) reported a study of BASF where occlusive exposure to 80% of PCOC in water was carried out (species used and amount applied not mentioned). It was concluded that PCOC was very corrosive. After only one minute of exposure necrosis was found. After 20 minutes the necrosis was very pronounced, and after 8 days it had not disappeared. On day 8 after application the skin was still scarred.

In the rabbits eye BUA (1994) citing BASF reports 50 mg PCOC in an 80% aqueous solution as strongly corrosive. The eye turned red and after 1 hour oedema and opacity of the cornea was found. After 8 days the clinical observations were the same and a staphyloma was found.

In conclusion, some of the studies concerning corrosive effects of PCOC are cited from secondary references, but together with the results of the irritation test (Scantox, 1982d), they indicate that PCOC, according to EU criteria, may be classified as corrosive with R35: causes severe burns, in agreement with classification by the manufacturers.

At least one human fatality attributed to PCOC poisoning has been reported following exposure of the face and neck to a momentary blast of PCOC and steam during a workplace accident. It was not possible to estimate the dose or concentration involved (Pers. comm., HSE, U.K. 1996).

4.1.2.4 Sensitization

In a Guinea Pig maximization test carried out according to OECD guidelines (Scantox, 1982e) PCOC caused no sensitization. 40 female albino Guinea Pigs were used in the study. As the provocation test with 30% solution of PCOC caused erythema, a further provocation test with 10% and 20% of PCOC applied on the left and right flank, respectively, was carried out a week later. No clear differences between the control group and the test group were found at this occasion. Some animals of both groups were reacting with erythema (score 1-2). The reactions in the two groups were of the same magnitude. Macroscopically none of the reactions appeared to be an allergic.

The report by BUA (1994) mentions another negative sensitization study. However, the study does not seem to have been reported properly.

4.1.2.5 Repeated dose toxicity

There are three available studies on repeated dose toxicity of PCOC.

In a guideline (407) study groups of five male and five female rats were given 0, 50, 200, or 800 mg PCOC/kg in oleum arachidis by gavage for 28 days (Scantox, 1982a). During the last three days of dosing three rats from the 800 mg/kg group showed salivation after dosing, and on the last day of dosing three rats from the group had ruffled fur. Body weight gain and feed consumption did not differ between groups. In blood parameters *the thromboplastin time and the number of leukocytes were statistically smaller in females from the 800 mg/kg group. In males from the same group the erythrocyte count was statistically significantly reduced. Serum alanine-aminotransferase (ALAT) was statistically significantly increased in males of the 800 mg/kg group, and marginally increased in females.* In females from the 800 mg/kg group relative and absolute liver weights were significantly increased.

No histopathological changes were seen in any organ at 800 mg/kg. The changes of ALAT and liver weights in the 800 mg/kg group indicated *mild toxicity to the liver*. It was concluded in the test report that 800 mg/kg is a LOAEL, and that 200 mg/kg is a NOAEL.

Hattula *et al.* (1979) dosed groups of ten male Wistar rats with 0, 100, 250, or 500 mg PCOC/kg in olive oil for 28 days by injection (gavage). It is very difficult to interpret the results of this study, basically because of lack of tables and explanations to the few tables given. However, at 100 mg/kg all investigated organs were normal except for the small intestine, which had necrotic areas of the mucosa. The dose relationship of the other histopathological observations mentioned is obscure. It is stated that

blood analyses showed that leukocytes were decreased with larger doses. *At 500 mg/kg a clear-cut leucopenia was found.*

In a combined *repeated dose/reproduction screening test* carried out according to *OECD draft guideline 422* (Ernst Hansen, "4-Chloro-2-methylphenol," National Food Agency, 1996) groups of 10 male and 10 female rats per dose were given 0, 50, 200, or 600 mg PCOC/kg in soybean oil by gavage for two weeks prior to mating until day 20 of gestation i.e. dosing was for a total of 40-45 days.

Weight gain was slightly reduced, and water consumption increased in the highest dose groups. *Males in the 600 mg/kg group showed a decrease in haemoglobin concentration ($p < 0.01$).* (A slight decrease in plasma creatine ($p < 0.05$) in the middle dose group was considered to be without physiological significance.)

A dose-related decrease in the absolute and relative weight of the adrenals of female rats was seen ($p < 0.05$ at 200mg/kg, $p < 0.01$ at 600 mg/kg) but was unaccompanied by histopathological changes, and without obvious toxicological significance.

No effects were seen in other macroscopic and histological examinations of the organs. No behavioural changes were found by a functional observational battery, or in motor activity. It was concluded that the NOAEL was 200 mg/kg.

With regard to respiratory irritation and corrosivity after repeated dosing no data are available. However, due to the caustic properties of the substance it seems unlikely that an inhalation study would add any new information on the systemic toxicity. Further, it seems that the way the substance is handled and used in the existing productions do not lead to any respiratory problems. At both production sites health surveillance programmes including examination of the respiratory function have been undertaken for several years. According to the medical reports submitted by the producers no significant increase in any specific symptoms such as sore throats, coughs and changes of lung function and no significant group changes of lung function have been observed (A.H. Marks, 1997b; Nufarm, 1997b).

4.1.2.6 Mutagenicity

Genetic toxicity *in vitro*

According to Ames, et. al. 1975, and/or OECD guideline 471 four direct plate Ames tests (Räsänen *et al.*, 1977 ; Teknologisk Inst, 1982; Strobel & Grummt, 1987; BASF, 1988) and one pre-incubation Ames test (BASF, 1988) have been carried out to study the mutagenicity of PCOC in the dose range 1-500 µg/plate.

Ames direct plate test was performed with the *Salmonella typhimurium* strains TA1537, TA1535, TA100, and TA98 at 0, 1, 5, 10, 50, 100, and 500 µg/plate with and without metabolic activation. The identity of the substance was as described in chapter 1. There was clear general toxicity in all strains at 500 µg/plate, but none of the strains showed an increase in the number of revertants/plate (Teknologisk Institut, 1982).

Ames direct plate test was performed with the *Salmonella typhimurium* strains TA1537, TA1535, TA100, and TA98 at 0, 0.5, 5, 50, and 500 µg/plate with and without metabolic activation. None of the strains showed an increase in the number of revertants/plate (Räsänen *et al.* 1977).

Ames direct plate test was performed with the *Salmonella typhimurium* strains TA1537, TA1535, TA100, and TA98 at 0, 20, 100, 500, 2500, and 5000 µg/plate and at 0, 4, 20, 100, 500, and 1500

µg/plate with and without metabolic activation. There was clear general toxicity in all strains at and above 500 µg/plate, and none of the strains showed an increase in the number of revertants/plate (BASF, 1988).

An Ames direct plate test using the strains TA98, TA100, TA97 and TA104 at 10, 25, 50, 100, 250, 500, and 1000 µg/plate with and without metabolic activation showed a 4.4 fold dose related increase with TA97-S9 and a 5.4 fold dose related increase with TA97+S9. Only these results were significant. At the highest dose a toxic effect was found in all the strains (Strobel & Grummt, 1987). The report of these results in the literature leaves open some questions with regard to the interpretation of results. For this reason an additional test was performed.

In this new test, 97% PCOC (Aldrich lot no. 3302005) was dissolved in DMSO and tested according to the Salmonella/microsome standard plate assay in *S. typhimurium* strains TA-97 and TA-98 at doses of 500, 250, 100, 50, 25 and 10 µg/plate with and without S9-mix (at 2 and 4 mg S9 protein/plate). No mutagenic effect was seen with or without metabolic activation in either strain. The experiments were repeated again with the same results. (Binderup, "4-Chloro-2-methylphenol: Assessment of mutagenic potential," National Food Agency of Denmark, 1996:)

In the Ames test with pre-incubation (BASF, 1988) *Salmonella typhimurium* strains TA1535, TA100, TA1537, and TA98 was used with and without metabolic activation in concentrations of 0, 4, 20, 100, 500, and 1000 µg/plate and 0, 15, 30, 60, 125, and 250 µg/plate (two separated series). General toxicity occurred at dose levels of 125 µg/plate or higher. There was no increase in the number of revertants/plate.

Genetic toxicity *in vivo*

In a micronucleus assay performed according to the first version of OECD guideline 474 male and female mice were dosed by gavage with 1600 mg PCOC/kg in 10 ml of peanut oil, corresponding to the maximum tolerable dose. Bone marrow cells were harvested at 24, 48, and 72 hours post dosing. A significant ($p < 0.0007$) increase (4-6 times) in the frequency of micronuclei was observed in the dosed animals at all harvesting times (Scantox, 1982f). It was noted that there was no clear evidence of a time-course for these effects. The incidences of micronucleated cells in treated animals were not particularly high compared to published data for untreated mice, while the incidence in the control group was lower than what would usually be expected. It was not possible to re-examine concurrent control data to obtain information on background rates, as the records are no longer available.

A new mouse micronucleus assay was performed in 1997 according to current guidelines (EEC, 29 December 1992, Official Journal of the European Communities No. L358B: Methods for determination of toxicity, B12: Mutagenicity (Micronucleus test) p. 124), including the OECD guideline revision (OECD 1996) recommending use of aqueous suspending agents for poorly soluble substances. The test substance, 99.3% pure PCOC consisting of 50% of current production lots from each of the two U.K. producers was suspended in aqueous 0.5% gum tragacanth. A preliminary toxicity test indicated that in this vehicle, the maximum dose which did not induce excessive lethality was approximately 400 mg/kg. For the Micronucleus test, groups of 5 male and 5 female mice were dosed by gavage with 20 ml/kg suspensions of test substance corresponding to 100, 200 and 400 mg/kg body weight of PCOC, using the vehicle alone as the negative, and Mitomycin C as the positive control.

Severe lethargy was noted shortly after dosing at 400 mg/kg. One female in the high dose group died, and was replaced by another female from the concurrently-treated satellite group. No adverse clinical signs were observed for the positive or negative control groups during the duration of the test.

Bone marrow samples were examined (1000 erythrocytes per smear) after 24 hours and 48 hours and did not show any substantial increase in the incidence of micronucleated immature erythrocytes or decrease in the proportion of immature erythrocytes. It was concluded that PCOC did not show any evidence of causing chromosome damage or bone marrow cell toxicity in this test. The positive control caused highly significant ($P < 0.001$) increases in the number of micronucleated immature erythrocytes at both 24 and 48 hours. Results for PCOC treated and control animals were within the expected range for unaffected mice based on published information and laboratory control data (Huntingdon, 1997).

While cytotoxic effects were not seen in the bone marrow, there is little to suggest that PCOC would not be absorbed, or would break down prior to reaching this site. Clear evidence of leukopenia seen in the two repeat-dose studies is highly suggestive of bone marrow effects. *In vivo* mutagenicity studies of the meta isomer of chlorocresol (4-Chloro-3-methyl phenol, Cas. no. 59-50-7) showed a similar pattern, with no change in the observed PCE/NCE ratio and no clastogenic activity (mouse micronucleus test, oral, 200 and 400 mg/kg, 24 hours; mouse micronucleus test, single i.p. injection of 125 mg/kg - 10 % mortality - investigations at 24, 48 and 72 hours post dosing, statistically significant response in cyclophosphamide control) (BUA, 1993 - U.S. EPA 1997).

Conclusion on mutagenicity.

PCOC was negative in 3 Ames tests, equivocal in one, and negative in repeat tests of the equivocal strain. An oral mouse micronucleus test performed in 1982 according to the first OECD guidelines was positive. A repeat of this test in 1997 using modern guideline recommendations and possibly a more suitable test vehicle was clearly negative. Using the best available data PCOC cannot be considered a mutagen.

4.1.2.7 Carcinogenicity

For 4-chloro-o-cresol (PCOC) no studies in humans or animals are available.

Human data on phenoxy herbicide production

A cohort study of workers employed in manufacturing of phenoxy herbicides, primarily MCPA, in Denmark before 1982 was carried out. The study seems to support the Swedish observation of an increased risk of soft tissue sarcomas following exposure to phenoxy herbicides. The purpose of the study was to shed further light on the potential carcinogenic effect indicated by a Swedish case control study of the 2,4-dichlorophenol and 4-chloro-o-cresol based phenoxy herbicides unlikely to be contaminated with 2,3,7,8-tetrachlorodibenzo-p-dioxin.

Cancer cases were identified by linkage with the National Cancer Register. Special attention was given to soft tissue sarcomas and malignant lymphomas. Five cases of soft tissue sarcomas were observed among male employees in contrast to 1.84 expected cases, $RR = 2.72$, $CI_{95} = 0.88-6.34$ (Lyngé, 1985).

An update of the above mentioned cohort study (Lyngé, 1993) adds data for the period 1983-87. Based on small numbers the study adds to the evidence for a possible association between phenoxy herbicide exposure and risk of soft tissue sarcomas. There are, however, a number of possible confounders in these studies, and the overall cancer incidence of workers employed in manufacturing and packaging of phenoxy herbicides was the same as for the Danish population (66 observed v. 64.27 expected, SIR 1.0, 95% CI 0.8-1.3).

IARC (1987) concluded that the chlorophenoxy herbicides should be placed in group 2B because of limited evidence for carcinogenicity to humans and because no adequate published data were available on the carcinogenicity of MCPA to animals.

While PCOC is a breakdown product and possible contaminant of (impurity in) MCPA, implications of these finding for the effects of PCOC itself can remain only speculative.

4.1.2.8 Toxicity for reproduction

In a combined repeated dose/reproduction screening test carried out according to OECD draft guideline 422 (Hansen, 1996) groups of 10 male and 10 female rats were given 0, 50, 200, or 600 mg PCOC/kg in soybean oil by gavage for two weeks prior to mating and until day 20 of gestation. No toxic effects on any reproductive or developmental parameters were observed, resulting in a no effect level for these endpoints of 600 mg/kg.

In a recently conducted *in vitro* assay for estrogenic effects using human breast cancer cells (Körner et al, 1996; Körner et al, 1997), PCOC was found to express activity corresponding to 1×10^{-6} that of 17- β -Estradiol. It is difficult to evaluate what possible influence this might have on reproductive parameters.

Risk characterisation

4.1.2.9 General aspects

Major effects of possible concern are corrosivity, acute inhalation toxicity and repeat dose toxicity. Direct exposure is possible for production workers, and indirect exposure for workers, consumers and the general population.

The human risk assessment according to the pesticide scenario is not conducted based on a decision at EU Technical meeting on risk assessment of existing substances (TM III, Nov.1996) referring to this part of the risk assessment being conducted by DGVI working group on risk assessment of plant protection products.

4.1.2.10 Workers⁴

Production facility workers (see 4.1.1.2. for exposure levels). Realistic worst case exposure is likely to be of the order of 0.7 mg/kg/day according to information provided by one of the producers (A.H. Marks, 1997b).

⁴ Herbicide application workers. (see 4.1.1.1. for exposure levels).

The exposure PCOC as a 1% impurity in MCPA can be in the order 0.28 mg/kg/day (agricultural) or 0.35 mg/kg/day (municipal weed control).

For the end-points irritation/corrosivity the concentration is below the level of concern. For repeat dose toxicity this should not present a major health problem, e.g. for repeat dose toxicity the margin of safety based on a NOAEL of 200 mg/kg/day is $200/0.35 = 571$.

The margin of safety for effects is in the order of 300-600, thus workplace exposure to PCOC does not seem to present a major risk.

Repeat dose toxicity is not likely to present a major health problem. The margin of safety based on a NOAEL of 200 mg/kg/day (slight effect on liver enzyme (ALAT), haemoglobin conc.) is $200/0.7 = 285$.

Also the end-point irritation/corrosivity does not seem to cause any health concern. In situations with possible contact with the substance safety measures, such as wearing appropriate PPE, are prescribed in the existing productions. Further, health surveillance programmes including examination of the respiratory function have been undertaken for several years. According to the medical reports submitted by the producers no significant effects on the respiratory system have been observed.

It should be stressed that direct skin contact with PCOC can lead to burns and/or irritation, but that adequate warning of this effect is given by the manufacturers classification (R-35) and that the wearing of appropriate PPE is compulsory when exposure at the workplace is possible (according to the UK Control Of Substances Hazardous to Health regulation - referred to in (Marks A H , 1997a)).

Conclusion of the risk assessment for workers:

- i) There is need for further information and/or testing
- ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied already
- iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account

4.1.2.11 Consumers

For this group exposure may be in the order of 0.07 mg/kg for each event corresponding to a daily dose of 9.6×10^{-4} mg/kg/day (see 4.1.1.3. for further details). With a NOAEL for repeat dose toxicity of 200 mg/kg/day the margin of safety is at least 20,000 for each single event.

Conclusion of the risk assessment for consumers:

- i) There is need for further information and/or testing
- ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied already
- iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account

4.1.2.12 Man exposed indirectly via the environment

The exposure of man indirectly via the environment through herbicide use is likely to be 10×10^{-8} mg/kg/day via human intake media.

Regional exposure resulting from production of PCOC is estimated as being low (1.3×10^{-5} mg/kg/day), while local indirect exposure estimates of 1.2×10^{-4} mg/kg/day does not give rise to immediate concern with regard to corrosivity or repeat dose toxicity.

Conclusions of the risk assessment for man exposed indirectly via the environment:

- i) There is need for further information and/or testing

- (X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied already
- () iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account

4.1.2.13 Combined exposure

On the basis of the conclusion made in 4.1.1.2. and 4.1.1.3. a consumer, who also works at a production site and sprays garden herbicides, will receive the highest dose of PCOC during work and during gardening activities of 1.05 mg/kg/day. The dose received indirectly via the environment is low compared to this, 1.2×10^{-4} mg/kg/day, but would occur regularly. A margin of safety of 190 (200 mg/kg / 1.05 mg/kg) would not seem to present undue risk.

Conclusions of the risk assessment for man during combined exposure:

- () i) There is need for further information and/or testing
- (X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied already
- () iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account

HUMAN HEALTH (PHYSICO-CHEMICAL PROPERTIES)

4.1.3 Exposure assessment

The substance PCOC gives no reason for concern in relation to the following physical-chemical properties. The tests performed all gave or were expected to give negative results.

4.1.3.1 Occupational exposure

4.1.3.2 Consumer exposure

Indirect exposure via the environment

Effects assessment: Hazard identification and Dose (concentration) - response (effect) assessment

4.1.3.3 Explosivity

Explosive properties have not been tested. No reports of explosive properties were found in the available literature, nor does the chemical structure contain any elements associated with explosivity.

4.1.3.4 Flammability

The substance does not burn according to methods used (EF 3.10 and EF 3.10 mod.), nor is it flammable in contact with water. (Quist Laboratory, 1983).

4.1.3.5 Oxidizing potential

The substance was classified as non oxidizing according to the test method from the working group PC II Annex V EEC/831/79, sixth amendment of Dir. 67/548/EEC. (Dantest, 1983).

4.1.4 Risk characterisation

It is not likely that any of the above mentioned adverse effects should occur under the conditions mentioned.

5 CONCLUSIONS

The documentation varies from original studies according to OECD test guidelines with GLP to literature references of varying quality. 4-Chloro-2-methylphenol (PCOC) is used in the industry as an intermediate in the synthesis of the phenoxy herbicides MCPA, MCPB and mecoprop (MCP). From the industrial production, processing and formulation PCOC is emitted to air and waste water. The produced pesticides contain PCOC as impurity (normally < 1%, 0,5% estimated as realistic worst case). The use of the pesticides in the agriculture as herbicides results in exposure to soil of PCOC as an impurity and degradation product.

As MCPA is transformed to PCOC, and PCOC has a high vapour pressure, the atmosphere will receive a contribution from application of the above mentioned pesticides. PCOC has a low to medium adsorption and may be considered mobile in some soils.

PCOC is according to an experiment primarily degradable by photolysis in clean water with a half-life of 4 days. However, a re-estimation of photolysis to typical EU surface water resulted in an estimated photolytic degradation half-life of 300-700 days and therefore photolysis is considered negligible. The available biodegradation data are somewhat conflicting but based on a judgement of the balance of evidence the "realistic worst case" aerobic biodegradation half-life of PCOC in soil is estimated to be 21 days, whereas no biodegradation has been found under anaerobic conditions. The aerobic biodegradation half-life in surface waters is also estimated to be 21 days. The estimated half-life in biological waste water treatment plants is 0.7 hour resulting in an estimated removal of 88% which is in general accordance with simple mass balance estimations from one of the main manufacturers sites. The substance is therefore considered to be ready biodegradable (borderline).

PCOC has been found in water, soil, air and groundwater. In water occurs mainly around emission sources, in air near fields applied with MCPA or MCP, and in soil and biota after the application of the herbicides. The findings in groundwater are assumed to be the result of mobility and reduced degradation under anaerobic conditions.

The exposure assessment is primarily based on monitoring data from the two main manufacturing sites where all production and all processing of PCOC takes place and where approximately 60% of the production volume is formulated. A worst case environmental exposure scenario for a separate formulation site is included in the risk assessment.

The emissions to surface water from production sites are local and the risk assessment based on monitoring data ($C_{\text{STP} + \text{influent}}$ and actual dilution in STPs) and TGD default environmental exposure assessment for formulation site where 10% of the production volume of phenoxy acids is formulated. Because only the STPs receiving waste water from one of the production sites and the formulation sites are using sludge application to soil, The sludge application is considered local.

PCOC is very toxic to aquatic organisms. The acute toxicity to fish LC_{50} (96h) was observed to be about 2.3-6.6 mg/l. The EC_{50} (48h) to daphnids were 0.29-1.0 mg/l. The EC_{50} (96h) to algae was 8.2 mg/l and the EC_{10} (96h) was 0.89 mg/l. The long term toxic effects were observed in fish to have a NOEC(28d) of 0.5 mg/l and the Daphnia reproduction NOEC(21d) was 0.55 mg/l.

The $PEC_{local(water)}/PNEC_{aquatic\ organisms}$ relationship is < 1 . Model calculation using EUSES version 1.0 supports the assumption of no risks for adverse effects in the aquatic environment and for the microorganisms of STPs.

There are no data available on the terrestrial toxicity. The equilibrium partitioning method is applied as a conservative calculation, comparing $PEC_{soil, porewater}$ with $PNEC_{aquatic\ organisms}$: $PEC_{soil}/PNEC < 1$.

PEC_{air} : There are no effect data present and no relation $PEC/PNEC$ can be calculated.

PCOC has a bioaccumulation potential based on $\log Kow$ 3.09, but BCF found in fish was low (≤ 30). The risk characterisation of secondary poisoning is therefore not performed.

The substance is considered to be of no concern to aquatic organisms and microorganisms of STPs, and no further information on environmental release from production and formulation facilities is required.

No current evidence was found for the use of PCOC as such in products, although it may formerly have been employed as a disinfectant. Direct exposure is therefore likely to be restricted to those involved in the manufacture and handling of PCOC, and in conjunction with its use in the manufacture of phenoxy herbicides. Based on limited information, exposures in the range of 0.02 - 0.7 mg/kg/day are estimated for these activities.

The main exposure of human beings to PCOC is likely to be via production, or use of phenoxy herbicides which may contain it as an impurity ($< 1\%$), or as a breakdown product following exposure of herbicides to sunlight, or to their metabolic transformation to the substance. It is difficult to quantify exposure occurring through transformation, but this is assumed to be less than 1%. During production, a realistic worst case exposure of 0.7 mg/kg/day is indicated. In conjunction with agricultural application of herbicides, a worst-case estimate of exposure to PCOC of 0.28 mg/kg/day is obtained. Municipal gardeners may be exposed to higher levels with an estimate of 0.35 mg/kg/day suggested as a realistic worst case.

Similarly, some consumer exposure should also be expected, as the same herbicides can be used in lawn treatment and similar gardening activities. While no detailed information was found on such exposures, it may be amount to 0.07 mg/kg per event. Assuming a really worst case of five events per year, the total yearly dose of PCOC would be 0.35 mg/kg/year corresponding to 9.6×10^{-4} mg/kg/day.

Indirect exposure via the environment resulting from partitioning into air/water/soil and biomagnification in food sources is low at a regional level, combined secondary exposure estimate being in the range of 1.40×10^{-5} mg/kg/day of PCOC. Local indirect exposure estimates are about 1.2×10^{-4} mg/kg/day.

The acute toxicity of PCOC (LD_{50} oral rat 2650-3196 mg/kg, LD_{50} dermal rat 2240 mg/kg, LC_{50} inhal. rat 4h 0.9mg/l or >30 mg/l) does not give rise to immediate concern, particularly considering that the substance (crystalline needles) is unlikely to form aerosols or dusts, and that PPE is mandated during handling of the substance.

PCOC is corrosive in high concentrations, and has been assigned risk phrase R-35 by the manufacturers which should provide adequate warning to those handling it in industrial settings. No consumer exposure is expected at concentrations which could approach that required for corrosivity. No sensitization was observed in a Guinea pig maximization test and no case studies indicating sensitization of persons handling the substance were found.

There were no effects on reproduction according to OECD screening test 422 at doses of up to 600 mg/kg for a total of 40 days.

In 28-day repeat dose studies in rats, the best NOAEL appears to be 200 mg/kg, with a LOAEL of 800 mg/kg where salivation after dosing and ruffled fur was seen in some animals. At this dose, levels of serum alanine-aminotransferase were increased in males, and effects were seen on blood parameters (reduced thromboplastin times, reduction of leukocyte and erythrocyte counts). Liver weights in females were increased, but no histopathological changes were seen in this, or any other organs examined. Decreased adrenal weights were also seen in females at 200 mg/kg and above, but were unaccompanied by histopathological changes.

PCOC has not been investigated for carcinogenicity. Two older tests were positive for mutagenicity, one *in vivo* (mouse micronucleus test) and one *in vitro* in a single strain (TA97) of Salmonella in the Ames test (while showing no activity in other strains in a number of separate tests). Repeated testing with TA97 gave unequivocally negative results. A repeat of the micronucleus test according to current guidelines also gave clearly negative results. On the balance, it is not felt that there is evidence for PCOC being a mutagen.

The estimated human local indirect exposure of 1.2×10^{-4} mg/kg/day is well below the repeat dose toxicity (NOAEL 200 mg/kg/day).

For the population with the highest potential exposure (production workers assuming inhalation exposure at 5 mg/m^3 for eight hours) a margin of safety of 285 ($200 \text{ mg/kg}/0.7 \text{ mg/kg/day}$) is obtained with regard to the repeat dose NOAEL. For agricultural workers engaged in spraying phenoxy herbicides the ratio is $200 \text{ mg/kg}/0.28 \text{ mg/kg}$, or 714. For municipal gardeners (0.35 mg/kg/day) a margin of safety of 571 is obtained. Consumers may be exposed to 0.07 mg/kg/day once, or a few times yearly. All other exposure scenarios result in much higher margins of safety.

6 REFERENCES

Ames B.N, J. McCann & E. Yamasaki (1975): Mutation Res. 31, 347-364.

AT: Arbejdstilsynet. (1994). Grænseværdier for stoffer og materialer. At-anvisning nr. 3.1.0.2. Direktoratet for Arbejdstilsynet, København, Denmark.

Atkinson R (1986): Kinetics and mechanisms of the gas-phase reaction of the hydroxyl radical with organic compounds under atmospheric conditions. Chem Rev 86: 69-201

BASF (1994). IUCLID Data Sheet Prepared by BASF 1994.

Benoit-Guyod JL, Andre C, Clavel K (1984): Chlorophenols: degradation and toxicity. J. Fr. Hydrol. 10(3): 249-63.

Benoit-Guyod JL, Crosby DG, Bowers JB (1986): Degradation of MCPA by ozone and light. Water. Res. 20(1): 67-72.

Bhamidimarri SMR, Petrie RA (1992): Adsorption and biodegradation of herbicide chemicals in silt loam soil. Proc. Ind. Waste Conf. 46: 591-5

Binderup, M-L, "4-chloro-2-methylphenol," Mutagenicity Study, Institute of Toxicology, National Food Agency, Denmark, 1996.

Blackman GE, Parke MH, Garton G (1955): The physiological activity of substituted phenols. I. Relationships between chemical structure and physiological activity. Arch. Biochem. Biophys. 54: 45-54.

Bollag JM, Alexander M (1967): Enzymatic degradation of phenoxyalkanoate herbicides. Bacteriol Proc. 1967: 8

Bollag JM, Helling CS, Alexander M (1967): Metabolism of 4-chloro-2-methylphenoxyacetic acid by soil bacteria. Appl. Microbiol 15(6): 1393-8.

Boethling *et al.* (1995): Factors for intermedia extrapolation in biodegradability assessment, Chemosphere 30, 741-52.

BUA (1993): 4-Chloro-3-methylphenol. BUA reprot 135, GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance, Stuttgart, December 1993, p. 103.

BUA (1994): 4-Chlor-2-methylphenol (p-Chlor-o-Kreol, PCOC). BUA-Stoffbericht 134. Beratergremium für umweltrelevante Altstoffe (BUA) der Gesellschaft Deutscher Chemiker.

Buccafusco, R.J. (1981): Acute toxicity of priority pollutants to Bluegill *Lepomis macrochirus*. Bulletin of Environmental Contamination and Toxicology 26: 446-52.

Buisson, RSK, Kirk, PWW, Lester, JN (1984): Determination of chlorinated phenols in water, wastewater and waste-water sludge by capillary gas chromatography-electron capture detector. J. Chromatogr. Sci. 22(8): 339-42.

Buisson RSK, Kirk PWW, Lester JN, Campbell JA (1986): Behavior of selected chlorinated organic micropollutants during batch anaerobic digestion. *Water Pollut. Control (Maidenstone, Engl)* 85(3): 387-94.

Buisson, RSK. Kirk, PWW, Lester, JN (1988): The behaviour of selected chlorinated organic micropollutants in the activated sludge process: A pilot plant Study. *Water Air Soil Pollut* 37: 419-32.

Buisson RSK, Kirk PWW, Lester JN (1990): Fate of selected chlorinated organic compounds during semi-continuous anaerobic sludge digestion. *Arch. Environ. Contam Toxicol.* 19: 428-32.

Chambers CW, Tabak HH, Kabler PW (1963): Degradation of aromatic compound by phenol-adapted bacteria. *J. Water Pollut. Control Fed.* 35: 1517-28.

Clapes P, Soley J, Vincente M, Rivera J, Caixach J, Ventura F (1986): Degradation of MCPA by photochemical methods. *Chemosphere* 15: 395-401.

Crosby DG, Bowers JB (1985): Composition and photochemical reactions of dimethylamine salt formulation of (4-chloro-2-methylphenoxy)acetic acid (MCPA). *J. Agric. Food Chem.* 33(4): 569-73.

Danish EPA (1995): Bekæmpelsesmiddelstatistik 1993. (The sale of plant protection active ingredients in 1991, 1992 and 1993). *Orientering fra Miljøstyrelsen 2/1995.* Danish Environmental Protection Agency, Copenhagen, Denmark.

Dantest (1983). Dantest study, prepared for the Danish-EPA.

Devilliers J, Chambon P, Zakarya D, Chastrette M (1986): Quantitative structure-activity relations of lethal effects of 38 halogenated compounds on *Lepomis macrochirus*. *C. R. Acad. Sci Ser.3* vol 303(14): 613-16.

DGU (1994): Grundvandsovervågning 1994.(Groundwater monitoring 1994 - in Danish). Danish Geological Survey Agency, Copenhagen, Denmark

Duah-Yentumi S, Kuwatsuka S (1980): Effects of organic matter and chemical fertilizers on the degradation of benthocarb and MCPA herbicides in the soil. *Soil Sci. Plant Nutri.* 26(4): 541-9.

EUSES (1997): The European Union System for the Evaluation of Substances, EUSES version 1.00. RIVM, NL for the European Chemical Bureau, JRC Environment Institute, Ispra, Italy.

Fiege H. Cresols and xlenols. In: Gerhartz W *et al.* (eds). *Ullmann's Encyclopedia of industrial chemistry.* VCH Verlag Germany 1986.

Folke J (1984): Organic micropollutants in the sewage from a phenoxyalkanoic acid production plant after biological treatment in a municipal trickling filters plant. *J.High Resolut. Chromatogr. Commun.* 7(1): 25-32.

Folke J, Lund U (1983): Occurrence of low- and high-chlorinated phenols in municipal sewage before and after passing through biological treatment plants. *J. Chromatogr.* 279: 189-98.

Freiberg MB, Crosby DG (1986): Loss of 4-chloro-2-methylphenoxyacetic acid from simulated spray droplets. *J.Agric.Food Chem.* 34(1): 92-95.

Gamar Y, Gaunt JK (1971): Bacterial metabolism of 4-chloro-2-methylphenoxyacetate. *Biochem* 122: 527-531.

Gaunt JK, Evans WC (1971): Metabolism of 4-chloro-2-methylphenoxyacetate by a soil Pseudomonad. *Biochem Journal* 122: 519-526.

Haldrup C, Kryger P, Nielsen GC, Jørgensen LN (1995). *Vejledning i planteværn*. Landbrugets Informationskontor, Århus, Denmark.

Hansch C, Leo A, Hoekman D (1995): Exploring QSAR. Hydrophobic, electronic, and steric constants. ACS Professional Reference Book. American Chemical Society, Washington DC.

Hansen, E., "4-Chloro-2-methylphenol," Combined Repeated dose and Toxicity study with the Reproductive/developmental Toxicity Screening Test on 1-Chloro-2-methylphenol in Rats, Institute of Toxicology, National Food Agency, Denmark, 1996.

Harries JE, Sheahan DA, Jobling S, Matthiessen P, Neall P, Sumpter JP, Taylor T, Zaman N (1997): Estrogenic activity in five United Kingdom rivers detected by measurement of vitellogenesis in caged male trout. *Environ. Toxicol. Chem.* 16(3): 534-542.

Hattula ML, Elo H, Reunanen H, Arstila AU, Sorvari TE (1977). Acute and subacute toxicity of 2-methyl-4-chlorophenoxyacetic acid (MCPA) in the male rat. I. Light microscopy and tissue concentrations of MCPA. *Bull Environ Contam Toxicol*, 18, 152-158.

Hattula ML, Reunanen H, Arstila AU (1979). Toxicity of 4-Chloro-*o*-Cresol to Rat: I. Light Microscopy and Chemical Observations. *Bull Environ Contam Toxicol*, 21, 492-497.

Hattula, M.L. *et al.* (1979): Toxicity of 4-chloro-*o*-cresol to fish. Light microscopy and chemical analysis of the tissue. *Bull. Environ. Contam. Toxicol.* 22: 508-511.

Hattula ML, Wasenius VM, Reunanen H, Arstila AU (1981): Acute toxicity of some chlorinated phenols catechols and cresols to trout *Salmo trutta*. *Bull. Environ. Contam. Toxicol.* 26(3): 295-298.

Hemmen van JJ (1993). Predictive exposure modelling for pesticide registration purposes. *Ann Occup Hyg* 37: 541-564.

HSE. (1995) EH40/95 Occupational exposure limits 1995. Her Majesty's Stationary Office, London, Great Britain.

Huntingdon (1997): Huntingdon Life Sciences. PCOC Mouse Micronucleus Test Report. Confidential AHM 114/970552, pp. 28, Apr. 24. 1997

IARC (1987). IARC Monographs on the evaluation of carcinogenic risks to humans. Overall evaluations of carcinogenicity: An updating of IARC Monographs volumes 1 to 42. IARC, Lyon. Suppl. 7, p. 156-160.

Jahanshahi J., Stow R.A. (1995). (14-C)-MCPA: Absorption, distribution, metabolism and excretion in the rat. Final report. Corning Hazleton, June, 1995.

Kincannon DF, Lin YS (1985): Microbial degradation of hazardous wastes by land treatment. *Proc. Ind. Waste Conf* 40: 607-9

Kirk P WW, Lester JN (1988): The behaviour of chlorinated organics during activated sludge treatment and anaerobic digestion. *Water Sci. Technol.* 20(11-12): 353-60.

Körner W, Hanf V, Schuller W, Bartsch H, Kreienberg R, Hagenmaier H (1997): Validation and application of a rapid *in vitro* assay for assessing the estrogenic potency of halogenated phenolic chemicals. *Chemosphere* (accepted 12. November 1997).

Leblanc, G.A. (1980): Acute toxicity of priority pollutants to Water flea (*Daphnia magna*) *Bulletin of Environmental Contamination and Toxicology* 24: 684-91.

Lindgaard-Joergensen P (1989): Biodegradability of chlorophenols and mixtures of chlorophenols in seawater. *Ecotoxicol. Environ. Saf.* 17(2): 216-20.

LST: National Food Agency of Denmark (in prep). Combined repeated dose and toxicity study with the reproductive/developmental toxicity screening test on 4-chloro-2-methylphenol in rats. *Levneds-middelstyrelsen, Søborg* (draft, 1995).

Lund I, Kirknel E (1995). Traktorførerens pesticidbelastning (Exposure of tractor drivers to pesticides). *Beretning nr. 62/1995. Statens Husdyrbrugsforsøg, Horsens, Denmark.*

Lyman W, Reehl WF, Rosenblatt DH (1982): *Handbook of chemical property estimation methods.* McGraw Hill, Inc. New York.

Lynge E (1985). A follow-up study of cancer incidence among workers in manufacture of phenoxy herbicides in Denmark. *Br J Cancer* 52: 259-70.

Lynge E (1993). Cancer in phenoxy herbicide manufacturing workers in Denmark, 1947-87. An update. *Cancer Causes Control* 4: 261-72.

Mackay D, Paterson S (1990): Fugacity models. In: Karcher W & Devillers J (eds.). *Practical applications of quantitative structure-activity Relationships (QSAR) in environmental chemistry and toxicology.* ECSC, EEC, EAEC, Brussels. Kluwer Acad. Publ. The Netherlands, 1990. p 433-460.

Marks A.H. & Co. LTD., letter of 1. July 1995.

Marks A.H. (1997a) & Co. LTD., letter of 15. October 1997.

Marks A.H. (1997b): The manufacture of PCOC and associated phenoxy acids: Worker exposure and emission report. **Confidential report.** A.H.Marks & Co. Ltd. Bradford, October 1997. **Submitted to the CAs.**

Milner CR, Goulder R (1986): Comparative toxicity of chlorophenols, nitrophenols and phenoxyalkanoic acids to freshwater bacteria. *Bull. Environ. Contam. Toxicol.* 37: 714-718.

Nufarm UK Ltd. (1997): Environmental release of 4-chloro-2-methylphenol (PCOC) during production and synthesis of phenoxy acid herbicides. **Confidential report,** Nufarm UK Ltd., Belvedere, UK. **Submitted to the CAs.**

Nufarm UK Ltd. 1997b: Further information on environmental release of 4-chloro-2-methylphenol (PCOC) as requested by the European Chemicals Bureau. **Confidential report.** Nufarm UK Ltd., Belvedere, UK, October 1997. **Submitted to the CAs.**

Oh, KH, Ahn SK, Yoon KH, Kim YS (1995): Biodegradation of the phenoxy herbicide MCPA by microbial consortia isolated from a rice field. *Bull. Environ. Contam. Toxicol.* 55: 539-545.

Paasivirta J, Sattar MA, Lahtipera M, Paukku R (1983): CG and MS analysis of MCPA and its two metabolites in the environment nearby a bush killing treatment zone. *Chemosphere* 12(9-10): 1277-89.

PCOC Task Force (1997); PCOC: Chronic toxicity to *Daphnia magna*. Brixham Environmental Laboratory Zeneca Ltd Report No. BL6032/B. September 1997.

Qvist Lab. (1983). Test report from Qvist Laboratories, Denmark, prepared for the Danish-EPA.

RIVM, VROM, WVC (1994): Uniform System for the Evaluation of Substances (USES), version 1.0. National Institute of Public Health and Environmental Protection (RIVM), Ministry of Housing, Spatial Planning and the Environment (VROM), Ministry of Welfare, Health and Cultural Affairs (WVC). VROM, The Hague.

Räsänen L, Hattula ML, Arstila AU (1977). Mutagenicity of MCPA and its soil metabolites, chlorinated phenols, catechols and some widely used slimicides in Finland. *Bull Environ Contam Toxicol*, 18, 565-571.

Russom CL, Bradbury SP, Broderius SJ (1997): Predicting modes of toxic action from chemicals structure: Acute toxicity in the fathead minnow (*Pimephales promelas*). *Envir. Tox Chem.* 16: 948-967.

Sattar, M.A. (1981): Persistence of 4-chloro-o-cresol and 5-chloro-3-methylcatechol in soil. *Chemosphere* 10(9): 1011-1018.

Sattar MA (1982): Persistence of 4-chloro-2-methylphenoxyacetic acid in soil. *Bull. Environ. Contam. Toxicol.* 28(3): 348-52.

Sattar, M.A. (1989): Fate of Chlorinated cresols from Environmental samples. *Chemosphere* 19(8-9): 1421-26.

Scantox (1982a). Report No. 10149, 27th December 1982. Scantox, Ejby, Denmark.

Scantox (1982b). Report No. 10150, 24th November 1982. Scantox, Ejby, Denmark.

Scantox (1982c). Report no. 10152, 26th November 1982. Scantox, Ejby, Denmark.

Scantox (1982d). Report No. 10154, November 17th 1982, Scantox, Ejby, Denmark.

Scantox (1982e). Report No. 10155, 28th December 1982. Scantox, Ejby, Denmark.

Scantox (1982f). Report No. 10156, 23th December 1982. Scantox, Ejby, Denmark.

Scantox (1983). Report No. 10153, February 28th 1983. Scantox, Ejby, Denmark.

Schrötter E, Tschäpe M, Meister A (1977). Organische synthetica und ihre vermiziden Eigenschaften. 5. Mitteilung. Ovozide Phenolderivate. *Pharmazie* 32: 171-174.

Seiber JN, McChesney MM, Sanders PF, Woodrow JE (1986): Models for assessing the volatilisation of herbicides applied to flooded rice fields. *Chemosphere* 15(2): 127-138.

Smith AE (1985): Identification of 4-chloro-2-methylphenol as a soil degradation product of ring-labeled ¹⁴C-Mecoprop. *Bull. Environ. Contam. Toxicol.* 34(5): 656-60.

Soderquist CJ, Crosby DG (1975): Dissipation of 4-chloro-2-methylphenoxyacetic acid (MCPA) in a rice field. *Pestic. Sci.* 6(1): 17-33.

Spliid NH, Mogensen BB (1995): Leaching of pesticides from arable soil (In Danish). *Bekæmpelsesmiddelforskning fra Miljøstyrelsen* Nr. 11. Danish Environmental Protection Agency.

Strobel K, Grummt T. (1987): Aliphatic and aromatic halocarbons as potential mutagens in drinking water. *Toxicol Environ Chem* 14, 143-156.

Teknologisk Institut (1982): Test report No. 2254851/60, December 1982. Teknologisk Institute, Microbiology, Taastrup, Denmark.

TETRATECH (1983): Water Quality Assessment. A Screening Procedure for Toxic and Conventional Pollutants in Surface Waters. Tetra Tech Inc. 1983.

TGD (1996): Technical Guidance Documents in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances. Part I-IV. European Communities, Brussels, 1996.

Ursin C (1985): Degradation of organic chemicals at trace levels in seawater and marine sediments. The effect of concentration of the initial fractional turnover rate. *Chemosphere* 14(10): 1539-1550.

US-EPA (1996): SIDS data summary for 4-chloro-2-methylphenol. Draft summary, October 18, 1996.

US-EPA (1997), Registration Eligibility Decisions: p-Chloro-m-cresol. Environmental Protection Agency, Washington D.C. Office of Prevention, Pesticides and Toxic Substances, 1997 (PB97-141733).

Weast RC (ed.) (1986): Handbook in chemistry and physics. Chemical Rubber Company, CRC 67th ed.

Woodrow JE, McChesney, Seiber JN (1990): Modelling the volatilisation of pesticides and their distribution in the atmosphere. In: Kurtz DA (Ed.): Long range transport of pesticides, Lewis Publ Inc. Chelsea, Michigan USA. ISBN 0-87371-168-8, p.61-82.

7 APPENDIX

Appendix 1

7.1 PHOTOLYSIS OF PCOC IN SURFACE WATER.

The effect of sunlight irradiation on aqueous solution of PCOC (100 µg/l = 0.7 mM) was studied. The PCOC-solution was sealed in a flask to prevent volatilisation. The exposure to "summer sunlight" (not further defined or specified) in California resulted in a stated photolytic half-life of 2.5 days (which from the presented graph rather seems to be 4 days) (Crosby & Bowers 1985). It is below assumed that the experimental data ($T^{1/2} = 4$ days) were obtained using quartz flask, i.e. at the surface of pure water at 40° latitude in the summer.

A photolytic half-life can be extrapolated from one set of conditions to another as a function of season, latitude, time of day, cloudiness, depth of water bodies and its content of dissolved and suspended matter (Zepp & Cline 1977: "Rates of direct photolysis in aquatic environment". Environmental Science and Technology 11: 359-366, "Water Quality Assessment. A Screening Procedure for Toxic and Conventional Pollutants in Surface Waters" (TETRATECH 1983), "Technical Guidance Document. Environmental Risk Assessment of New and Existing substances", Draft Sept. 1995 (TGD Sept.95), "Direct Phototransformation of Chemicals in Water. A draft guidance document" Febr.1995, OECD).

Like hydrolysis, photolysis only results in primarily degradation (transformation) of substance. Furthermore, extrapolation of photolytic half-lives from one set of conditions to another is generally very uncertain. A substantial part of the uncertainty may be due to lack of information of the conditions under which the half-life was measured. On the other hand it is rather easy to define the conditions of the environment of the "standard EU region" (cf. TGD Sept.95). However the representativeness of such a "standard EU" environment for the whole EU may be questioned (e.g. how to define the "standard" water body as regards water depth and content of dissolved and suspended matter? The latitude range of EU covers the latitudes from 35° to 70° giving a tremendous difference in the incoming sun light intensity in the relevant wave length interval). Below it is assumed that the standard EU environment is at the latitude 50°. As regard the content of dissolved and suspended matter and the depth of water in the EU "standard environment" cf. below.

Two types of extrapolation guidance have been considered:

- TGD (Sept.1995 ver.)
- TETRATECH (1983)

According to TGD (Sept.95):

The extrapolation methods recommended in TGD require use of computer models which were not available.

According to TETRATECH:

Photolytic rate constant $K_{\text{photo}} = K_{\text{photo},0} * (I/I_0) * 1/K * Z$

where

$K_{\text{photo},0}$ = Experimentally determined photolytic rate constant at surface of pure water

I: light intensity at the conditions under consideration

I_0 : light intensity at the surface of pure water at which $K_{\text{photo},0}$ was measured

K: light reduction (diffuse light attenuation coefficient) in water = R/Z_{sd} ,

Z_{sd} : Secchi disc depth (m)

R: proportionality constant 1.44-1.7 for visible light (400nm to 800nm). In the middle UV portion of the spectrum (i.e.near 312 nm) R = 9.15

Z: water depth (m)

The experimentally determined photolytic rate constant at the surface of pure water (summer, 40 °): $T_{1/2}$ of 4 days, is calculated to be $K_{\text{photo,CA}}: \ln 2/4 \text{ (d}^{-1}\text{)} = 0.17325 \text{ (d}^{-1}\text{)}$, and Annual mean: $I_{\text{EU}}: 460 \text{ langley/d (TETRATECH)}$,

Winter mean: $I_{\text{EU}}: 190 \text{ langley/d (TETRATECH)}$

Summer mean $I_{\text{CA}}: 740 \text{ langley/d (TETRATECH)}$

In the table below extrapolations according to various Z_{sd} and Z of the "standard EU environment" for the whole year (upper four rows) and for the winter season (lower four rows, "realistic worst case" according to suggestion of draft TGD (sept.)) are presented;

Z_{sd} m	K m^{-1}	Z	$1/(K*Z)$	I_{EU} ly/d	$K_{\text{photo,EU}}$ d^{-1}	$T_{1/2\text{photo,EU}}$ days
1	9.15	1	0.1093	460	0.0118	58
0.5	18.3	1	0.0546	460	0.0059	117
0.3	30.5	1	0.0328	460	0.0035	198
0.6	15.3	3	0.0218	460	0.0023	301
1	9.15	1	0.1093	190	0.0049	141
0.5	18.3	1	0.0546	190	0.0024	289
0.3	30.5	1	0.0328	190	0.0015	475
0.6	15.3	3	0.0218	190	0.0009	715

Remark: The relevant dimensions of the "standard environment" employed in the regional model for calculation of $\text{PEC}_{\text{water, regional}}$ for EU is a water depth of 3 m and a concentration of suspended solids of 15 mg/l. The latter is equivalent with $Z_{\text{sd}} = 0.6 \text{ m}$ (pers. comm. O. Sortkær, Danish Environmental Research Inst.). Therefore it seems most reasonable to choose these values when extrapolating the experimental data on photolysis to photolytic degradation half-lives in EU surface waters. The estimated photolytic half-life in surface waters of EU is therefore 301 days for the annual mean and 715 days for the winter season.

Based on the above estimations, the photolytic degradation of PCOC in surface waters of EU is concluded to be negligible.

Appendix 2

7.2 QSAR ESTIMATIONS ON TOXICITY

Comparison between QSAR predicted and experimental L(E)C₅₀-values for fish and daphnia using the preferred log Kow 3.09 and the log Kow 2.63 by Hansch *et al.* (1995)..

The QSARs employed are those recommended in the TGD for polar narcotic acting substances. Recommended QSAR for polar narcotic acting substances on algae has not been agreed upon.

Log Kow = 3.09	QSAR L(E)C₅₀ (mg/l)	Experimental L(E)C₅₀ (mg/l)	Ratio QSAR/experimental
Fish	5	2.3	2.2
Daphnia	4	0.63 *	6.3

Log Kow = 2.63	QSAR L(E)C₅₀ (mg/l)	Experimental L(E)C₅₀ (mg/l)	Ratio QSAR/experimental
Fish	12	2.3	5.2
Daphnia	8	0.63 *	12.5

*: Geometric mean og nominal acute toxicity by three independent authors.

The comparisons illustrate the reliability of the nominal experimental values may be invalid or that excess acute toxicity towards daphnids may occur. However, as the results are not used in the risk assessment, the validity is not further discussed.

Appendix 3

7.3 TGD ESTIMATIONS ON EXPOSURE

7.3.1 PEC_{local, water} estimations

For illustrative purposes, estimations according to TGD are calculated below. The calculations of the predicted environmental concentrations are presented according to TGD, Appendix I, Table A1.2, A2.1, A3.3 and B1.6, B2 and B3.2. Measured data from the two main production sites are included as average values to preserve confidentiality.

The calculation of PEC_{local} for the aquatic compartment includes the calculation of the discharge concentration of STP to a water body, dilution effects and removal from the aqueous medium by adsorption to suspended matter.

The local emission during episode to the aquatic compartment, E_{local,water}, is calculated by using the regional values in section 3.1.1.4 multiplied with the estimated fractions.

Fractions of total production volume used for local calculations:

Production: 0.5

Processing: 0.5

Formulation: $0.5 \times 0.6 = 0.3$

Days of emission is according to TGD: 300 days/year. The calculation of the local concentration in untreated waste water, C_{local,influent}, is performed by the equation:

$$C_{\text{local,influent}} = E_{\text{local,water}} * 10^6 / \text{EFFLUENT}_{\text{STP}}$$

where the EFFLUENT_{STP} is the capacity of the STP multiplied with the sewage flow per inhabitant (default $10000 \times 200 = 2 \times 10^6$ l/d). For comparison the site specific EFFLUENT_{STP} of 1.3×10^8 l/d is included. Because this value is the lowest flow of the STPs receiving waste water from the two known manufacturers, the resulting values are used in the further estimations.

Concentration in waste water before treatment in municipal STP

Life cycle stage	Emission (t/y)	Emission (kg/d)	C _{site effluent} ** (mg/l)	C _{STP influent} (mg/l)	
				TGD	Site***
Production	22.5	75.0		37.5	0.58
Processing	3.75	12.5		6.3	0.10
Formulation ⁵	13.5	45.0		7.5	0.12
Specific site	2.5 *	7.8 *	30 **		0.004**

*: Monitoring data from an actual production site representing the average of two production plants where all three processes are included (cf. Confidential appendix, submitted to CAs).

** : Monitoring data, average value from two sites, 95% percentile.

***: Dilution during entrance to STP with other waste water, STP flow $130000 \text{ m}^3/\text{d}$.

The concentration in the STP effluent is found by including the fraction of emission directed to water by STP:

⁵ The release estimations from the formulation performed outside the specific sites are calculated according to TGD using 10% of total production and a PCOC content of the formulation of 1% (worst case). The default local waste water volume is according to TGD: $2000 \text{ m}^3/\text{d}$, and number of days of emission is according to TGD: 300.

$$\text{Clocal}_{\text{effluent}} = \text{Clocal}_{\text{influent}} * \text{Fstp}_{\text{water}}$$

The EUSES model includes the model SimpleTreat 3.0 in the calculations and estimate 12% is directed to water (i.e.: 0.5% to air, 12,1% to water, 3.6% to sludge and 83.8% degraded, and a removal of 88%).

The local concentration in surface water is calculated according to the equation:

$$\text{Clocal}_{\text{water}} = \text{Clocal}_{\text{effluent}} / (1 + K_{p(\text{susp})} * \text{SUSP}_{\text{water}} * 10^{-6}) * D,$$

where

$K_{p(\text{susp})}$ = the solids-water partitioning coefficient of suspended matter = $K_{oc} * F_{oc_{\text{susp}}} = 401 * 0.1 = 40.1$ l/kg, and $\text{SUSP}_{\text{water}}$ = the concentration of suspended matter in the river (default: 15 mg/l), and D = dilution factor (default 10). The dilution of EFFLUENT_{STP} to river based on river flows varies between 2.5 to 1700. But since unknown formulation sites are also included in the estimations the default value is used in the risk assessment.

The concentration at the regional scale ($\text{PEC}_{\text{regional}_{\text{water}}}$) is used as background concentration for the local scale. Therefore, these concentrations are summed for the predicted environmental concentration in surface water during episode and in the annual average:

$$\text{PEC}_{\text{local}_{\text{water}}} = \text{Clocal}_{\text{water}} + \text{PEC}_{\text{regional}_{\text{water}}}$$

$$\text{PEC}_{\text{local}_{\text{water,ann}}} = \text{Clocal}_{\text{water,ann}} + \text{PEC}_{\text{regional}_{\text{water}}}$$

Predicted environmental local concentration in surface water during episode ($\text{PEC}_{\text{local}_{\text{water}}}$). The site specific dilution data are used in the estimations.

Life cycle stage	Clocal _{effluent} (mg/l)	Clocal _{water} (mg/l)	PEC local _{water} * (mg/l)
Production	0.070	0.0070	0.0071
Processing	0.012	0.0012	0.0013
Formulation	0.042	0.0042	0.0043
Site specific measurements	0.004	0.0036	0.0038

*: including $\text{PEC}_{\text{regional}_{\text{water}}}$ 0.000169 mg/l

The predicted annual average concentration in surface water ($\text{PEC}_{\text{local}_{\text{water,ann}}}$)

Life cycle stage	Clocal _{water} (mg/l)	Clocal _{water,ann} (mg/l)	PEC _{local_{water,ann}} * (mg/l)
Production	0.0070	0.0057	0.0059
Processing	0.0012	0.0010	0.0011
Formulation	0.0042	0.0034	0.0036
Specific site **	0.0036	0.0036	0.0037

*: including $\text{PEC}_{\text{regional}_{\text{water}}}$: 0.000169 mg/l

** : Based on monitoring data

Calculation of PEC local for sediment

The local concentration in sediments during emission episode is calculated according to TGD. The concentration in the bulk sediment is derived from the corresponding water body concentration, assuming a thermodynamical partition equilibrium:

$$\text{PEC}_{\text{local}_{\text{sed}}} = (K_{\text{susp-water}} / \text{RHO}_{\text{susp}}) * \text{PEC}_{\text{local}_{\text{water}}} * 1000$$

$K_{\text{susp-water}}$ = the suspended matter partitioning coefficient = 10.9
 RHO_{susp} = bulk density of (wet) suspended matter = 1150 kg/m³

Predicted environmental local concentration in sediments (PEC_{local, sed})

Life cycle stage	PEC local _{water} (mg/l)	PEC local _{sed} (mg/kg)
Production	0.0071	0.0676
Processing	0.0013	0.0126
Formulation	0.0043	0.0412
Specific site*	0.0038	0.038

*Estimated, using monitoring data

7.3.2 Atmospheric exposure estimations.

Exposure from production, processing and formulation

The concentration in air at a distance of 100 meters from the point source is estimated according to TGD. In the calculation for PEC_{local} for air both emissions from a point source as well as the emission from a STP is taken into account. The maximum from the two concentrations (direct and via STP) is used as the PEC_{local}.

E_{local,air} is the local direct emission rate to air during emission episode

E_{stp,air} is the local indirect emission to air from STP during episode:

$$E_{\text{stp,air}} = F_{\text{stp,air}} * E_{\text{local,water}}$$

C_{local,air} is the local concentration in air during emission episode:

$$C_{\text{local,air}} = \max \text{Emission} (E_{\text{local,air}} \text{ or } E_{\text{stp,air}}) * C_{\text{std,air}}$$

where C_{std,air} is the standard concentration in air at source strength of 1 kg/d = 2.78x10⁻⁴ mg/m³.

C_{local,air,ann} is the annual average concentration in air, 100 m from point source:

$$C_{\text{local,air,ann}} = C_{\text{local,air}} * 300/365$$

The annual average predicted environmental concentration in air, PEC_{local,air,ann}, is the local annual average added to the regional concentration in air.

PEC_{regional,air} : 1.18x10⁻⁶ mg/m³ (EUSES)

PEC_{local,air} calculations

	Emission (t/yr)	E _{local,air} (kg/d)	E _{stp,air} (kg/d)	C _{local,air} (mg/m ³)	C _{local,air,ann} (mg/m ³)	PEC _{local,air,ann} (mg/m ³)
Production	0.075	0.25	0.482	0.00013	0.00011	0.00011
Processing	0.075	0.25	0.075	0.00007	0.00006	0.00006
Formulation	4.5	15.0	0.289	0.00417	0.00343	0.00343
Specific site**		0.57	0.047	0.00016	0.00013	0.00013

** : Estimated using monitoring data

Deposition from air

The deposition from air includes the emissions from the two sources (direct and STP)

The annual average total deposition flux is defined as:

$$\text{DEPtotal ann} = \text{DEPtotal} * 300/365$$

The total deposition from air during emission episode is calculated as;

$$\text{DEPtotal} = (\text{Elocal}_{\text{air}} + \text{Estp}_{\text{air}}) * [\text{Fass}_{\text{aer}} * \text{DEPstd}_{\text{aer}} + (1 - \text{Fass}_{\text{aer}}) * \text{DEPstd}_{\text{gas}}]$$

where the fraction of PCOC associated with aerosol particles can be estimated on basis of the chemicals vapour pressure (TGD):

$$\begin{aligned} \text{Fass}_{\text{aer}} &= (\text{CON}_{\text{junge}} * \text{SURF}_{\text{aer}}) / (\text{VP} + \text{CON}_{\text{junge}} * \text{SURF}_{\text{aer}}) \\ &= 1 \times 10^{-4} / (26.66 + 1 \times 10^{-4}) = 3.75 \times 10^{-6} \end{aligned}$$

$\text{DEPstd}_{\text{air}}$, the standard deposition flux of aerosol-bound compound at a source strength of 1 kg/d is default $1 \times 10^{-2} \text{ mg/m}^2/\text{d}$

$\text{DEPstd}_{\text{gas}}$, the deposition flux of gaseous compounds as a function of Henry's Law coefficient, at a source strength of 1 kg/d, is for PCOC $4 \times 10^{-4} \text{ mg/m}^2/\text{d}$

Deposition from the atmosphere calculations

	$\text{Elocal}_{\text{air}}$ (kg/d)	Estp_{air} (kg/d)	DEPtotal ($\text{mg/m}^2/\text{d}$)	$\text{DEPtotal}_{\text{ann}}$ ($\text{mg/m}^2/\text{d}$)
Production	0.25	0.482	0.00029	0.00024
Processing	0.25	0.075	0.00013	0.00011
Formulation	15.0	0.289	0.00612	0.00503
Site specific*	0.57	0.047	0.00025	0.00020

* Estimated from monitoring data

7.3.3 PEC_{local, soil} estimations

The estimated concentration of PCOC in soil may be a results of atmospheric deposition and sludge application.

Deposition from air

The contribution from atmospheric deposition, D_{air} is derived by converting the total deposition flux $\text{DEPtotal}_{\text{ann}}$ (calculated in the previous appendix) by the equation:

$$D_{\text{air}} = \text{DEPtotal}_{\text{ann}} / (\text{DEPTH}_{\text{soil}} * \text{RHO}_{\text{soil}})$$

where RHO_{soil} is the bulk density of (wet) soil: 1700 kg/m^3

Deposition from the atmosphere per kg of soil

	$\text{DEPtotal}_{\text{ann}}$ ($\text{mg/m}^2/\text{d}$)	D_{air} 0.2 m soil (mg/kg/d)	D_{air} 0.1 m soil (mg/kg/d)	D_{air} 0.05 m soil (mg/kg/d)	$\text{Cdep}_{\text{soil } 10(0)}$ 0.2 m soil (mg/kg)	$\text{Cdep}_{\text{soil } 10(0)}$ 0.1 m soil (mg/kg)	$\text{Cdep}_{\text{soil } 10(0)}$ 0.05 m soil (mg/kg)
Production	0.00024	7.08×10^{-7}	1.42×10^{-6}	2.83×10^{-6}	2.12×10^{-5}	4.20×10^{-5}	8.23×10^{-5}
Processing	0.00011	3.19×10^{-7}	6.39×10^{-7}	1.28×10^{-6}	9.58×10^{-6}	1.90×10^{-5}	3.71×10^{-5}
Formulation	0.00503	1.48×10^{-5}	2.96×10^{-5}	5.91×10^{-5}	4.43×10^{-4}	8.77×10^{-4}	1.72×10^{-3}
Site specific	0.00020	5.88×10^{-7}	1.18×10^{-6}	2.35×10^{-6}	1.76×10^{-5}	3.49×10^{-5}	6.84×10^{-5}

The initial concentration after 10 years of continuous deposition was calculated as:

$$C_{dep_{soil\ 10}(0)} = (D_{air}/k) - (D_{air}/k) * e^{-365*10*k}$$

where k is the first order rate constant for removal from top soil (calculated below).

Sludge application

The concentration in soil will be high just after sludge application and reduced in time due to removal processes (degradation, volatilisation, leaching, etc.). Therefore, the concentration is averaged over a certain time period for different endpoints:

	Depth of soil (m)	Averaging time (days)	Sludge application (kg _{dw} /m ² /year)	Endpoint
PEC _{local} _{soil}	0.20	30	0.5	terrestrial ecosystem
PEC _{local} _{agr. soil}	0.20	180	0.5	crops
PEC _{local} _{grassland}	0.10	180	0.1	grass for cattle

The concentration in dry sewage sludge, C_{sludge}, is calculated from the emission rate to water, the fraction of emission sorbed to sludge and the rate of sewage sludge production:

$$C_{sludge} = (F_{stp_{sludge}} * E_{local_{water}} * 10^6) / SLUDGERATE$$

Where SLUDGERATE is the rate of sewage sludge production (default 710 kg/d, local STP). F_{stp_{sludge}} is 3.59%. The estimated values consider the site specific data known from the manufacturers in using STP flow of 130000 m³/d and 700000 personequivalents.

Predicted environmental local concentration in sludge (PEC_{local}_{sludge})

Life cycle stage	E _{local} _{water} (kg/d)	C _{sludge} (mg/kg dw)
Production	75.0	52.5
Processing	12.5	8.7
Formulation	45.0	31.5
Site specific**	7.8	0.002

*Estimated, using monitoring data

The concentration in soil just after the first year of sludge application is calculated by:

$$C_{sludge_{soil\ 1}(0)} = C_{sludge} * APPL_{sludge} / (DEPTH_{soil} * RHO_{soil})$$

where dry sludge application rate, APPL_{sludge}, the soil depth, DEPTH_{soil} and the bulk density of soil is presented in the table above.

Concentration in soil just after sludge application

	C _{sludge, local} _{agr. soil} (mg/kg)	C _{sludge, local} _{grassland} (mg/kg)
Production	0.077	0.031
Processing	0.013	0.005
Formulation	0.045	0.018
Site specific**	0.000003	0.000001

*Estimated, using monitoring data

The concentration in soil after sludge application for 10 consecutive years is assumed to be a realistic worst case. The initial concentration after 10 applications of sludge including the fraction that remains from previous year(s) is calculated by:

$$C_{\text{sludge}_{\text{soil } 10}(0)} = C_{\text{sludge}_{\text{soil } 1}(0)} * (1 + \sum \text{Facc}^n)$$

where the fraction accumulated in one year, $\text{Facc} = e^{-365*k} = 5.16 \times 10^{-6}$ for 0.2 m soil depth and 4.54×10^{-6} for 0.1 m soil depth.

The initial concentration in soil after 10 years of sludge application is estimated to be the same as after first year. There is no indication of accumulation in top soil.

Removal rates

The first order constant for removal from top soil, k , is derived by adding the biodegradation ($k_{\text{bio}_{\text{soil}}}$), volatilisation (k_{volat}) and leaching rate constant (k_{leach}) calculated for PCOC according to TGD.

Removal rate constants

Soil depth	$K_{\text{bio}_{\text{soil}}}$ (d ⁻¹)	k_{volat} (d ⁻¹)	k_{leach} (d ⁻¹)	k (d ⁻¹)
0.2 m	0.033007	0.000156	0.000197	0.033353
0.1 m	0.033007	0.000312	0.000393	0.033705
0.05 m	0.033007	0.000624	0.000785	0.034416

Local concentration in soil

The sum of both the concentration due to deposition and sludge application as the initial concentration in year 10 is calculated by the equation:

$$C_{\text{soil } 10}(0) = C_{\text{dep}_{\text{soil } 10}(0)} + C_{\text{sludge}_{\text{soil } 10}(0)}$$

Initial concentration in soil after 10 years of deposition and sludge application

	$C_{\text{local}_{\text{agr. soil } 10}(0)}$ (mg/kg)	$C_{\text{local}_{\text{grassland } 10}(0)}$ (mg/kg)
Production	0.077	0.031
Processing	0.013	0.005
Formulation	0.045	0.018
Site specific**	0.000003	0.000001

*Estimated, using monitoring data

The initial concentration is used to calculate the average concentration over a certain time period by:

$$C_{\text{local}_{\text{soil}}} = (D_{\text{air}}/k) + (1/(k*T)) [(C_{\text{soil}}(0)) - (D_{\text{air}}/k)] * 1 - e^{-k*T}$$

For natural soil is deposition from air included only as no sludge application is assumed.

$$PEC_{\text{local}_{\text{soil}}} = C_{\text{local}_{\text{soil}}} + PEC_{\text{regional}_{\text{natural soil}}}$$

$$PEC_{\text{regional}_{\text{natural soil}}}: 8.5 \times 10^{-7} \text{ mg/kg ww.}$$

$PEC_{\text{local}_{\text{soil}}}$ is set equal to $C_{\text{local}_{\text{soil}}}$ because the regional contribution is estimated to be very much lower than the estimated values except for the specific site estimated from C_{sludge} monitoring data (cf. the table below).

Estimated local concentration in soil

	$PEC_{\text{local}_{\text{soil}}}$ (mg/kg)	$PEC_{\text{local}_{\text{agr. soil}}}$ (mg/kg)	$PEC_{\text{local}_{\text{grassland}}}$ (mg/kg)	$PEC_{\text{local}_{\text{natural soil}}}$ (mg/kg)
Production	0.049	0.0128	0.0058	0.00003

Processing	0.008	0.0021	0.0009	0.00001
Formulation	0.030	0.0081	0.0039	0.00336
Specific site**	0.000002	0.0000014	0.0000011	0.00000088

*Estimated, using monitoring data

Concentration in pore water

The concentration in porewater is calculated by the equation

$$PEC_{local, soil, porew} = PEC_{local, soil} * RHO_{soil} / (K_{soil-water} * 1000)$$

where $K_{soil-water}$ is the soil-water partition coefficient calculated to be 12.2

Local concentration in soil porewater

	$C_{local, soil, porewater}$ (mg/l)	$C_{local, agr. soil, porewater}$ (mg/l)	$C_{local, grassland, porewater}$ (mg/l)	$C_{local, natural soil, porewater}$ (mg/l)
Production	0.0066	0.00178	0.00071	0.000004
Processing	0.0012	0.00030	0.00012	0.000002
Formulation	0.0036	0.00113	0.00054	0.000468
Site specific*	0.0000003	0.0000002	0.00000015	0.00000012

*: Estimated using monitoring data

Concentration in groundwater

The concentration in groundwater calculated for indirect exposure to humans through drinking water is initially assessed by the concentration in porewater in agricultural soil for a worst case estimation according to TGD.

$$PEC_{local, grw} = PEC_{local, agr. soil, porew}$$

Local concentration in groundwater

	$PEC_{local, grw}$ (mg/l)
Production	0.00178
Processing	0.00030
Formulation	0.00113
Site specific	0.0000002

Appendix 4

7.4 EUSES V. 1.0 ESTIMATIONS.

Two versions of EUSES estimations have been performed. One as in the risk assessment report assuming ready biodegradability and one assuming inherent biodegradability. The last is included for illustrative purposes.

When using EUSES, it should be noted that the regional and continental distribution models are nested, i.e. the continental production volume and tonnage are calculated as the total EU production minus regional production.

Appendix 4A

EUSES Full report	Single substance
Printed on	21-11-97 09.11.48
Study	new
Substance	4-chloro-2-methylphenol
Defaults	Standard
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	Yes

Name	Reference	Value	Units	Status
DEFAULTS				
DEFAULT IDENTIFICATION				
General name	Standard	Standard		D
Description	According to TGDS	According to TGDS		D
RELEASE ESTIMATION				
Fraction of EU production volume for region	0.5	0.5	[-]	S
Fraction connected to sewer systems	0.7	0.7	[-]	D
CHARACTERISTICS OF COMPARTMENTS				
GENERAL				
Density of solid phase	2.5	2.5	[kg.l-1]	D
Density of water phase	1	1	[kg.l-1]	D
Density of air phase	1.3E-03	1.3E-03	[kg.l-1]	D
Environmental temperature	12	12	[oC]	D
Constant of Junge equation	0.01	0.01	[Pa.m]	D
Surface area of aerosol particles	0.01	0.01	[m2.m-3]	D
Gas constant (8.314)	8.314	8.314	[Pa.m3.mol-1.K-1]	D
SUSPENDED MATTER				
Volume fraction solids in suspended matter	0.1	0.1	[m3.m-3]	D
Volume fraction water in suspended matter	0.9	0.9	[m3.m-3]	D
Weight fraction of organic carbon in suspended matter	0.1	0.1	[kg.kg-1]	D
Wet bulk density of suspended matter	1.15E+03	1.15E+03	[kg.m-3]	O
SEDIMENT				
Volume fraction solids in sediment	0.2	0.2	[m3.m-3]	D
Volume fraction water in sediment	0.8	0.8	[m3.m-3]	D
Weight fraction of organic carbon in sediment	0.05	0.05	[kg.kg-1]	D
Bulk density of sediment	1.3E+03	1.3E+03	[kgwwt.m-3]	O
Conversion factor wet-dry sediment	2.6	2.6	[kgwwt.kgdwt-1]	O
SOIL				
Volume fraction solids in soil	0.6	0.6	[m3.m-3]	D
Volume fraction water in soil	0.2	0.2	[m3.m-3]	D
Volume fraction air in soil	0.2	0.2	[m3.m-3]	D
Weight fraction of organic carbon in soil	0.02	0.02	[kg.kg-1]	D
Bulk density of soil	1.7E+03	1.7E+03	[kgwwt.m-3]	O
Conversion factor wet-dry soil	1.13	1.13	[kgwwt.kgdwt-1]	O
STP SLUDGE				
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D
DEGRADATION AND TRANSFORMATION RATES				
Concentration of OH-radicals in atmosphere	5E+05	5E+05	[molec.cm-3]	D
Rate constant for abiotic degradation in STP	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk soil	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk sediment	0	0	[d-1]	D
Rate constant for anaerobic biodegradation in sediment	0	0	[d-1]	D
Fraction of sediment compartment that is aerated	0.1	0.1	[m3.m-3]	D
SEWAGE TREATMENT				
GENERAL				
Number of inhabitants feeding one STP	1E+04	1E+04	[eq]	D
Sewage flow	200	200	[l.eq-1.d-1]	D

Effluent discharge rate of local STP	2E+06	2E+06	[l.d-1]	O
Temperature dependency correction	No	No		D
Temperature of air above aeration tank	15	15	[oC]	D
Temperature of water in aeration tank	15	15	[oC]	D
Height of air column above STP	10	10	[m]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Windspeed in the system	3	3	[m.s-1]	D
RAW SEWAGE				
Mass of O2 binding material per person per day	54	54	[g.eq-1.d-1]	D
Dry weight solids produced per person per day	0.09	0.09	[kg.eq-1.d-1]	D
Density solids in raw sewage	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
PRIMARILY SETTLER				
Depth of primarily settler	4	4	[m]	D
Hydraulic retention time of primarily settler	2	2	[hr]	D
Density suspended and settled solids in primarily settler	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
ACTIVATED SLUDGE TANK				
Depth of aeration tank	3	3	[m]	D
Density solids of activated sludge	1.3	1.3	[kg.l-1]	D
Concentration solids of activated sludge	4	4	[kg.m-3]	D
Steady state O2 concentration in activated sludge	2E-03	2E-03	[kg.m-3]	D
Mode of aeration	Surface	Surface		D
Aeration rate of bubble aeration	1.31E-05	1.31E-05	[m3.s-1.eq-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Sludge loading rate	0.15	0.15	[kg.kg-1.d-1]	D
Hydraulic retention time in aerator (9-box STP)	6.9	6.9	[hr]	O
Hydraulic retention time in aerator (6-box STP)	10.8	10.8	[hr]	O
Sludge retention time of aeration tank	9.2	9.2	[d]	O
SOLIDS-LIQUIDS SEPARATOR				
Depth of solids-liquid separator	3	3	[m]	D
Density suspended and settled solids in solids-liquid separator	1.3	1.3	[kg.l-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Hydraulic retention time of solids-liquid separator	6	6	[hr]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D
REGIONAL AND CONTINENTAL DISTRIBUTION				
CONTINENTAL				
Area of EU	3.56E+06	3.56E+06	[km2]	D
Area of continental system	3.52E+08	3.52E+08	[km2]	O
Number of inhabitants in the EU	3.7E+08	3.7E+08	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Area fraction of water of the continental system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from global scale to continent	0	0	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of continental system	25	25	[mg.l-1]	D
Residence time of water in system	166	166	[d]	O
Residence time of air in system	6.41	6.41	[d]	O
Net sedimentation rate	2.59	2.59	[mm.yr-1]	O
REGIONAL				
Area of regional system	4E+04	4E+04	[km2]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Area fraction of water of the regional system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from continental scale to region	0.034	0.034	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of regional	15	15	[mg.l-1]	D

system				
Residence time of water in system	40.1	40.1	[d]	O
Residence time of air in system	0.684	0.684	[d]	O
Net sedimentation rate	3.13	3.13	[mm.yr-1]	O
AIR				
Atmospheric mixing height	1000	1000	[m]	D
Windspeed in the system	3	3	[m.s-1]	D
Aerosol deposition velocity	1E-03	1E-03	[m.s-1]	D
Aerosol collection efficiency	2E+05	2E+05	[-]	D
Average annual precipitation	700	700	[mm.yr-1]	D
WATER AND SEDIMENT				
Concentration biota	1	1	[mg.l-1]	D
Sediment mixing depth	0.03	0.03	[m]	D
Settling velocity of suspended solids	2.5	2.5	[m.d-1]	D
(biogenic) production of suspended solids in water	0	0	[kg.d-1]	D
Sewage flow	200	200	[l.eq-1.d-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Fraction connected to sewer systems	0.7	0.7	[-]	D
SOIL				
Mixing depth natural soil	0.05	0.05	[m]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Mixing depth industrial/urban soil	0.05	0.05	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D
Fraction of rain water running off soil	0.25	0.25	[-]	D
Soil erosion rate of regional system	0.03	0.03	[mm.yr-1]	D
MASS TRANSFER				
Air-film PMTC (air-water interface)	1.39E-03	1.39E-03	[m.s-1]	D
Water-film PMTC (air-water interface)	1.39E-05	1.39E-05	[m.s-1]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Water-film PMTC (sediment-water interface)	2.78E-06	2.78E-06	[m.s-1]	D
Pore water PMTC (sediment-water interface)	2.78E-08	2.78E-08	[m.s-1]	D
LOCAL DISTRIBUTION				
AIR AND SURFACE WATER				
Concentration in air at source strength 1 [kg.d-1]	2.78E-04	2.78E-04	[mg.m-3]	D
Standard deposition flux of aerosol-bound compounds	0.01	0.01	[mg.m-2.d-1]	D
Standard deposition flux of gaseous compounds	4E-04	4E-04	[mg.m-2.d-1]	O
Suspended solids concentration of regional system	15	15	[mg.l-1]	D
Dilution factor	10	10	[-]	D
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	D
Calculate dilution from river flow rate	No	No		D
SOIL				
Mixing depth of grassland soil	0.1	0.1	[m]	D
Dry sludge application rate on agricultural soil	5E+03	5E+03	[kg.ha-1.yr-1]	D
Dry sludge application rate on grassland	1000	1000	[kg.ha-1.yr-1]	D
Averaging time soil (for terrestrial ecosystem)	30	30	[d]	D
Averaging time agricultural soil	180	180	[d]	D
Averaging time grassland	180	180	[d]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D
Average annual precipitation	700	700	[mm.yr-1]	D
CHARACTERISTICS OF PLANTS AND CATTLE				
PLANTS				
Volume fraction of water in plant tissue	0.65	0.65	[m3.m-3]	D
Volume fraction of lipids in plant tissue	0.01	0.01	[m3.m-3]	D
Volume fraction of air in plant tissue	0.3	0.3	[m3.m-3]	D
Correction for differences between plant lipids and octanol	0.95	0.95	[-]	D
Bulk density of plant tissue (wet weight)	0.7	0.7	[kg.l-1]	D
Rate constant for metabolism in plants	0	0	[d-1]	D
Rate constant for photolysis in plants	0	0	[d-1]	D
Leaf surface area	5	5	[m2]	D

Conductance	1E-03	1E-03	[m.s-1]	D
Shoot volume	2	2	[l]	D
Rate constant for dilution by growth	0.035	0.035	[d-1]	D
Transpiration stream	1	1	[l.d-1]	D
CATTLE				
Daily intake for cattle of grass (dryweight)	16.9	16.9	[kg.d-1]	D
Conversion factor grass from dryweight to wetweight	4	4	[kg.kg-1]	D
Daily intake of soil (dryweight)	0.41	0.41	[kg.d-1]	D
Daily inhalation rate for cattle	122	122	[m3.d-1]	D
Daily intake of drinking water for cattle	55	55	[l.d-1]	D
CHARACTERISTICS OF HUMANS				
Daily intake of drinking water	2	2	[l.d-1]	D
Daily intake of fish	0.115	0.115	[kg.d-1]	D
Daily intake of leaf crops (incl. fruit and cereals)	1.2	1.2	[kg.d-1]	D
Daily intake of root crops	0.384	0.384	[kg.d-1]	D
Daily intake of meat	0.301	0.301	[kg.d-1]	D
Daily intake of dairy products	0.561	0.561	[kg.d-1]	D
Inhalation rate for humans	20	20	[m3.d-1]	D
Bioavailability for oral uptake	1	1	[-]	D
Bioavailability for inhalation	0.75	0.75	[-]	D
Bioavailability for dermal uptake	1	1	[-]	D
Bodyweight of the human considered	70	70	[kg]	D
Oral to inhalatory extrapolation	Using adsorption rates	Using adsorption rates		D
SUBSTANCE IDENTIFICATION				
General name	4-chloro-2-methyl-phenol	4-chloro-2-methyl-phenol		S
Description	cresol	cresol		S
CAS-No	1570-64-5	1570-64-5		S
EC-notification no.				D
EINECS no.	216-381-3	216-381-3		S
PHYSICO-CHEMICAL PROPERTIES				
Molecular weight	142.59	142.59	[g.mol-1]	S
Melting point	50	50	[oC]	S
Boiling point	231	231	[oC]	S
Vapour pressure at 25 [oC]	26.66	26.66	[Pa]	S
Octanol-water partition coefficient.	3.09	3.09	[log10]	S
Water solubility	2.3E+03	2.3E+03	[mg.l-1]	S
RELEASE ESTIMATION CHARACTERIZATION AND TONNAGE				
High Production Volume Chemical	Yes	Yes		S
Production volume of chemical in EU	1.5E+04	1.5E+04	[tonnes.yr-1]	S
Volume of chemical imported to EU	0	0	[tonnes.yr-1]	D
Volume of chemical exported from EU	0	0	[tonnes.yr-1]	S
Intermittent release	No	No		D
INTERMEDIATE RESULTS PRODUCTION VOLUMES				
Tonnage of substance in Europe	1.5E+04	1.5E+04	[tonnes.yr-1]	O
Regional production volume of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	S
Continental production volume of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	O
USE PATTERNS EMISSION INPUT DATA				
Industry category	3 Chemical industry: chemicals used in synthesis	3 Chemical industry: chemicals used in synthesis		S
Use category	33 Intermediates	33 Intermediates		S
Emission scenario document available	Yes	Yes		O
Extra details on use category	Substance processed elsewhere	Substance processed elsewhere		S
Extra details on use category	No extra details necessary	No extra details necessary		D
Fraction of tonnage for application	1	1	[-]	O
Fraction of chemical in formulation	1	0.01	[-]	S
Production	Yes	Yes		S
Formulation	Yes	Yes		D
Processing	Yes	Yes		D

Private use	No	No		S
Recovery	No	No		S
Main category production	Ib Intermed. stored on-site/continuous prod.	Ib Intermed. stored on-site/continuous prod.		S
Main category formulation	Ib Dedicated equipment, (very) little cleaning	Ib Dedicated equipment, (very) little cleaning		S
Main category processing	Ic Dedicated equipment	Ic Dedicated equipment		S
INTERMEDIATE RESULTS				
USE PATTERN 1				
INTERMEDIATE RESULTS TONNAGES PER USE PATTERN				
Relevant tonnage for application	1.5E+04	1.5E+04	[tonnes.yr-1]	O
Regional tonnage of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	S
Continental tonnage of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	O
RELEASE FRACTIONS AND EMISSION DAYS				
[PRODUCTION]				
Fraction of tonnage released to air	1E-05	1E-05	[-]	O
Fraction of tonnage released to waste water	3E-03	3E-03	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-05	1E-05	[-]	O
Source of A-table data	Specific IC/UC combination	Specific IC/UC combination		O
Fraction of the main local source	1	1	[-]	O
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O
[FORMULATION]				
Fraction of tonnage released to air	1E-03	1E-03	[-]	O
Fraction of tonnage released to waste water	3E-03	3E-03	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-04	1E-04	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0.8	0.6	[-]	S
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O
[PROCESSING]				
Fraction of tonnage released to air	1E-05	1E-05	[-]	O
Fraction of tonnage released to waste water	7E-03	5E-04	[-]	S
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-04	1E-04	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0.25	1	[-]	S
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O
[PRIVATE USE]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	1	1	[-]	O
Source of B-table data	No applicable data found	No applicable data found		O
[RECOVERY]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
[RECOVERY] (Continued)				
Number of emission days per year	1	1	[-]	O
Source of B-table data	No applicable data found	No applicable data found		O

CONTINENTAL				
[PRODUCTION]				
Continental release to air	0.205	0.205	[kg.d-1]	0
Continental release to waste water	61.6	61.6	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	0.205	0.205	[kg.d-1]	0
[FORMULATION]				
Continental release to air	20.5	20.5	[kg.d-1]	0
Continental release to waste water	61.6	61.6	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	2.05	2.05	[kg.d-1]	0
[PROCESSING]				
Continental release to air	0.205	0.205	[kg.d-1]	0
Continental release to waste water	143	10.2	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	2.05	2.05	[kg.d-1]	0
[PRIVATE USE]				
Continental release to air	0	0	[kg.d-1]	0
Continental release to waste water	0	0	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	0	0	[kg.d-1]	0
[RECOVERY]				
Continental release to air	0	0	[kg.d-1]	0
Continental release to waste water	0	0	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	0	0	[kg.d-1]	0
REGIONAL				
[PRODUCTION]				
Regional release to air	0.205	0.205	[kg.d-1]	0
Regional release to waste water	61.6	61.6	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	0.205	0.205	[kg.d-1]	0
[FORMULATION]				
Regional release to air	20.5	20.5	[kg.d-1]	0
Regional release to waste water	61.6	61.6	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	2.05	2.05	[kg.d-1]	0
[PROCESSING]				
Regional release to air	0.205	0.205	[kg.d-1]	0
Regional release to waste water	143	10.2	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	2.05	2.05	[kg.d-1]	0
[PRIVATE USE]				
Regional release to air	0	0	[kg.d-1]	0
Regional release to waste water	0	0	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	0	0	[kg.d-1]	0
[RECOVERY]				
Regional release to air	0	0	[kg.d-1]	0
Regional release to waste water	0	0	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	0	0	[kg.d-1]	0
CONTINENTAL				
Total continental emission to air	21	21	[kg.d-1]	0
Total continental emission to wastewater	187	93.5	[kg.d-1]	0
Total continental emission to surface water	80	40.1	[kg.d-1]	0
Total continental emission to industrial soil	4.31	4.31	[kg.d-1]	0
Total continental emission to agricultural soil	0	0	[kg.d-1]	0
REGIONAL				
Total regional emission to air	21	21	[kg.d-1]	0
Total regional emission to wastewater	187	93.5	[kg.d-1]	0
Total regional emission to surface water	80	40.1	[kg.d-1]	0
Total regional emission to industrial soil	4.31	4.31	[kg.d-1]	0
Total regional emission to agricultural soil	0	0	[kg.d-1]	0

LOCAL				
[PRODUCTION]				
Local emission to air during episode	0.25	0.25	[kg.d-1]	O
Local emission to wastewater during episode	75	75	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[FORMULATION]				
Local emission to air during episode	20	15	[kg.d-1]	O
Local emission to wastewater during episode	60	45	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[PROCESSING]				
Local emission to air during episode	0.0622	0.249	[kg.d-1]	O
Local emission to wastewater during episode	43.6	12.4	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[PRIVATE USE]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[RECOVERY]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
DISTRIBUTION				
PARTITION COEFFICIENTS				
SOLIDS WATER PARTITIONING				
Organic carbon-water partition coefficient	401	401	[l.kg-1]	O
Solids-water partition coefficient in soil	8.02	8.02	[l.kg-1]	O
Solids-water partition coefficient in sediment	20.1	20.1	[l.kg-1]	O
Solids-water partition coefficient suspended matter	40.1	40.1	[l.kg-1]	O
Solids-water partition coefficient in raw sewage sludge	120	120	[l.kg-1]	O
Solids-water partition coefficient in settled sewage sludge	120	120	[l.kg-1]	O
Solids-water partition coefficient in activated sewage sludge	148	148	[l.kg-1]	O
Solids-water partition coefficient in effluent sewage sludge	148	148	[l.kg-1]	O
Suspended matter-water partition coefficient	10.9	10.9	[m3.m-3]	O
Soil-water partition coefficient	12.2	12.2	[m3.m-3]	O
Sediment-water partition coefficient	10.8	10.8	[m3.m-3]	O
AIR-WATER PARTITIONING AND ADSORPTION TO AEROSOL PARTICLES				
Sub-cooled liquid vapour pressure	65.9	65.9	[Pa]	O
Fraction of chemical associated with aerosol particles	1.52E-06	1.52E-06	[-]	O
Henry's law constant	1.65	1.65	[Pa.m3.mol-1]	O
Air-water partitioning coefficient	6.98E-04	6.98E-04	[m3.m-3]	O
BIOTA-WATER				
Bioconcentration factor for aquatic biota	84.4	84.4	[l.kg-1]	O
DEGRADATION AND TRANSFORMATION RATES				
CHARACTERIZATION AND STP				
Characterization of biodegradability	Readily biodegradable	Readily biodegradable		S
Degradation calculation method in STP	First order, standard OECD/EU tests	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	24	24	[d-1]	O
Total rate constant for degradation in STP	24	24	[d-1]	O
Maximum growth rate of specific microorganisms	2	2	[d-1]	D
Half saturation concentration	0.5	0.5	[g.m-3]	D
ENVIRONMENTAL				
Specific degradation rate constant with OH-radicals	0	0	[cm3.molec-1.s-1]	D

Rate constant for degradation in air	0	0	[d-1]	O
Rate constant for hydrolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for photolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for biodegradation in surface water	15	21	[d] (Dt50)	S
Total rate constant for degradation in bulk surface water	0.0462	0.033	[d-1]	O
Rate constant for biodegradation in bulk soil	30	21	[d] (Dt50)	S
Total rate constant for degradation in bulk soil	0.0231	0.033	[d-1]	O
Rate constant for biodegradation in aerated sediment	0.0231	0.0231	[d-1]	O
Total rate constant for degradation in bulk sediment	2.31E-03	2.31E-03	[d-1]	O
SEWAGE TREATMENT				
CONTINENTAL				
Fraction of emission directed to air	5.1E-03	5.1E-03	[-]	O
Fraction of emission directed to water	0.121	0.121	[-]	O
Fraction of emission directed to sludge	0.0359	0.0359	[-]	O
Fraction of the emission degraded	0.838	0.838	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	0.952	0.477	[kg.d-1]	O
Indirect emission to surface water	22.6	11.3	[kg.d-1]	O
Indirect emission to agricultural soil	6.7	3.36	[kg.d-1]	O
REGIONAL				
Fraction of emission directed to air	6.11E-03	6.11E-03	[-]	O
Fraction of emission directed to water	0.121	0.121	[-]	O
Fraction of emission directed to sludge	0.0359	0.0359	[-]	O
Fraction of the emission degraded	0.837	0.837	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	1.14	0.571	[kg.d-1]	O
Indirect emission to surface water	22.5	11.3	[kg.d-1]	O
Indirect emission to agricultural soil	6.7	3.36	[kg.d-1]	O
LOCAL				
[PRODUCTION]				
INPUT AND CONFIGURATION [PRODUCTION]				
Use or bypass STP	Use STP	Use STP		D
Local emission to wastewater during episode	75	75	[kg.d-1]	O
Concentration in untreated wastewater	37.5	0.577	[mg.l-1]	O
Local emission entering the STP	75	75	[kg.d-1]	O
Type of local STP	With primarily settler (9-box)	With primarily settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	6.5E+05	[eq]	S
Effluent discharge rate of this STP	2E+06	1.3E+08	[l.d-1]	O
Calculate dilution from river flow rate	No	No		S
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O
Dilution factor	10	10	[-]	D
OUTPUT [PRODUCTION]				
Fraction of emission directed to air by STP	6.51E-03	6.43E-03	[-]	O
Fraction of emission directed to water by STP	0.12	0.12	[-]	O
Fraction of emission directed to sludge by STP	0.0359	0.0359	[-]	O
Fraction of the emission degraded in STP	0.837	0.837	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	0.488	0.482	[kg.d-1]	O
Concentration in untreated wastewater	37.5	0.577	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	4.51	0.0695	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	3.41E+03	52.5	[mg.kg-1]	O
PEC for micro-organisms in the STP	4.51	0.0695	[mg.l-1]	O
[FORMULATION]				
INPUT AND CONFIGURATION [FORMULATION]				
Use or bypass STP	Use STP			D
Local emission to wastewater during episode	60	45	[kg.d-1]	O
Concentration in untreated wastewater	30	0.346	[mg.l-1]	O
Local emission entering the STP	60	45	[kg.d-1]	O
Type of local STP	With primarily settler (9-box)	With primarily settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	6.5E+05	[eq]	S
Effluent discharge rate of this STP	2E+06	1.3E+08	[l.d-1]	O
Calculate dilution from river flow rate	No	No		O
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O

Dilution factor	10	10	[-]	D
OUTPUT [FORMULATION]				
Fraction of emission directed to air by STP	6.51E-03	6.43E-03	[-]	O
Fraction of emission directed to water by STP	0.12	0.12	[-]	O
Fraction of emission directed to sludge by STP	0.0359	0.0359	[-]	O
Fraction of the emission degraded in STP	0.837	0.837	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	0.39	0.289	[kg.d-1]	O
Concentration in untreated wastewater	30	0.346	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	3.61	0.0417	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	2.73E+03	31.5	[mg.kg-1]	O
PEC for micro-organisms in the STP	3.61	0.0417	[mg.l-1]	O
[PROCESSING]				
INPUT AND CONFIGURATION [PROCESSING]				
Use or bypass STP	Use STP	Use STP		D
Local emission to wastewater during episode	43.6	12.4	[kg.d-1]	O
Concentration in untreated wastewater	21.8	0.0958	[mg.l-1]	O
Local emission entering the STP	43.6	12.4	[kg.d-1]	O
Type of local STP	With primarily settler (9-box)	With primarily settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	6.5E+05	[eq]	S
Effluent discharge rate of this STP	2E+06	1.3E+08	[l.d-1]	O
Calculate dilution from river flow rate	No	No		O
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O
Dilution factor	10	10	[-]	D
OUTPUT [PROCESSING]				
Fraction of emission directed to air by STP	6.51E-03	6.43E-03	[-]	O
Fraction of emission directed to water by STP	0.12	0.12	[-]	O
Fraction of emission directed to sludge by STP	0.0359	0.0359	[-]	O
Fraction of the emission degraded in STP	0.837	0.837	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	0.284	0.08	[kg.d-1]	O
Concentration in untreated wastewater	21.8	0.0958	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	2.62	0.0115	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	1.98E+03	8.71	[mg.kg-1]	O
PEC for micro-organisms in the STP	2.62	0.0115	[mg.l-1]	O
CONTINENTAL AND REGIONAL				
CONTINENTAL				
Continental PEC in surface water (total)	4.22E-06	2.57E-06	[mg.l-1]	O
Continental PEC in surface water (dissolved)	4.21E-06	2.57E-06	[mg.l-1]	O
Continental PEC in air (total)	1.86E-07	1.4E-07	[mg.m-3]	O
Continental PEC in agricultural soil (total)	9.53E-07	3.5E-07	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.33E-07	4.87E-08	[mg.l-1]	O
Continental PEC in natural soil (total)	2.85E-07	1.54E-07	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	5.97E-06	4.24E-06	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	3.82E-05	2.33E-05	[mg.kgwwt-1]	O
REGIONAL				
Regional PEC in surface water (total)	2.94E-04	1.7E-04	[mg.l-1]	O
Regional PEC in surface water (dissolved)	2.93E-04	1.7E-04	[mg.l-1]	O
Regional PEC in air (total)	1.03E-06	7.8E-07	[mg.m-3]	O
Regional PEC in agricultural soil (total)	7.76E-05	2.75E-05	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	1.08E-05	3.82E-06	[mg.l-1]	O
Regional PEC in natural soil (total)	1.58E-06	8.59E-07	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	5.02E-04	3.61E-04	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	2.41E-03	1.4E-03	[mg.kgwwt-1]	O
LOCAL				
REMOVAL RATE CONSTANTS SOIL				
Total rate constant for degradation in bulk soil	0.0231	0.033	[d-1]	O
Rate constant for volatilisation from agricultural soil	1.56E-04	1.56E-04	[d-1]	O
Rate constant for volatilisation from grassland soil	3.12E-04	3.12E-04	[d-1]	O
Rate constant for leaching from agricultural soil	1.96E-04	1.96E-04	[d-1]	O

Rate constant for leaching from grassland soil	3.92E-04	3.92E-04	[d-1]	0
Total rate constant for removal from agricultural top soil	0.0235	0.0334	[d-1]	0
Total rate constant for removal from grassland top soil	0.0238	0.0337	[d-1]	0
[PRODUCTION]				
LOCAL CONCENTRATIONS AND DEPOSITIONS [PRODUCTION]				
Concentration in air during emission episode	1.36E-04	1.34E-04	[mg.m-3]	0
Annual average concentration in air, 100 m from point source	1.12E-04	1.1E-04	[mg.m-3]	0
Total deposition flux during emission episode	2.95E-04	2.93E-04	[mg.m-2.d-1]	0
Annual average total deposition flux	2.43E-04	2.41E-04	[mg.m-2.d-1]	0
Concentration in surface water during emission episode	0.451	6.94E-03	[mg.l-1]	0
Annual average concentration in surface water	0.371	5.71E-03	[mg.l-1]	0
Concentration in agric. soil averaged over 30 days	3.6	0.0488	[mg.kgwwt-1]	0
Concentration in agric. soil averaged over 180 days	1.17	0.0128	[mg.kgwwt-1]	0
Concentration in grassland averaged over 180 days	0.462	5.12E-03	[mg.kgwwt-1]	0
Fraction of steady-state (agricultural soil)	1	1	[-]	0
Fraction of steady-state (grassland soil)	1	1	[-]	0
LOCAL PECS [PRODUCTION]				
Annual average local PEC in air (total)	1.13E-04	1.11E-04	[mg.m-3]	0
Local PEC in surface water during emission episode	0.451	7.11E-03	[mg.l-1]	0
Annual average local PEC in surface water (dissolved)	0.371	5.88E-03	[mg.l-1]	0
Local PEC in sediment during emission episode	4.29	0.0676	[mg.kgwwt-1]	0
Local PEC in agric. soil (total) averaged over 30 days	3.6	0.0488	[mg.kgwwt-1]	0
Local PEC in agric. soil (total) averaged over 180 days	1.17	0.0128	[mg.kgwwt-1]	0
Local PEC in grassland (total) averaged over 180 days	0.462	5.12E-03	[mg.kgwwt-1]	0
Local PEC in pore water of agricultural soil	0.163	1.78E-03	[mg.l-1]	0
Local PEC in pore water of grassland	0.0642	7.11E-04	[mg.l-1]	0
Local PEC in groundwater under agricultural soil	0.163	1.78E-03	[mg.l-1]	0
[FORMULATION]				
LOCAL CONCENTRATIONS AND DEPOSITIONS [FORMULATION]				
Concentration in air during emission episode	5.56E-03	4.17E-03	[mg.m-3]	0
Annual average concentration in air, 100 m from point source	4.57E-03	3.43E-03	[mg.m-3]	0
Total deposition flux during emission episode	8.16E-03	6.12E-03	[mg.m-2.d-1]	0
Annual average total deposition flux	6.7E-03	5.03E-03	[mg.m-2.d-1]	0
Concentration in surface water during emission episode	0.361	4.17E-03	[mg.l-1]	0
Annual average concentration in surface water	0.297	3.42E-03	[mg.l-1]	0
Concentration in agric. soil averaged over 30 days	2.88	0.0297	[mg.kgwwt-1]	0
Concentration in agric. soil averaged over 180 days	0.938	8.14E-03	[mg.kgwwt-1]	0
Concentration in grassland averaged over 180 days	0.371	3.92E-03	[mg.kgwwt-1]	0
Fraction of steady-state (agricultural soil)	1	1	[-]	0
Fraction of steady-state (grassland soil)	1	1	[-]	0
LOCAL PECS [FORMULATION]				
Annual average local PEC in air (total)	4.57E-03	3.43E-03	[mg.m-3]	0
Local PEC in surface water during emission episode	0.361	4.34E-03	[mg.l-1]	0
Annual average local PEC in surface water (dissolved)	0.297	3.59E-03	[mg.l-1]	0
Local PEC in sediment during emission episode	3.43	0.0412	[mg.kgwwt-1]	0
Local PEC in agric. soil (total) averaged over 30 days	2.88	0.0297	[mg.kgwwt-1]	0
Local PEC in agric. soil (total) averaged over 180 days	0.938	8.14E-03	[mg.kgwwt-1]	0
Local PEC in grassland (total) averaged over 180 days	0.371	3.92E-03	[mg.kgwwt-1]	0
Local PEC in pore water of agricultural soil	0.13	1.13E-03	[mg.l-1]	0
Local PEC in pore water of grassland	0.0516	5.45E-04	[mg.l-1]	0

Local PEC in groundwater under agricultural soil	0.13	1.13E-03	[mg.l-1]	O
[PROCESSING]				
LOCAL CONCENTRATIONS AND DEPOSITIONS [PROCESSING]				
Concentration in air during emission episode	7.88E-05	6.92E-05	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	6.48E-05	5.69E-05	[mg.m-3]	O
Total deposition flux during emission episode	1.38E-04	1.32E-04	[mg.m-2.d-1]	O
Annual average total deposition flux	1.14E-04	1.08E-04	[mg.m-2.d-1]	O
Concentration in surface water during emission episode	0.262	1.15E-03	[mg.l-1]	O
Annual average concentration in surface water	0.215	9.47E-04	[mg.l-1]	O
Concentration in agric. soil averaged over 30 days	2.09	8.1E-03	[mg.kgwwt-1]	O
Concentration in agric. soil averaged over 180 days	0.68	2.14E-03	[mg.kgwwt-1]	O
Concentration in grassland averaged over 180 days	0.268	8.61E-04	[mg.kgwwt-1]	O
Fraction of steady-state (agricultural soil)	1	1	[-]	O
Fraction of steady-state (grassland soil)	1	1	[-]	O
LOCAL PECS [PROCESSING]				
Annual average local PEC in air (total)	6.58E-05	5.77E-05	[mg.m-3]	O
Local PEC in surface water during emission episode	0.262	1.32E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	0.216	1.12E-03	[mg.l-1]	O
Local PEC in sediment during emission episode	2.49	0.0126	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	2.09	8.1E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.68	2.14E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	0.268	8.62E-04	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	0.0945	2.97E-04	[mg.l-1]	O
Local PEC in pore water of grassland	0.0373	1.2E-04	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	0.0945	2.97E-04	[mg.l-1]	O
EXPOSURE				
BIOCONCENTRATION FACTORS				
Partition coefficient worm-porewater	49.2	49.2	[l.kg-1]	O
Bioconcentration factor for earthworms	6.84	6.84	[kg.kg-1]	O
Bioconcentration factor for fish	84.4306	30	[l.kg-1]	S
Partition coefficient between plant tissue and water	9.27	9.27	[m3.m-3]	O
Partition coefficient between leaves and air	1.33E+04	1.33E+04	[m3.m-3]	O
Transpiration-stream concentration factor	0.388	0.388	[-]	O
Bioaccumulation factor for meat	3.09E-05	3.09E-05	[d.kg-1]	O
Bioaccumulation factor for milk	9.77E-06	9.77E-06	[d.kg-1]	O
Purification factor for surface water	1	1	[-]	O
SECONDARY POISONING				
SECONDARY POISONING [PRODUCTION]				
Concentration in fish from surface water for predators	15.7	0.0907	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	4	0.044	[mg.kg-1]	O
SECONDARY POISONING [FORMULATION]				
Concentration in fish from surface water for predators	12.5	0.0565	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	3.21	0.0279	[mg.kg-1]	O
SECONDARY POISONING [PROCESSING]				
Concentration in fish from surface water for predators	9.12	0.0193	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	2.33	7.41E-03	[mg.kg-1]	O
HUMANS EXPOSED TO OR VIA THE ENVIRONMENT				
REGIONAL				
CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER				
Regional concentration in wet fish	0.0248	5.11E-03	[mg.kg-1]	O
Regional concentration in root tissue of plant	1.43E-04	5.06E-05	[mg.kg-1]	O
Regional concentration in leaves of plant	1.98E-05	1.48E-05	[mg.kg-1]	O

Regional concentration in grass (wet weight)	1.98E-05	1.48E-05	[mg.kg-1]	0
Fraction of total uptake by crops from pore water	9.29E-03	4.38E-03	[-]	0
Fraction of total uptake by crops from air	0.991	0.996	[-]	0
Fraction of total uptake by grass from pore water	9.29E-03	4.38E-03	[-]	0
Fraction of total uptake by grass from air	0.991	0.996	[-]	0
Regional concentration in drinking water	2.93E-04	1.7E-04	[mg.l-1]	0
CONCENTRATIONS IN MEAT AND MILK				
Regional concentration in meat (wet weight)	5.45E-07	3.24E-07	[mg.kg-1]	0
Regional concentration in milk (wet weight)	1.72E-07	1.02E-07	[mg.kg-1]	0
Fraction of total intake by cattle through grass	0.0757	0.0958	[-]	0
Fraction of total intake by cattle through drinking water	0.915	0.894	[-]	0
Fraction of total intake by cattle through air	7.15E-03	9.08E-03	[-]	0
Fraction of total intake by cattle through soil	2.05E-03	1.22E-03	[-]	0
DAILY HUMAN DOSES				
Daily dose through intake of drinking water	8.38E-06	4.86E-06	[mg.kg-1.d-1]	0
Fraction of total dose through intake of drinking water	0.166	0.349	[-]	0
Daily dose through intake of fish	4.07E-05	8.39E-06	[mg.kg-1.d-1]	0
Fraction of total dose through intake of fish	0.807	0.601	[-]	0
Daily dose through intake of leaf crops	3.39E-07	2.54E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of leaf crops	6.72E-03	0.0182	[-]	0
Daily dose through intake of root crops	7.84E-07	2.77E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of root crops	0.0155	0.0199	[-]	0
Daily dose through intake of meat	2.34E-09	1.39E-09	[mg.kg-1.d-1]	0
Fraction of total dose through intake of meat	4.65E-05	9.97E-05	[-]	0
Daily dose through intake of milk	1.38E-09	8.2E-10	[mg.kg-1.d-1]	0
Fraction of total dose through intake of milk	2.74E-05	5.88E-05	[-]	0
Daily dose through intake of air	2.21E-07	1.67E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of air	4.39E-03	0.012	[-]	0
Regional total daily intake for humans	5.04E-05	1.4E-05	[mg.kg-1.d-1]	0
LOCAL [PRODUCTION]				
CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER, [PRODUCTION]				
Local concentration in wet fish	31.3	0.176	[mg.kg-1]	0
Local concentration in root tissue of plant	2.15	0.0236	[mg.kg-1]	0
Local concentration in leaves of plant	4.9E-03	2.13E-03	[mg.kg-1]	0
Local concentration in grass (wet weight)	3.22E-03	2.11E-03	[mg.kg-1]	0
Fraction of total uptake by crops from pore water	0.565	0.0142	[-]	0
Fraction of total uptake by crops from air	0.435	0.986	[-]	0
Fraction of total uptake by grass from pore water	0.339	5.73E-03	[-]	0
Fraction of total uptake by grass from air	0.661	0.994	[-]	0
Local concentration in drinking water	0.371	5.88E-03	[mg.l-1]	0
Annual average local PEC in air (total)	1.13E-04	1.11E-04	[mg.m-3]	0
CONCENTRATIONS IN MEAT AND MILK, [PRODUCTION]				
Local concentration in meat (wet weight)	6.45E-04	1.49E-05	[mg.kg-1]	0
Local concentration in milk (wet weight)	2.04E-04	4.71E-06	[mg.kg-1]	0
Fraction of total intake by cattle through grass	0.0105	0.296	[-]	0
Fraction of total intake by cattle through drinking water	0.979	0.671	[-]	0
Fraction of total intake by cattle through air	6.58E-04	0.0281	[-]	0
Fraction of total intake by cattle through soil	0.0103	4.94E-03	[-]	0
DAILY HUMAN DOSES, [PRODUCTION]				
Daily dose through intake of drinking water	0.0106	1.68E-04	[mg.kg-1.d-1]	0
Fraction of total dose through intake of drinking water	0.143	0.259	[-]	0
Daily dose through intake of fish	0.0515	2.9E-04	[mg.kg-1.d-1]	0
Fraction of total dose through intake of fish	0.695	0.447	[-]	0
Daily dose through intake of leaf crops	8.4E-05	3.65E-05	[mg.kg-1.d-1]	0
Fraction of total dose through intake of leaf crops	1.14E-03	0.0564	[-]	0
Daily dose through intake of root crops	0.0118	1.3E-04	[mg.kg-1.d-1]	0
Fraction of total dose through intake of root crops	0.16	0.2	[-]	0
Daily dose through intake of meat	2.77E-06	6.4E-08	[mg.kg-1.d-1]	0
Fraction of total dose through intake of meat	3.74E-05	9.89E-05	[-]	0
Daily dose through intake of milk	1.63E-06	3.77E-08	[mg.kg-1.d-1]	0
Fraction of total dose through intake of milk	2.21E-05	5.83E-05	[-]	0
Daily dose through intake of air	2.41E-05	2.38E-05	[mg.kg-1.d-1]	0
Fraction of total dose through intake of air	3.26E-04	0.0367	[-]	0
Local total daily intake for humans	0.074	6.48E-04	[mg.kg-1.d-1]	0

[FORMULATION]

CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER, [FORMULATION]

Local concentration in wet fish	25.1	0.108	[mg.kg-1]	O
Local concentration in root tissue of plant	1.73	0.015	[mg.kg-1]	O
Local concentration in leaves of plant	0.0888	0.065	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.0875	0.065	[mg.kg-1]	O
Fraction of total uptake by crops from pore water	0.025	2.96E-04	[-]	O
Fraction of total uptake by crops from air	0.975	1	[-]	O
Fraction of total uptake by grass from pore water	0.01	1.43E-04	[-]	O
Fraction of total uptake by grass from air	0.99	1	[-]	O
Local concentration in drinking water	0.297	3.59E-03	[mg.l-1]	O
Annual average local PEC in air (total)	4.57E-03	3.43E-03	[mg.m-3]	O

CONCENTRATIONS IN MEAT AND MILK, [FORMULATION]

Local concentration in meat (wet weight)	7.1E-04	1.55E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	2.25E-04	4.89E-05	[mg.kg-1]	O
Fraction of total intake by cattle through grass	0.257	0.877	[-]	O
Fraction of total intake by cattle through drinking water	0.711	0.0395	[-]	O
Fraction of total intake by cattle through air	0.0243	0.0835	[-]	O
Fraction of total intake by cattle through soil	7.51E-03	3.64E-04	[-]	O

DAILY HUMAN DOSES, [FORMULATION]

Daily dose through intake of drinking water	8.48E-03	1.03E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of drinking water	0.138	0.0464	[-]	O
Daily dose through intake of fish	0.0412	1.77E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of fish	0.668	0.0801	[-]	O
Daily dose through intake of leaf crops	1.52E-03	1.11E-03	[mg.kg-1.d-1]	O
Fraction of total dose through intake of leaf crops	0.0247	0.504	[-]	O
Daily dose through intake of root crops	9.47E-03	8.21E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of root crops	0.154	0.0371	[-]	O
Daily dose through intake of meat	3.05E-06	6.66E-07	[mg.kg-1.d-1]	O
Fraction of total dose through intake of meat	4.95E-05	3.01E-04	[-]	O
Daily dose through intake of milk	1.8E-06	3.92E-07	[mg.kg-1.d-1]	O
Fraction of total dose through intake of milk	2.92E-05	1.77E-04	[-]	O
Daily dose through intake of air	9.79E-04	7.35E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of air	0.0159	0.332	[-]	O
Local total daily intake for humans	0.0616	2.21E-03	[mg.kg-1.d-1]	O

[PROCESSING]

CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER, [PROCESSING]

Local concentration in wet fish	18.2	0.0335	[mg.kg-1]	O
Local concentration in root tissue of plant	1.25	3.94E-03	[mg.kg-1]	O
Local concentration in leaves of plant	2.86E-03	1.1E-03	[mg.kg-1]	O
Local concentration in grass (wet weight)	1.88E-03	1.09E-03	[mg.kg-1]	O
Fraction of total uptake by crops from pore water	0.563	4.61E-03	[-]	O
Fraction of total uptake by crops from air	0.437	0.995	[-]	O
Fraction of total uptake by grass from pore water	0.337	1.86E-03	[-]	O
Fraction of total uptake by grass from air	0.663	0.998	[-]	O
Local concentration in drinking water	0.216	1.12E-03	[mg.l-1]	O
Annual average local PEC in air (total)	6.58E-05	5.77E-05	[mg.m-3]	O

CONCENTRATIONS IN MEAT AND MILK, [PROCESSING]

Local concentration in meat (wet weight)	3.75E-04	4.42E-06	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.18E-04	1.4E-06	[mg.kg-1]	O
Fraction of total intake by cattle through grass	0.0105	0.518	[-]	O
Fraction of total intake by cattle through drinking water	0.979	0.43	[-]	O
Fraction of total intake by cattle through air	6.62E-04	0.0492	[-]	O
Fraction of total intake by cattle through soil	0.0103	2.8E-03	[-]	O

DAILY HUMAN DOSES, [PROCESSING]

Daily dose through intake of drinking water	6.16E-03	3.19E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of drinking water	0.143	0.228	[-]	O
Daily dose through intake of fish	0.0299	5.51E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of fish	0.696	0.394	[-]	O
Daily dose through intake of leaf crops	4.9E-05	1.88E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of leaf crops	1.14E-03	0.135	[-]	O
Daily dose through intake of root crops	6.87E-03	2.16E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of root crops	0.16	0.154	[-]	O
Daily dose through intake of meat	1.61E-06	1.9E-08	[mg.kg-1.d-1]	O

Fraction of total dose through intake of meat	3.75E-05	1.36E-04	[-]	O
Daily dose through intake of milk	9.49E-07	1.12E-08	[mg.kg-1.d-1]	O
Fraction of total dose through intake of milk	2.21E-05	8.01E-05	[-]	O
Daily dose through intake of air	1.41E-05	1.24E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of air	3.28E-04	0.0884	[-]	O
Local total daily intake for humans	0.043	1.4E-04	[mg.kg-1.d-1]	O
EFFECTS				
INPUT OF EFFECTS DATA				
MICRO-ORGANISMS				
EC50 for micro-organisms in a STP	55	55	[mg.l-1]	S
Specific bacterial population?	No	No		D
EC10 for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
NOEC for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
AQUATIC ORGANISMS				
LC50 for fish	2.3	2.3	[mg.l-1]	S
L(E)C50 for Daphnia	0.63	0.63	[mg.l-1]	S
EC50 for algae	8.2	8.2	[mg.l-1]	S
LC50 for other aquatic species	??	??	[mg.l-1]	D
Species	other	other		D
NOEC for fish	0.5	0.5	[mg.l-1]	S
NOEC for Daphnia	0.55	0.55	[mg.l-1]	S
NOEC for algae	0.89	0.89	[mg.l-1]	S
NOEC for other aquatic species	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
TERRESTRIAL ORGANISMS				
LC50 for plants	??	??	[mg.kgwwt-1]	D
LC50 for earthworms	??	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	??	[mg.kgwwt-1]	D
Species	other	other		D
NOEC for plants	??	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	??	[mg.kgwwt-1]	D
NOEC for other terrestrial species	??	??	[mg.kgwwt-1]	D
NOEC for other terrestrial species	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
BIRDS				
LC50 in avian dietary study (5 days)	??	??	[mg.kg-1]	D
NOAEL	??	??	[mg.kg-1.d-1]	D
NOEC via food	??	??	[mg.kg-1]	O
Duration of (sub-)chronic oral test	Chronic	Chronic		D
Conversion factor NOAEL to NOEC	8	8	[kg.d.kg-1]	D
MAMMALS				
ACUTE				
Oral LD50	2.65E+03	2.65E+03	[mg.kg-1]	S
Oral Discriminatory Dose	??	??	[mg.kg-1]	D
Dermal LD50	2.65E+03	2.65E+03	[mg.kg-1]	O
Inhalatory LC50	900	900	[mg.m-3]	S
(SUB)CHRONIC				
Oral NOAEL	200	200	[mg.kg-1.d-1]	S
Oral LOAEL	800	800	[mg.kg-1.d-1]	S
Inhalatory NOAEL	933	933	[mg.m-3]	O
Inhalatory LOAEL	3.73E+03	3.73E+03	[mg.m-3]	O
Dermal NOAEL	200	200	[mg.kg-1.d-1]	O
Dermal LOAEL	800	800	[mg.kg-1.d-1]	O
NOEC via food	2E+03	2E+03	[mg.kg-1]	O
LOEC via food	??	??	[mg.kg-1]	D
Duration of (sub-)chronic oral test	28 days	28 days		D

Species for conversion of NOAEL to NOEC	Rattus norvegicus (<6 weeks)	Rattus norvegicus (<6 weeks)		D
Conversion factor NOAEL to NOEC	10	10	[kg.d.kg-1]	O
HUMANS				
(SUB)CHRONIC				
Oral NOAEL	??	??	[mg.kg-1.d-1]	D
Oral LOAEL	??	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium	??	??	[mg.cm-3]	D
Dermal LOEC in a medium	??	??	[mg.cm-3]	D
Inhalatory (fibre) NOAEL	??	??	[fibres.m-3]	D
Inhalatory (fibre) LOAEL	??	??	[fibres.m-3]	D
Dermal LOAEL	??	??	[mg.kg-1.d-1]	O
Dermal NOAEL	??	??	[mg.kg-1.d-1]	O
Inhalatory LOAEL	??	??	[mg.m-3]	O
Inhalatory NOAEL	??	??	[mg.m-3]	O
CURRENT CLASSIFICATION				
Corrosive (C, R34 or R35)	No	No		D
Irritating to skin (Xi, R38)	No	No		D
Irritating to eyes (Xi, R36)	No	No		D
Risk of serious damage to eyes (Xi, R41)	No	No		D
Irritating to respiratory system (Xi, R37)	No	No		D
May cause sensitisation by inhalation (Xn, R42)	No	No		D
May cause sensitisation by skin contact (Xi, R43)	No	No		D
May cause cancer (T, R45)	No	No		D
May cause cancer by inhalation (T, R49)	No	No		D
Possible risk of irreversible effects (Xn, R40)	No	No		D
ENVIRONMENTAL EFFECTS ASSESSMENT				
INTERMEDIATE RESULTS AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
Toxicological data used for extrapolation to PNEC Aqua	0.5	0.5	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	10	10	[-]	O
Toxicological data used for extrapolation to PNEC Aqua	0.63	0.63	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	100	100	[-]	O
Toxicological data used for extrapolation to PNEC micro	55	55	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	100	100	[-]	O
Toxicological data used for extrapolation to PNEC oral	2E+03	2E+03	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	100	100	[-]	O
INTERMEDIATE RESULTS TERRESTRIAL AND SEDIMENT ORGANISMS				
Toxicological data used for extrapolation to PNEC Terr	0.36	0.36	[mg.kgwwt-1]	O
Assessment factor applied in extrapolation to PNEC Terr	1	1	[-]	O
Equilibrium partitioning used for PNEC in soil?	Yes	Yes		O
Equilibrium partitioning used for PNEC in sediment?	Yes	Yes		O
PNECS FOR AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
PNEC for aquatic organisms	0.05	0.05	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	6.3E-03	6.3E-03	[mg.l-1]	O
PNEC for micro-organisms in a STP	0.55	0.55	[mg.l-1]	O
PNEC for secondary poisoning of birds and mammals	20	20	[mg.kg-1]	O
PNEC for aquatic organisms with statistical method	??	??	[mg.l-1]	O
PNECS FOR TERRESTRIAL AND SEDIMENT ORGANISMS				
PNEC for terrestrial organisms	0.36	0.36	[mg.kgwwt-1]	O
PNEC for terrestrial organisms with statistical method	??	??	[mg.kgwwt-1]	O
PNEC for sediment-dwelling organisms	0.416	0.416	[mg.kgwwt-1]	O
RISK CHARACTERIZATION				
ENVIRONMENTAL EXPOSURE				
LOCAL				

RISK CHARACTERIZATION OF [PRODUCTION]

ENVIRONMENTAL

RCR for the local water compartment	9.03	0.142	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	10	0.136	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	10.3	0.162	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the sewage treatment plant	8.21	0.126	[-]	O

PREDATORS

RCR for fish-eating birds and mammals	0.784	4.54E-03	[-]	O
RCR for worm-eating birds and mammals	0.2	2.2E-03	[-]	O

HUMANS

MOS local, total exposure via all media	2.7E+03	3.09E+05	[-]	O
MOS local, exposure via air	8.29E+06	8.41E+06	[-]	O

RISK CHARACTERIZATION OF [FORMULATION]

ENVIRONMENTAL

RCR for the local water compartment	7.22	0.0867	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	8.01	0.0826	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	8.24	0.0989	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the sewage treatment plant	6.57	0.0758	[-]	O

PREDATORS

RCR for fish-eating birds and mammals	0.627	2.82E-03	[-]	O
RCR for worm-eating birds and mammals	0.16	1.4E-03	[-]	O

HUMANS

MOS local, total exposure via all media	3.24E+03	9.04E+04	[-]	O
MOS local, exposure via air	2.04E+05	2.72E+05	[-]	O

RISK CHARACTERIZATION OF [PROCESSING]

ENVIRONMENTAL

RCR for the local water compartment	5.25	0.0265	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	5.82	0.0225	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	5.99	0.0302	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the sewage treatment plant	4.77	0.021	[-]	O

PREDATORS

RCR for fish-eating birds and mammals	0.456	9.66E-04	[-]	O
RCR for worm-eating birds and mammals	0.116	3.7E-04	[-]	O

HUMANS

MOS local, total exposure via all media	4.65E+03	1.43E+06	[-]	O
MOS local, exposure via air	1.42E+07	1.62E+07	[-]	O

REGIONAL

ENVIRONMENT

RCR for the regional water compartment	5.87E-03	3.4E-03	[-]	O
RCR for the regional soil compartment	2.16E-04	7.64E-05	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the regional sediment compartment	5.78E-03	3.35E-03	[-]	O
Extra factor 10 applied to PEC	No	No		O

HUMANS

MOS regional, total exposure via all media	3.97E+06	1.43E+07	[-]	O
MOS regional, exposure via air	9.03E+08	1.2E+09	[-]	O

Appendix 4B

EUSES Full report	Single substance			
Printed on	21-11-97 09.16.14			
Substance	4-chloro-2-methylphenol			
Defaults	Standard			
Assessment types	1A, 1B, 2, 3A, 3B			
Base set complete	Yes			
Explanation status column	'O' = Output; 'D' = Default; 'S' = Set; 'I' = Imported			
Name	Reference	Value	Units	Status
DEFAULTS				
DEFAULT IDENTIFICATION				
General name	Standard	Standard		D
Description	According to TGDs	According to TGDs		D
RELEASE ESTIMATION				
Fraction of EU production volume for region	0.5	0.5	[-]	S
Fraction connected to sewer systems	0.7	0.7	[-]	D
CHARACTERISTICS OF COMPARTMENTS				
GENERAL				
Density of solid phase	2.5	2.5	[kg.l-1]	D
Density of water phase	1	1	[kg.l-1]	D
Density of air phase	1.3E-03	1.3E-03	[kg.l-1]	D
Environmental temperature	12	12	[oC]	D
Constant of Junge equation	0.01	0.01	[Pa.m]	D
Surface area of aerosol particles	0.01	0.01	[m2.m-3]	D
Gas constant (8.314)	8.314	8.314	[Pa.m3.mol-1.K-1]	D
SUSPENDED MATTER				
Volume fraction solids in suspended matter	0.1	0.1	[m3.m-3]	D
Volume fraction water in suspended matter	0.9	0.9	[m3.m-3]	D
Weight fraction of organic carbon in suspended matter	0.1	0.1	[kg.kg-1]	D
Wet bulk density of suspended matter	1.15E+03	1.15E+03	[kg.m-3]	O
SEDIMENT				
Volume fraction solids in sediment	0.2	0.2	[m3.m-3]	D
Volume fraction water in sediment	0.8	0.8	[m3.m-3]	D
Weight fraction of organic carbon in sediment	0.05	0.05	[kg.kg-1]	D
Bulk density of sediment	1.3E+03	1.3E+03	[kgwwt.m-3]	O
Conversion factor wet-dry sediment	2.6	2.6	[kgwwt.kgdwt-1]	O
SOIL				
Volume fraction solids in soil	0.6	0.6	[m3.m-3]	D
Volume fraction water in soil	0.2	0.2	[m3.m-3]	D
Volume fraction air in soil	0.2	0.2	[m3.m-3]	D
Weight fraction of organic carbon in soil	0.02	0.02	[kg.kg-1]	D
Bulk density of soil	1.7E+03	1.7E+03	[kgwwt.m-3]	O
Conversion factor wet-dry soil	1.13	1.13	[kgwwt.kgdwt-1]	O
STP SLUDGE				
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D
DEGRADATION AND TRANSFORMATION RATES				
Concentration of OH-radicals in atmosphere	5E+05	5E+05	[molec.cm-3]	D
Rate constant for abiotic degradation in STP	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk soil	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk sediment	0	0	[d-1]	D
Rate constant for anaerobic biodegradation in sediment	0	0	[d-1]	D
Fraction of sediment compartment that is aerated	0.1	0.1	[m3.m-3]	D
SEWAGE TREATMENT				
GENERAL				
Number of inhabitants feeding one STP	1E+04	1E+04	[eq]	D
Sewage flow	200	200	[l.eq-1.d-1]	D

Effluent discharge rate of local STP	2E+06	2E+06	[l.d-1]	O
Temperature dependency correction	No	No		D
Temperature of air above aeration tank	15	15	[oC]	D
Temperature of water in aeration tank	15	15	[oC]	D
Height of air column above STP	10	10	[m]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Windspeed in the system	3	3	[m.s-1]	D
RAW SEWAGE				
Mass of O2 binding material per person per day	54	54	[g.eq-1.d-1]	D
Dry weight solids produced per person per day	0.09	0.09	[kg.eq-1.d-1]	D
Density solids in raw sewage	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
PRIMARILY SETTLER				
Depth of primarily settler	4	4	[m]	D
Hydraulic retention time of primarily settler	2	2	[hr]	D
Density suspended and settled solids in primarily settler	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
ACTIVATED SLUDGE TANK				
Depth of aeration tank	3	3	[m]	D
Density solids of activated sludge	1.3	1.3	[kg.l-1]	D
Concentration solids of activated sludge	4	4	[kg.m-3]	D
Steady state O2 concentration in activated sludge	2E-03	2E-03	[kg.m-3]	D
Mode of aeration	Surface	Surface		D
Aeration rate of bubble aeration	1.31E-05	1.31E-05	[m3.s-1.eq-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Sludge loading rate	0.15	0.15	[kg.kg-1.d-1]	D
Hydraulic retention time in aerator (9-box STP)	6.9	6.9	[hr]	O
Hydraulic retention time in aerator (6-box STP)	10.8	10.8	[hr]	O
Sludge retention time of aeration tank	9.2	9.2	[d]	O
SOLIDS-LIQUIDS SEPARATOR				
Depth of solids-liquid separator	3	3	[m]	D
Density suspended and settled solids in solids-liquid separator	1.3	1.3	[kg.l-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Hydraulic retention time of solids-liquid separator	6	6	[hr]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D
REGIONAL AND CONTINENTAL DISTRIBUTION				
CONTINENTAL				
Area of EU	3.56E+06	3.56E+06	[km2]	D
Area of continental system	3.52E+08	3.52E+08	[km2]	O
Number of inhabitants in the EU	3.7E+08	3.7E+08	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Area fraction of water of the continental system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from global scale to continent	0	0	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of continental system	25	25	[mg.l-1]	D
Residence time of water in system	166	166	[d]	O
Residence time of air in system	6.41	6.41	[d]	O
Net sedimentation rate	2.59	2.59	[mm.yr-1]	O
REGIONAL				
Area of regional system	4E+04	4E+04	[km2]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Area fraction of water of the regional system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from continental scale to region	0.034	0.034	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of regional	15	15	[mg.l-1]	D

system				
Residence time of water in system	40.1	40.1	[d]	O
Residence time of air in system	0.684	0.684	[d]	O
Net sedimentation rate	3.13	3.13	[mm.yr-1]	O
AIR				
Atmospheric mixing height	1000	1000	[m]	D
Windspeed in the system	3	3	[m.s-1]	D
Aerosol deposition velocity	1E-03	1E-03	[m.s-1]	D
Aerosol collection efficiency	2E+05	2E+05	[-]	D
Average annual precipitation	700	700	[mm.yr-1]	D
WATER AND SEDIMENT				
Concentration biota	1	1	[mg.l-1]	D
Sediment mixing depth	0.03	0.03	[m]	D
Settling velocity of suspended solids	2.5	2.5	[m.d-1]	D
(biogenic) production of suspended solids in water	0	0	[kg.d-1]	D
Sewage flow	200	200	[l.eq-1.d-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Fraction connected to sewer systems	0.7	0.7	[-]	D
SOIL				
Mixing depth natural soil	0.05	0.05	[m]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Mixing depth industrial/urban soil	0.05	0.05	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D
Fraction of rain water running off soil	0.25	0.25	[-]	D
Soil erosion rate of regional system	0.03	0.03	[mm.yr-1]	D
MASS TRANSFER				
Air-film PMTC (air-water interface)	1.39E-03	1.39E-03	[m.s-1]	D
Water-film PMTC (air-water interface)	1.39E-05	1.39E-05	[m.s-1]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Water-film PMTC (sediment-water interface)	2.78E-06	2.78E-06	[m.s-1]	D
Pore water PMTC (sediment-water interface)	2.78E-08	2.78E-08	[m.s-1]	D
LOCAL DISTRIBUTION				
AIR AND SURFACE WATER				
Concentration in air at source strength 1 [kg.d-1]	2.78E-04	2.78E-04	[mg.m-3]	D
Standard deposition flux of aerosol-bound compounds	0.01	0.01	[mg.m-2.d-1]	D
Standard deposition flux of gaseous compounds	4E-04	4E-04	[mg.m-2.d-1]	O
Suspended solids concentration of regional system	15	15	[mg.l-1]	D
Dilution factor	10	10	[-]	D
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	D
Calculate dilution from river flow rate	No	No		D
SOIL				
Mixing depth of grassland soil	0.1	0.1	[m]	D
Dry sludge application rate on agricultural soil	5E+03	5E+03	[kg.ha-1.yr-1]	D
Dry sludge application rate on grassland	1000	1000	[kg.ha-1.yr-1]	D
Averaging time soil (for terrestrial ecosystem)	30	30	[d]	D
Averaging time agricultural soil	180	180	[d]	D
Averaging time grassland	180	180	[d]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D
Average annual precipitation	700	700	[mm.yr-1]	D
CHARACTERISTICS OF PLANTS AND CATTLE				
PLANTS				
Volume fraction of water in plant tissue	0.65	0.65	[m3.m-3]	D
Volume fraction of lipids in plant tissue	0.01	0.01	[m3.m-3]	D
Volume fraction of air in plant tissue	0.3	0.3	[m3.m-3]	D
Correction for differences between plant lipids and octanol	0.95	0.95	[-]	D
Bulk density of plant tissue (wet weight)	0.7	0.7	[kg.l-1]	D
Rate constant for metabolism in plants	0	0	[d-1]	D
Rate constant for photolysis in plants	0	0	[d-1]	D
Leaf surface area	5	5	[m2]	D

Conductance	1E-03	1E-03	[m.s-1]	D
Shoot volume	2	2	[l]	D
Rate constant for dilution by growth	0.035	0.035	[d-1]	D
Transpiration stream	1	1	[l.d-1]	D
CATTLE				
Daily intake for cattle of grass (dryweight)	16.9	16.9	[kg.d-1]	D
Conversion factor grass from dryweight to wetweight	4	4	[kg.kg-1]	D
Daily intake of soil (dryweight)	0.41	0.41	[kg.d-1]	D
Daily inhalation rate for cattle	122	122	[m3.d-1]	D
Daily intake of drinking water for cattle	55	55	[l.d-1]	D
CHARACTERISTICS OF HUMANS				
Daily intake of drinking water	2	2	[l.d-1]	D
Daily intake of fish	0.115	0.115	[kg.d-1]	D
Daily intake of leaf crops (incl. fruit and cereals)	1.2	1.2	[kg.d-1]	D
Daily intake of root crops	0.384	0.384	[kg.d-1]	D
Daily intake of meat	0.301	0.301	[kg.d-1]	D
Daily intake of dairy products	0.561	0.561	[kg.d-1]	D
Inhalation rate for humans	20	20	[m3.d-1]	D
Bioavailability for oral uptake	1	1	[-]	D
Bioavailability for inhalation	0.75	0.75	[-]	D
Bioavailability for dermal uptake	1	1	[-]	D
Bodyweight of the human considered	70	70	[kg]	D
Oral to inhalatory extrapolation	Using adsorption rates	Using adsorption rates		D
SUBSTANCE IDENTIFICATION				
General name	4-chloro-2-methyl-phenol	4-chloro-2-methyl-phenol		S
Description	cresol	cresol		S
CAS-No	1570-64-5	1570-64-5		S
EC-notification no.				D
EINECS no.	216-381-3	216-381-3		S
PHYSICO-CHEMICAL PROPERTIES				
Molecular weight	142.59	142.59	[g.mol-1]	S
Melting point	50	50	[oC]	S
Boiling point	231	231	[oC]	S
Vapour pressure at 25 [oC]	26.66	26.66	[Pa]	S
Octanol-water partition coefficient.	3.09	3.09	[log10]	S
Water solubility	2.3E+03	2.3E+03	[mg.l-1]	S
RELEASE ESTIMATION				
CHARACTERIZATION AND TONNAGE				
High Production Volume Chemical	Yes	Yes		S
Production volume of chemical in EU	1.5E+04	1.5E+04	[tonnes.yr-1]	S
Volume of chemical imported to EU	0	0	[tonnes.yr-1]	D
Volume of chemical exported from EU	0	0	[tonnes.yr-1]	S
Intermittent release	No	No		D
INTERMEDIATE RESULTS PRODUCTION VOLUMES				
Tonnage of substance in Europe	1.5E+04	1.5E+04	[tonnes.yr-1]	O
Regional production volume of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	S
Continental production volume of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	O
USE PATTERNS				
EMISSION INPUT DATA				
Industry category	3 Chemical industry: chemicals used in synthesis	3 Chemical industry: chemicals used in synthesis		S
Use category	33 Intermediates	33 Intermediates		S
Emission scenario document available	Yes	Yes		O
Extra details on use category	Substance processed elsewhere	Substance processed elsewhere		S
Extra details on use category	No extra details necessary	No extra details necessary		D
Fraction of tonnage for application	1	1	[-]	O
Fraction of chemical in formulation	1	0.01	[-]	S
Production	Yes	Yes		S
Formulation	Yes	Yes		D

Processing	Yes	Yes		D
Private use	No	No		S
Recovery	No		S	
Main category production	Ib Intermed. stored on-site/continuous prod.	Ib Intermed. stored on-site/continuous prod.		S
Main category formulation	Ib Dedicated equipment, (very) little cleaning	Ib Dedicated equipment, (very) little cleaning		S
Main category processing	Ic Dedicated equipment	Ic Dedicated equipment		S

INTERMEDIATE RESULTS

USE PATTERN 1

INTERMEDIATE RESULTS TONNAGES PER USE PATTERN

Relevant tonnage for application	1.5E+04	1.5E+04	[tonnes.yr-1]	O
Regional tonnage of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	S
Continental tonnage of substance	7.5E+03	7.5E+03	[tonnes.yr-1]	O

RELEASE FRACTIONS AND EMISSION DAYS

[PRODUCTION]

Fraction of tonnage released to air	1E-05	1E-05	[-]	O
Fraction of tonnage released to waste water	3E-03	3E-03	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-05	1E-05	[-]	O
Source of A-table data	Specific IC/UC combination	Specific IC/UC combination		O
Fraction of the main local source	1	1	[-]	O
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O

[FORMULATION]

Fraction of tonnage released to air	1E-03	1E-03	[-]	O
Fraction of tonnage released to waste water	3E-03	3E-03	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-04	1E-04	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0.8	0.6	[-]	S
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O

[PROCESSING]

Fraction of tonnage released to air	1E-05	1E-05	[-]	O
Fraction of tonnage released to waste water	7E-03	5E-04	[-]	S
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-04	1E-04	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0.25	1	[-]	S
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O

[PRIVATE USE]

Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	1	1	[-]	O
Source of B-table data	No applicable data found	No applicable data found		O

[RECOVERY]

Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	1	1	[-]	O
Source of B-table data	No applicable data found	No applicable data found		O

CONTINENTAL

[PRODUCTION]				
Continental release to air	0.205	0.205	[kg.d-1]	0
Continental release to waste water	61.6	61.6	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	0.205	0.205	[kg.d-1]	0
[FORMULATION]				
Continental release to air	20.5	20.5	[kg.d-1]	0
Continental release to waste water	61.6	61.6	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	2.05	2.05	[kg.d-1]	0
[PROCESSING]				
Continental release to air	0.205	0.205	[kg.d-1]	0
Continental release to waste water	143	10.2	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	2.05	2.05	[kg.d-1]	0
[PRIVATE USE]				
Continental release to air	0	0	[kg.d-1]	0
Continental release to waste water	0	0	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	0	0	[kg.d-1]	0
[RECOVERY]				
Continental release to air	0	0	[kg.d-1]	0
Continental release to waste water	0	0	[kg.d-1]	0
Continental release to surface water	0	0	[kg.d-1]	0
Continental release to industrial soil	0	0	[kg.d-1]	0
REGIONAL				
[PRODUCTION]				
Regional release to air	0.205	0.205	[kg.d-1]	0
Regional release to waste water	61.6	61.6	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	0.205	0.205	[kg.d-1]	0
[FORMULATION]				
Regional release to air	20.5	20.5	[kg.d-1]	0
Regional release to waste water	61.6	61.6	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	2.05	2.05	[kg.d-1]	0
[PROCESSING]				
Regional release to air	0.205	0.205	[kg.d-1]	0
Regional release to waste water	143	10.2	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	2.05	2.05	[kg.d-1]	0
[PRIVATE USE]				
Regional release to air	0	0	[kg.d-1]	0
Regional release to waste water	0	0	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	0	0	[kg.d-1]	0
[RECOVERY]				
Regional release to air	0	0	[kg.d-1]	0
Regional release to waste water	0	0	[kg.d-1]	0
Regional release to surface water	0	0	[kg.d-1]	0
Regional release to industrial soil	0	0	[kg.d-1]	0
CONTINENTAL				
Total continental emission to air	21	21	[kg.d-1]	0
Total continental emission to wastewater	187	93.5	[kg.d-1]	0
Total continental emission to surface water	80	40.1	[kg.d-1]	0
Total continental emission to industrial soil	4.31	4.31	[kg.d-1]	0
Total continental emission to agricultural soil	0	0	[kg.d-1]	0
REGIONAL				
Total regional emission to air	21	21	[kg.d-1]	0
Total regional emission to wastewater	187	93.5	[kg.d-1]	0
Total regional emission to surface water	80	40.1	[kg.d-1]	0
Total regional emission to industrial soil	4.31	4.31	[kg.d-1]	0
Total regional emission to agricultural soil	0	0	[kg.d-1]	0
LOCAL				

[PRODUCTION]				
Local emission to air during episode	0.25	0.25	[kg.d-1]	O
Local emission to wastewater during episode	75	75	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[FORMULATION]				
Local emission to air during episode	20	15	[kg.d-1]	O
Local emission to wastewater during episode	60	45	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[PROCESSING]				
Local emission to air during episode	0.0622	0.249	[kg.d-1]	O
Local emission to wastewater during episode	43.6	12.4	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[PRIVATE USE]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[RECOVERY]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
DISTRIBUTION				
PARTITION COEFFICIENTS				
SOLIDS WATER PARTITIONING				
Organic carbon-water partition coefficient	401	401	[l.kg-1]	O
Solids-water partition coefficient in soil	8.02	8.02	[l.kg-1]	O
Solids-water partition coefficient in sediment	20.1	20.1	[l.kg-1]	O
Solids-water partition coefficient suspended matter	40.1	40.1	[l.kg-1]	O
Solids-water partition coefficient in raw sewage sludge	120	120	[l.kg-1]	O
Solids-water partition coefficient in settled sewage sludge	120	120	[l.kg-1]	O
Solids-water partition coefficient in activated sewage sludge	148	148	[l.kg-1]	O
Solids-water partition coefficient in effluent sewage sludge	148	148	[l.kg-1]	O
Suspended matter-water partition coefficient	10.9	10.9	[m3.m-3]	O
Soil-water partition coefficient	12.2	12.2	[m3.m-3]	O
Sediment-water partition coefficient	10.8	10.8	[m3.m-3]	O
AIR-WATER PARTITIONING AND ADSORPTION TO AEROSOL PARTICLES				
Sub-cooled liquid vapour pressure	65.9	65.9	[Pa]	O
Fraction of chemical associated with aerosol particles	1.52E-06	1.52E-06	[-]	O
Henry's law constant	1.65	1.65	[Pa.m3.mol-1]	O
Air-water partitioning coefficient	6.98E-04	6.98E-04	[m3.m-3]	O
BIOTA-WATER				
Bioconcentration factor for aquatic biota	84.4	84.4	[l.kg-1]	O
DEGRADATION AND TRANSFORMATION RATES				
CHARACTERIZATION AND STP				
Characterization of biodegradability	Inherently biodegr., fulfilling criteria	Inherently biodegr., fulfilling criteria		S
Degradation calculation method in STP	First order, standard OECD/EU tests	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	2.4	2.4	[d-1]	O
Total rate constant for degradation in STP	2.4	2.4	[d-1]	O
Maximum growth rate of specific microorganisms	2	2	[d-1]	D
Half saturation concentration	0.5	0.5	[g.m-3]	D
ENVIRONMENTAL				
Specific degradation rate constant with OH-radicals	0	0	[cm3.molec-1.s-1]	D
Rate constant for degradation in air	0	0	[d-1]	O

Rate constant for hydrolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for photolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for biodegradation in surface water	150	21	[d] (Dt50)	S
Total rate constant for degradation in bulk surface water	4.62E-03	0.033	[d-1]	O
Rate constant for biodegradation in bulk soil	300	21	[d] (Dt50)	S
Total rate constant for degradation in bulk soil	2.31E-03	0.033	[d-1]	O
Rate constant for biodegradation in aerated sediment	2.31E-03	2.31E-03	[d-1]	O
Total rate constant for degradation in bulk sediment	2.31E-04	2.31E-04	[d-1]	O
SEWAGE TREATMENT CONTINENTAL				
Fraction of emission directed to air	0.0149	0.0149	[-]	O
Fraction of emission directed to water	0.557	0.557	[-]	O
Fraction of emission directed to sludge	0.0421	0.0421	[-]	O
Fraction of the emission degraded	0.386	0.386	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	2.78	1.39	[kg.d-1]	O
Indirect emission to surface water	104	52	[kg.d-1]	O
Indirect emission to agricultural soil	7.86	3.94	[kg.d-1]	O
REGIONAL				
Fraction of emission directed to air	0.0178	0.0178	[-]	O
Fraction of emission directed to water	0.555	0.555	[-]	O
Fraction of emission directed to sludge	0.0421	0.0421	[-]	O
Fraction of the emission degraded	0.385	0.385	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	3.32	1.67	[kg.d-1]	O
Indirect emission to surface water	103	51.8	[kg.d-1]	O
Indirect emission to agricultural soil	7.85	3.93	[kg.d-1]	O
LOCAL [PRODUCTION]				
INPUT AND CONFIGURATION [PRODUCTION]				
Use or bypass STP	Use STP	Use STP		D
Local emission to wastewater during episode	75	75	[kg.d-1]	O
Concentration in untreated wastewater	37.5	0.577	[mg.l-1]	O
Local emission entering the STP	75	75	[kg.d-1]	O
Type of local STP	With primarily settler (9-box)	With primarily settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	6.5E+05	[eq]	S
Effluent discharge rate of this STP	2E+06	1.3E+08	[l.d-1]	O
Calculate dilution from river flow rate	No	No		S
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O
Dilution factor	10	10	[-]	D
OUTPUT [PRODUCTION]				
Fraction of emission directed to air by STP	0.019	0.0187	[-]	O
Fraction of emission directed to water by STP	0.554	0.554	[-]	O
Fraction of emission directed to sludge by STP	0.0421	0.0421	[-]	O
Fraction of the emission degraded in STP	0.385	0.385	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	1.42	1.4	[kg.d-1]	O
Concentration in untreated wastewater	37.5	0.577	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	20.8	0.32	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	4E+03	61.5	[mg.kg-1]	O
PEC for micro-organisms in the STP	20.8	0.32	[mg.l-1]	O
[FORMULATION]				
INPUT AND CONFIGURATION [FORMULATION]				
Use or bypass STP	Use STP	Use STP		D
Local emission to wastewater during episode	60	45	[kg.d-1]	O
Concentration in untreated wastewater	30	0.346	[mg.l-1]	O
Local emission entering the STP	60	45	[kg.d-1]	O
Type of local STP	With primarily settler (9-box)	With primarily settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	6.5E+05	[eq]	S
Effluent discharge rate of this STP	2E+06	1.3E+08	[l.d-1]	O
Calculate dilution from river flow rate	No	No		O
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O
Dilution factor	10	10	[-]	D

OUTPUT [FORMULATION]

Fraction of emission directed to air by STP	0.019	0.0187	[-]	O
Fraction of emission directed to water by STP	0.554	0.554	[-]	O
Fraction of emission directed to sludge by STP	0.0421	0.0421	[-]	O
Fraction of the emission degraded in STP	0.385	0.385	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	1.14	0.843	[kg.d-1]	O
Concentration in untreated wastewater	30	0.346	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	16.6	0.192	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	3.2E+03	36.9	[mg.kg-1]	O
PEC for micro-organisms in the STP	16.6	0.192	[mg.l-1]	O

[PROCESSING]

INPUT AND CONFIGURATION [PROCESSING]

Use or bypass STP	Use STP	Use STP		D
Local emission to wastewater during episode	43.6	12.4	[kg.d-1]	O
Concentration in untreated wastewater	21.8	0.0958	[mg.l-1]	O
Local emission entering the STP	43.6	12.4	[kg.d-1]	O
Type of local STP	With primarily settler (9-box)	With primarily settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	6.5E+05	[eq]	S
Effluent discharge rate of this STP	2E+06	1.3E+08	[l.d-1]	O
Calculate dilution from river flow rate	No	No		O
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O
Dilution factor	10	10	[-]	D

OUTPUT [PROCESSING]

Fraction of emission directed to air by STP	0.019	0.0187	[-]	O
Fraction of emission directed to water by STP	0.554	0.554	[-]	O
Fraction of emission directed to sludge by STP	0.0421	0.0421	[-]	O
Fraction of the emission degraded in STP	0.385	0.385	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	0.826	0.233	[kg.d-1]	O
Concentration in untreated wastewater	21.8	0.0958	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	12.1	0.053	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	2.32E+03	10.2	[mg.kg-1]	O
PEC for micro-organisms in the STP	12.1	0.053	[mg.l-1]	O

CONTINENTAL AND REGIONAL

CONTINENTAL

Continental PEC in surface water (total)	1.64E-05	4.58E-06	[mg.l-1]	O
Continental PEC in surface water (dissolved)	1.64E-05	4.58E-06	[mg.l-1]	O
Continental PEC in air (total)	4.77E-07	1.95E-07	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.01E-05	4.19E-07	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.41E-06	5.83E-08	[mg.l-1]	O
Continental PEC in natural soil (total)	4.11E-06	2.15E-07	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.61E-05	4.3E-06	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.76E-04	4.89E-05	[mg.kgwwt-1]	O

REGIONAL

Regional PEC in surface water (total)	9.28E-04	3.05E-04	[mg.l-1]	O
Regional PEC in surface water (dissolved)	9.27E-04	3.05E-04	[mg.l-1]	O
Regional PEC in air (total)	2.39E-06	1.07E-06	[mg.m-3]	O
Regional PEC in agricultural soil (total)	7.56E-04	3.22E-05	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	1.05E-04	4.48E-06	[mg.l-1]	O
Regional PEC in natural soil (total)	2.06E-05	1.18E-06	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	2.83E-03	3.61E-04	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	9.18E-03	3.02E-03	[mg.kgwwt-1]	O

LOCAL

REMOVAL RATE CONSTANTS SOIL

Total rate constant for degradation in bulk soil	2.31E-03	0.033	[d-1]	O
Rate constant for volatilisation from agricultural soil	1.56E-04	1.56E-04	[d-1]	O
Rate constant for volatilisation from grassland soil	3.12E-04	3.12E-04	[d-1]	O
Rate constant for leaching from agricultural soil	1.96E-04	1.96E-04	[d-1]	O
Rate constant for leaching from grassland soil	3.92E-04	3.92E-04	[d-1]	O

Total rate constant for removal from agricultural top soil	2.66E-03	0.0334	[d-1]	O
Total rate constant for removal from grassland top soil	3.01E-03	0.0337	[d-1]	O
[PRODUCTION]				
LOCAL CONCENTRATIONS AND DEPOSITIONS [PRODUCTION]				
Concentration in air during emission episode	3.95E-04	3.9E-04	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	3.25E-04	3.21E-04	[mg.m-3]	O
Total deposition flux during emission episode	6.69E-04	6.62E-04	[mg.m-2.d-1]	O
Annual average total deposition flux	5.5E-04	5.44E-04	[mg.m-2.d-1]	O
Concentration in surface water during emission episode	2.08	0.0319	[mg.l-1]	O
Annual average concentration in surface water	1.71	0.0263	[mg.l-1]	O
Concentration in agric. soil averaged over 30 days	9.08	0.0572	[mg.kgwwt-1]	O
Concentration in agric. soil averaged over 180 days	7.51	0.0151	[mg.kgwwt-1]	O
Concentration in grassland averaged over 180 days	2.72	6.04E-03	[mg.kgwwt-1]	O
Fraction of steady-state (agricultural soil)	1	1	[-]	O
Fraction of steady-state (grassland soil)	1	1	[-]	O
LOCAL PECS [PRODUCTION]				
Annual average local PEC in air (total)	3.27E-04	3.22E-04	[mg.m-3]	O
Local PEC in surface water during emission episode	2.08	0.0322	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	1.71	0.0266	[mg.l-1]	O
Local PEC in sediment during emission episode	19.7	0.306	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	9.08	0.0572	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	7.51	0.0151	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	2.72	6.04E-03	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	1.04	2.09E-03	[mg.l-1]	O
Local PEC in pore water of grassland	0.378	8.4E-04	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.04	2.09E-03	[mg.l-1]	O
[FORMULATION]				
LOCAL CONCENTRATIONS AND DEPOSITIONS [FORMULATION]				
Concentration in air during emission episode	5.56E-03	4.17E-03	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	4.57E-03	3.43E-03	[mg.m-3]	O
Total deposition flux during emission episode	8.46E-03	6.34E-03	[mg.m-2.d-1]	O
Annual average total deposition flux	6.95E-03	5.21E-03	[mg.m-2.d-1]	O
Concentration in surface water during emission episode	1.66	0.0192	[mg.l-1]	O
Annual average concentration in surface water	1.36	0.0158	[mg.l-1]	O
Concentration in agric. soil averaged over 30 days	7.27	0.0347	[mg.kgwwt-1]	O
Concentration in agric. soil averaged over 180 days	6.01	9.47E-03	[mg.kgwwt-1]	O
Concentration in grassland averaged over 180 days	2.19	4.48E-03	[mg.kgwwt-1]	O
Fraction of steady-state (agricultural soil)	1	1	[-]	O
Fraction of steady-state (grassland soil)	1	1	[-]	O
LOCAL PECS [FORMULATION]				
Annual average local PEC in air (total)	4.57E-03	3.43E-03	[mg.m-3]	O
Local PEC in surface water during emission episode	1.66	0.0195	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	1.37	0.0161	[mg.l-1]	O
Local PEC in sediment during emission episode	15.8	0.185	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	7.27	0.0347	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	6.01	9.47E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	2.19	4.48E-03	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	0.836	1.32E-03	[mg.l-1]	O
Local PEC in pore water of grassland	0.304	6.22E-04	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	0.836	1.32E-03	[mg.l-1]	O

[PROCESSING]

LOCAL CONCENTRATIONS AND DEPOSITIONS [PROCESSING]

Concentration in air during emission episode	2.3E-04	6.92E-05	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	1.89E-04	5.69E-05	[mg.m-3]	O
Total deposition flux during emission episode	3.55E-04	1.93E-04	[mg.m-2.d-1]	O
Annual average total deposition flux	2.92E-04	1.59E-04	[mg.m-2.d-1]	O
Concentration in surface water during emission episode	1.21	5.3E-03	[mg.l-1]	O
Annual average concentration in surface water	0.991	4.36E-03	[mg.l-1]	O
Concentration in agric. soil averaged over 30 days	5.28	9.49E-03	[mg.kgwwt-1]	O
Concentration in agric. soil averaged over 180 days	4.36	2.51E-03	[mg.kgwwt-1]	O
Concentration in grassland averaged over 180 days	1.58	1.01E-03	[mg.kgwwt-1]	O
Fraction of steady-state (agricultural soil)	1	1	[-]	O
Fraction of steady-state (grassland soil)	1	1	[-]	O

LOCAL PECS [PROCESSING]

Annual average local PEC in air (total)	1.91E-04	5.8E-05	[mg.m-3]	O
Local PEC in surface water during emission episode	1.21	5.61E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	0.992	4.66E-03	[mg.l-1]	O
Local PEC in sediment during emission episode	11.5	0.0533	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.28	9.5E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	4.36	2.51E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.58	1.02E-03	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	0.606	3.48E-04	[mg.l-1]	O
Local PEC in pore water of grassland	0.22	1.41E-04	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	0.606	3.48E-04	[mg.l-1]	O

EXPOSURE

BIOCONCENTRATION FACTORS

Partition coefficient worm-porewater	49.2	49.2	[l.kg-1]	O
Bioconcentration factor for earthworms	6.84	6.84	[kg.kg-1]	O
Bioconcentration factor for fish	84.4306	30	[l.kg-1]	S
Partition coefficient between plant tissue and water	9.27	9.27	[m3.m-3]	O
Partition coefficient between leaves and air	1.33E+04	1.33E+04	[m3.m-3]	O
Transpiration-stream concentration factor	0.388	0.388	[-]	O
Bioaccumulation factor for meat	3.09E-05	3.09E-05	[d.kg-1]	O
Bioaccumulation factor for milk	9.77E-06	9.77E-06	[d.kg-1]	O
Purification factor for surface water	1	1	[-]	O

SECONDARY POISONING

SECONDARY POISONING [PRODUCTION]

Concentration in fish from surface water for predators	72.1	0.403	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	25.7	0.0516	[mg.kg-1]	O

SECONDARY POISONING [FORMULATION]

Concentration in fish from surface water for predators	57.7	0.245	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	20.6	0.0325	[mg.kg-1]	O

SECONDARY POISONING [PROCESSING]

Concentration in fish from surface water for predators	41.9	0.0745	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	14.9	8.69E-03	[mg.kg-1]	O

HUMANS EXPOSED TO OR VIA THE ENVIRONMENT

REGIONAL

CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER

Regional concentration in wet fish	0.0783	9.15E-03	[mg.kg-1]	O
Regional concentration in root tissue of plant	1.39E-03	5.93E-05	[mg.kg-1]	O
Regional concentration in leaves of plant	4.71E-05	2.03E-05	[mg.kg-1]	O
Regional concentration in grass (wet weight)	4.71E-05	2.03E-05	[mg.kg-1]	O

Fraction of total uptake by crops from pore water	0.038	3.75E-03	[-]	0
Fraction of total uptake by crops from air	0.962	0.996	[-]	0
Fraction of total uptake by grass from pore water	0.038	3.75E-03	[-]	0
Fraction of total uptake by grass from air	0.962	0.996	[-]	0
Regional concentration in drinking water	9.27E-04	3.05E-04	[mg.l-1]	0
CONCENTRATIONS IN MEAT AND MILK				
Regional concentration in meat (wet weight)	1.69E-06	5.66E-07	[mg.kg-1]	0
Regional concentration in milk (wet weight)	5.36E-07	1.79E-07	[mg.kg-1]	0
Fraction of total intake by cattle through grass	0.058	0.0751	[-]	0
Fraction of total intake by cattle through drinking water	0.93	0.917	[-]	0
Fraction of total intake by cattle through air	5.32E-03	7.12E-03	[-]	0
Fraction of total intake by cattle through soil	6.41E-03	8.18E-04	[-]	0
DAILY HUMAN DOSES				
Daily dose through intake of drinking water	2.65E-05	8.72E-06	[mg.kg-1.d-1]	0
Fraction of total dose through intake of drinking water	0.161	0.353	[-]	0
Daily dose through intake of fish	1.29E-04	1.5E-05	[mg.kg-1.d-1]	0
Fraction of total dose through intake of fish	0.784	0.61	[-]	0
Daily dose through intake of leaf crops	8.07E-07	3.48E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of leaf crops	4.92E-03	0.0141	[-]	0
Daily dose through intake of root crops	7.63E-06	3.25E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of root crops	0.0465	0.0132	[-]	0
Daily dose through intake of meat	7.29E-09	2.43E-09	[mg.kg-1.d-1]	0
Fraction of total dose through intake of meat	4.44E-05	9.86E-05	[-]	0
Daily dose through intake of milk	4.29E-09	1.43E-09	[mg.kg-1.d-1]	0
Fraction of total dose through intake of milk	2.62E-05	5.81E-05	[-]	0
Daily dose through intake of air	5.12E-07	2.29E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of air	3.12E-03	9.28E-03	[-]	0
Regional total daily intake for humans	1.64E-04	2.47E-05	[mg.kg-1.d-1]	0
LOCAL				
[PRODUCTION]				
CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER, [PRODUCTION]				
Local concentration in wet fish	144	0.797	[mg.kg-1]	0
Local concentration in root tissue of plant	13.8	0.0277	[mg.kg-1]	0
Local concentration in leaves of plant	0.024	6.14E-03	[mg.kg-1]	0
Local concentration in grass (wet weight)	0.0126	6.11E-03	[mg.kg-1]	0
Fraction of total uptake by crops from pore water	0.741	5.81E-03	[-]	0
Fraction of total uptake by crops from air	0.259	0.994	[-]	0
Fraction of total uptake by grass from pore water	0.509	2.34E-03	[-]	0
Fraction of total uptake by grass from air	0.491	0.998	[-]	0
Local concentration in drinking water	1.71	0.0266	[mg.l-1]	0
Annual average local PEC in air (total)	3.27E-04	3.22E-04	[mg.m-3]	0
CONCENTRATIONS IN MEAT AND MILK, [PRODUCTION]				
Local concentration in meat (wet weight)	2.97E-03	5.92E-05	[mg.kg-1]	0
Local concentration in milk (wet weight)	9.38E-04	1.87E-05	[mg.kg-1]	0
Fraction of total intake by cattle through grass	8.89E-03	0.216	[-]	0
Fraction of total intake by cattle through drinking water	0.978	0.762	[-]	0
Fraction of total intake by cattle through air	4.16E-04	0.0205	[-]	0
Fraction of total intake by cattle through soil	0.0132	1.47E-03	[-]	0
DAILY HUMAN DOSES, [PRODUCTION]				
Daily dose through intake of drinking water	0.0488	7.59E-04	[mg.kg-1.d-1]	0
Fraction of total dose through intake of drinking water	0.135	0.317	[-]	0
Daily dose through intake of fish	0.237	1.31E-03	[mg.kg-1.d-1]	0
Fraction of total dose through intake of fish	0.654	0.547	[-]	0
Daily dose through intake of leaf crops	4.11E-04	1.05E-04	[mg.kg-1.d-1]	0
Fraction of total dose through intake of leaf crops	1.14E-03	0.0439	[-]	0
Daily dose through intake of root crops	0.0758	1.52E-04	[mg.kg-1.d-1]	0
Fraction of total dose through intake of root crops	0.21	0.0635	[-]	0
Daily dose through intake of meat	1.28E-05	2.55E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of meat	3.53E-05	1.06E-04	[-]	0
Daily dose through intake of milk	7.52E-06	1.5E-07	[mg.kg-1.d-1]	0
Fraction of total dose through intake of milk	2.08E-05	6.27E-05	[-]	0
Daily dose through intake of air	7.01E-05	6.9E-05	[mg.kg-1.d-1]	0
Fraction of total dose through intake of air	1.94E-04	0.0288	[-]	0
Local total daily intake for humans	0.362	2.39E-03	[mg.kg-1.d-1]	0

[FORMULATION]

CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER, [FORMULATION]

Local concentration in wet fish	115	0.482	[mg.kg-1]	O
Local concentration in root tissue of plant	11.1	0.0174	[mg.kg-1]	O
Local concentration in leaves of plant	0.101	0.065	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.0918	0.065	[mg.kg-1]	O
Fraction of total uptake by crops from pore water	0.141	3.45E-04	[-]	O
Fraction of total uptake by crops from air	0.859	1	[-]	O
Fraction of total uptake by grass from pore water	0.0564	1.63E-04	[-]	O
Fraction of total uptake by grass from air	0.944	1	[-]	O
Local concentration in drinking water	1.37	0.0161	[mg.l-1]	O
Annual average local PEC in air (total)	4.57E-03	3.43E-03	[mg.m-3]	O

CONCENTRATIONS IN MEAT AND MILK, [FORMULATION]

Local concentration in meat (wet weight)	2.56E-03	1.76E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	8.1E-04	5.57E-05	[mg.kg-1]	O
Fraction of total intake by cattle through grass	0.0749	0.771	[-]	O
Fraction of total intake by cattle through drinking water	0.906	0.155	[-]	O
Fraction of total intake by cattle through air	6.73E-03	0.0734	[-]	O
Fraction of total intake by cattle through soil	0.0123	3.65E-04	[-]	O

DAILY HUMAN DOSES, [FORMULATION]

Daily dose through intake of drinking water	0.039	4.59E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of drinking water	0.134	0.144	[-]	O
Daily dose through intake of fish	0.189	7.91E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of fish	0.649	0.248	[-]	O
Daily dose through intake of leaf crops	1.73E-03	1.11E-03	[mg.kg-1.d-1]	O
Fraction of total dose through intake of leaf crops	5.92E-03	0.349	[-]	O
Daily dose through intake of root crops	0.0607	9.56E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of root crops	0.208	0.0299	[-]	O
Daily dose through intake of meat	1.1E-05	7.57E-07	[mg.kg-1.d-1]	O
Fraction of total dose through intake of meat	3.77E-05	2.37E-04	[-]	O
Daily dose through intake of milk	6.49E-06	4.46E-07	[mg.kg-1.d-1]	O
Fraction of total dose through intake of milk	2.22E-05	1.4E-04	[-]	O
Daily dose through intake of air	9.8E-04	7.35E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of air	3.36E-03	0.23	[-]	O
Local total daily intake for humans	0.292	3.2E-03	[mg.kg-1.d-1]	O

[PROCESSING]

CONCENTRATIONS IN FISH, PLANTS AND DRINKING WATER, [PROCESSING]

Local concentration in wet fish	83.7	0.14	[mg.kg-1]	O
Local concentration in root tissue of plant	8.03	4.62E-03	[mg.kg-1]	O
Local concentration in leaves of plant	0.0139	1.1E-03	[mg.kg-1]	O
Local concentration in grass (wet weight)	7.36E-03	1.1E-03	[mg.kg-1]	O
Fraction of total uptake by crops from pore water	0.74	5.37E-03	[-]	O
Fraction of total uptake by crops from air	0.26	0.995	[-]	O
Fraction of total uptake by grass from pore water	0.508	2.18E-03	[-]	O
Fraction of total uptake by grass from air	0.492	0.998	[-]	O
Local concentration in drinking water	0.992	4.66E-03	[mg.l-1]	O
Annual average local PEC in air (total)	1.91E-04	5.8E-05	[mg.m-3]	O

CONCENTRATIONS IN MEAT AND MILK, [PROCESSING]

Local concentration in meat (wet weight)	1.72E-03	1.05E-05	[mg.kg-1]	O
Local concentration in milk (wet weight)	5.45E-04	3.31E-06	[mg.kg-1]	O
Fraction of total intake by cattle through grass	8.91E-03	0.22	[-]	O
Fraction of total intake by cattle through drinking water	0.978	0.758	[-]	O
Fraction of total intake by cattle through air	4.18E-04	0.0209	[-]	O
Fraction of total intake by cattle through soil	0.0132	1.39E-03	[-]	O

DAILY HUMAN DOSES, [PROCESSING]

Daily dose through intake of drinking water	0.0283	1.33E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of drinking water	0.135	0.317	[-]	O
Daily dose through intake of fish	0.138	2.3E-04	[mg.kg-1.d-1]	O
Fraction of total dose through intake of fish	0.654	0.547	[-]	O
Daily dose through intake of leaf crops	2.39E-04	1.89E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of leaf crops	1.14E-03	0.0451	[-]	O
Daily dose through intake of root crops	0.044	2.53E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of root crops	0.209	0.0603	[-]	O
Daily dose through intake of meat	7.42E-06	4.5E-08	[mg.kg-1.d-1]	O
Fraction of total dose through intake of meat	3.53E-05	1.07E-04	[-]	O

Daily dose through intake of milk	4.37E-06	2.65E-08	[mg.kg-1.d-1]	O
Fraction of total dose through intake of milk	2.08E-05	6.31E-05	[-]	O
Daily dose through intake of air	4.1E-05	1.24E-05	[mg.kg-1.d-1]	O
Fraction of total dose through intake of air	1.95E-04	0.0296	[-]	O
Local total daily intake for humans	0.21	4.2E-04	[mg.kg-1.d-1]	O
EFFECTS				
INPUT OF EFFECTS DATA				
MICRO-ORGANISMS				
EC50 for micro-organisms in a STP	55	55	[mg.l-1]	S
Specific bacterial population?	No	No		D
EC10 for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
NOEC for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
AQUATIC ORGANISMS				
LC50 for fish	2.3	2.3	[mg.l-1]	S
L(E)C50 for Daphnia	0.63	0.63	[mg.l-1]	S
EC50 for algae	8.2	8.2	[mg.l-1]	S
LC50 for other aquatic species	??	??	[mg.l-1]	D
Species	other	other		D
NOEC for fish	0.5	0.5	[mg.l-1]	S
NOEC for Daphnia	0.55	0.55	[mg.l-1]	S
NOEC for algae	0.89	0.89	[mg.l-1]	S
NOEC for other aquatic species	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
TERRESTRIAL ORGANISMS				
LC50 for plants	??	??	[mg.kgwwt-1]	D
LC50 for earthworms	??	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	??	[mg.kgwwt-1]	D
Species	other	other		D
NOEC for plants	??	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	??	[mg.kgwwt-1]	D
NOEC for other terrestrial species	??	??	[mg.kgwwt-1]	D
NOEC for other terrestrial species	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
BIRDS				
LC50 in avian dietary study (5 days)	??	??	[mg.kg-1]	D
NOAEL	??	??	[mg.kg-1.d-1]	D
NOEC via food	??	??	[mg.kg-1]	O
Duration of (sub-)chronic oral test	Chronic	Chronic		D
Conversion factor NOAEL to NOEC	8	8	[kg.d.kg-1]	D
MAMMALS				
ACUTE				
Oral LD50	2.65E+03	2.65E+03	[mg.kg-1]	S
Oral Discriminatory Dose	??	??	[mg.kg-1]	D
Dermal LD50	2.65E+03	2.65E+03	[mg.kg-1]	O
Inhalatory LC50	900	900	[mg.m-3]	S
(SUB)CHRONIC				
Oral NOAEL	200	200	[mg.kg-1.d-1]	S
Oral LOAEL	800	800	[mg.kg-1.d-1]	S
Inhalatory NOAEL	933	933	[mg.m-3]	O
Inhalatory LOAEL	3.73E+03	3.73E+03	[mg.m-3]	O
Dermal NOAEL	200	200	[mg.kg-1.d-1]	O
Dermal LOAEL	800	800	[mg.kg-1.d-1]	O
NOEC via food	2E+03	2E+03	[mg.kg-1]	O
LOEC via food	??	??	[mg.kg-1]	D
Duration of (sub-)chronic oral test	28 days	28 days		D
Species for conversion of NOAEL to NOEC	Rattus norvegicus	Rattus norvegicus		D

Conversion factor NOAEL to NOEC	(<6 weeks) 10	(<6 weeks) 10	[kg.d.kg-1]	O
HUMANS				
(SUB)CHRONIC				
Oral NOAEL	??	??	[mg.kg-1.d-1]	D
Oral LOAEL	??	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium	??	??	[mg.cm-3]	D
Dermal LOEC in a medium	??	??	[mg.cm-3]	D
Inhalatory (fibre) NOAEL	??	??	[fibres.m-3]	D
Inhalatory (fibre) LOAEL	??	??	[fibres.m-3]	D
Dermal LOAEL	??	??	[mg.kg-1.d-1]	O
Dermal NOAEL	??	??	[mg.kg-1.d-1]	O
Inhalatory LOAEL	??	??	[mg.m-3]	O
Inhalatory NOAEL	??	??	[mg.m-3]	O
CURRENT CLASSIFICATION				
Corrosive (C, R34 or R35)	No	No		D
Irritating to skin (Xi, R38)	No	No		D
Irritating to eyes (Xi, R36)	No	No		D
Risk of serious damage to eyes (Xi, R41)	No	No		D
Irritating to respiratory system (Xi, R37)	No	No		D
May cause sensitisation by inhalation (Xn, R42)	No	No		D
May cause sensitisation by skin contact (Xi, R43)	No	No		D
May cause cancer (T, R45)	No	No		D
May cause cancer by inhalation (T, R49)	No	No		D
Possible risk of irreversible effects (Xn, R40)	No	No		D
ENVIRONMENTAL EFFECTS ASSESSMENT				
INTERMEDIATE RESULTS AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
Toxicological data used for extrapolation to PNEC Aqua	0.5	0.5	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	10	10	[-]	O
Toxicological data used for extrapolation to PNEC Aqua	0.63	0.63	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	100	100	[-]	O
Toxicological data used for extrapolation to PNEC micro	55	55	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	100	100	[-]	O
Toxicological data used for extrapolation to PNEC oral	2E+03	2E+03	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	100	100	[-]	O
INTERMEDIATE RESULTS TERRESTRIAL AND SEDIMENT ORGANISMS				
Toxicological data used for extrapolation to PNEC Terr	0.36	0.36	[mg.kgwwt-1]	O
Assessment factor applied in extrapolation to PNEC Terr	1	1	[-]	O
Equilibrium partitioning used for PNEC in soil?	Yes	Yes		O
Equilibrium partitioning used for PNEC in sediment?	Yes	Yes		O
PNECS FOR AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
PNEC for aquatic organisms	0.05	0.05	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	6.3E-03	6.3E-03	[mg.l-1]	O
PNEC for micro-organisms in a STP	0.55	0.55	[mg.l-1]	O
PNEC for secondary poisoning of birds and mammals	20	20	[mg.kg-1]	O
PNEC for aquatic organisms with statistical method	??	??	[mg.l-1]	O
PNECS FOR TERRESTRIAL AND SEDIMENT ORGANISMS				
PNEC for terrestrial organisms	0.36	0.36	[mg.kgwwt-1]	O
PNEC for terrestrial organisms with statistical method	??	??	[mg.kgwwt-1]	O
PNEC for sediment-dwelling organisms	0.416	0.416	[mg.kgwwt-1]	O
RISK CHARACTERIZATION				
ENVIRONMENTAL EXPOSURE				
LOCAL				
RISK CHARACTERIZATION OF [PRODUCTION]				

ENVIRONMENTAL				
RCR for the local water compartment	41.5	0.645	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	25.3	0.159	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	47.4	0.736	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the sewage treatment plant	37.8	0.581	[-]	O
PREDATORS				
RCR for fish-eating birds and mammals	3.6	0.0201	[-]	O
RCR for worm-eating birds and mammals	1.28	2.58E-03	[-]	O
HUMANS				
MOS local, total exposure via all media	553	8.35E+04	[-]	O
MOS local, exposure via air	2.85E+06	2.9E+06	[-]	O
RISK CHARACTERIZATION OF [FORMULATION]				
ENVIRONMENTAL				
RCR for the local water compartment	33.2	0.389	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	20.2	0.0965	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	37.9	0.444	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the sewage treatment plant	30.2	0.349	[-]	O
PREDATORS				
RCR for fish-eating birds and mammals	2.88	0.0123	[-]	O
RCR for worm-eating birds and mammals	1.03	1.62E-03	[-]	O
HUMANS				
MOS local, total exposure via all media	685	6.26E+04	[-]	O
MOS local, exposure via air	2.04E+05	2.72E+05	[-]	O
RISK CHARACTERIZATION OF [PROCESSING]				
ENVIRONMENTAL				
RCR for the local water compartment	24.1	0.112	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	14.7	0.0264	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	27.5	0.128	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the sewage treatment plant	21.9	0.0964	[-]	O
PREDATORS				
RCR for fish-eating birds and mammals	2.1	3.73E-03	[-]	O
RCR for worm-eating birds and mammals	0.746	4.34E-04	[-]	O
HUMANS				
MOS local, total exposure via all media	951	4.76E+05	[-]	O
MOS local, exposure via air	4.88E+06	1.61E+07	[-]	O
REGIONAL ENVIRONMENT				
RCR for the regional water compartment	0.0185	6.1E-03	[-]	O
RCR for the regional soil compartment	2.1E-03	8.96E-05	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the regional sediment compartment	0.0221	7.26E-03	[-]	O
Extra factor 10 applied to PEC	No	No		O
HUMANS				
MOS regional, total exposure via all media	1.22E+06	8.11E+06	[-]	O
MOS regional, exposure via air	3.91E+08	8.73E+08	[-]	O

Appendix 5

7.5 ESTIMATION OF INHALATION AND DERMAL EXPOSURE EASE-MODEL

Results from Ease model:

This file was created by the EASE system
EASE for Windows version: 2.0

Standard data (inhalation):

Name of the substance: 4-chloro-2-methylphenol
The temperature of the proces: 150 C
The physical state of the substance: Liquid
The exposure type: gas/vapour/liquid aerosol
The status vp is measured at a different temperature
The measurement-temperature is 70
The vp value of the substance is 0.16 KPa at 70 C
The calculated vp is 4.023 Kpa
The volatility of the substance is moderate
The ability-airborne-vapour of the substance is moderate

Scenario: Production (or processing)of PCOC:

aerosol-formed is false
The use-pattern is Closed system
Significant-breaching is false
The pattern of control is Full containment
The predicted gas/vapour/liquid aerosol exposure to 4-chloro-2-methylphenol is 0-0.1 ppm

Standard data (dermal):

Name of the substance: 4-chloro-2-methylphenol
The temperature of the proces: 150 C
The physical state of the substance: Liquid
The exposure type is dermal

Scenario: Production (or processing)of PCOC:

The use-pattern is Closed system
Significant-breaching is false
The pattern of control is not direct handling

Conclusion: The predicted dermal exposure to 4-chloro-2-methylphenol is very low.

H E D S E T

D a t a S h e e t

CAS-No.: 1570-64-5
EINECS-No.: 216-381-3
IUPAC-Name: 4-chloro-2-methylphenol

Producer related part
Company: Danish technological
Institute
Creation date: 27/05/94

Substance related part
Company: Danish technological
Institute
Creation date: 27/05/94

Printing date: 18/12/97
Revision date: 27/05/94
Date of last Update: 18/12/97

1. General Information

1.1 General Substance Information

Molecular Formula: C7-H7-Cl-O
Molecular Weight: 142.59
Smiles Code: Cl-c(ccc1O)cc1C

Substance Type	Physical Status	Purity
Organic	solid	ca. 97.09. % w/w

1.2 Synonyms

4-chloro-o-cresol
 4-chloro-2-cresol
 p-chloro-o-cresol
 5-chloro-2-hydroxy-toluene

1.3 Impurities

CAS-No	EINECS-No	IUPAC-Name	Value
87-64-9	201-760-8	2-chloro-6-methylphenol	ca. 1.21 .. % w/w
95-48-7	202-423-8	2-methylphenol	ca. 0.92 .. % w/w
1570-65-6	216-382-9	2,4-dichloro-6-methylphenol	ca. 0.78 .. % w/w

1.4 Additives

CAS-No	EINECS-No	IUPAC-Name	Value .. % w/w
--------	-----------	------------	-------------------

Remark No information

1.6.1 Labelling

Labelling no labelling required (no data available)
 Specific Limits
 Symbols Nota
 R Phrases 23-34
 S Phrases 22-26-36/37/39-44
 Text Do not breath dust--In close contact with eyes, rinse immediately with plenty of water and seek medical advice--Wear suitable protective clothing, gloves and eye/face protection--If you feel unwell, seek medical advice (show the label where Separate the phrases with '-' and the text for S-phrases with '--'.

Remark Not on official list for labelling. Provisional labelling based on the data given in this document T, R23,34, S 22, 26, 36/37/39, 44

Labelling other, as in legislation
 Specific Limits
 Symbols N Nota
 R Phrases 50/53
 S Phrases
 Text Separate the phrases with '-' and the text for S-phrases with '--'.

1.6.2 Classification

Classification provisionally by manufacturer/importer
 Class of Danger toxic
 R Phrases 23

Classification as in Directive 67/548/EEC
 Class of Danger dangerous for the environment
 R Phrases 50/53

1.7 Use Pattern

Type of Use industrial
 Category Chemical industry: used in synthesis
 Remark Used as chemical intermediate in the synthesis of chlorophenoxyacetic acid herbicides, e.g. MCPA, MCPB, and mecoprop.
 Reference US-EPA (1980): Ambient Water Quality Criteria Document: Chlorinated Phenols. EPA 440/5-80-032.

1.8 Occupational Exposure Limit Values

Type of Limit
 Value

Short Term Exposure Limit Value
 Value

Time Schedule
 Frequency

Remark None known

2. Physico-chemical Data

2.1 Melting Point

Value = 50 .. degree C

Decomposition
 Sublimation

Method OECD Guide-line 102

Year 1981

GLP yes

Remark OECD 102: capillary method

Test substance 97% 4-chloro-o-cresol in test substance

Reference Test report from Qvist Laboratory, Denmark, 1983

Value = 51 .. degree C

Decomposition
 Sublimation

Method

Year

GLP no data

Reference Weast RC (editor) (1974): CRC Handbook of Chemistry and Physics. 56th edition. Chemical Rubber Co., USA

2.2 Boiling Point

Value = 231 .. degree C
 Pressure
 Decomposition
 Method OECD Guide-line 103 Year 1981
 GLP yes
 Remark Method: OECD 103, Siwoloboff method. Chlorocresols decomposes when heated, evolving extremely toxic fumes (phosgene) according to IMDG-Code.
 Test substance Test substance 97% purity
 Reference Test report from Qvist Laboratory, Denmark, 1983

Value = 223 .. degree C
 Pressure
 Decomposition
 Method Year
 GLP no data
 Reference Weast RC (Ed.)(1975): CRC Handbook of Chemistry and Physics, 56th edition. Chemical Rubber Company.

2.3 Density

Type relative density
 Value = 0.4769 .. g/cm3
 Temperature 20 degree C
 Method OECD Guide-line 109 Year 1981
 GLP yes
 Remark OECD 109, pycnometer method (not comprimated)
 Reference Test report from Qvist Laboratory, Denmark, 1983

Type density
 Value = 1.2 .. g/cm3
 Temperature 50 degree C
 Method
 Year
 GLP no data
 Reference A.H.Marks internal data

2.4 Vapour Pressure

Value = 0.2666 .. hPa
 Temperature 20 degree C
 Method OECD Guide-line 104 Year 1981
 GLP yes
 Remark Vapour pressure = 0.2 mmHg, recalculated to 26.66 Pa. Information from notification form, Danish-EPA 1983.
 Reference Dantest, Denmark, for the Danish EPA

Value = 0.032 .. hPa
 Temperature 25 degree C
 Method other (measured) Year 1986
 GLP no data
 Remark The vapour pressure is measured in a laboratory test without further information. The vapour pressure was 0.024 Torr, recalculated to 3.199 Pa.
 Reference Seiber JN, McChesney MM, Sanders PF and Woodrow JE (1986): Models for Assessing the Volatilization of Herbicides Applied to Flooded Rice Fields. Chemosphere 15(2): 127-138.

Value = 0.1623 .. hPa
 Temperature degree C
 Method Year
 GLP
 Remark The QSAR database states 0.122 mmHg, which is recalculated to 16.23 Pa or 0.1623 hPa. Method and validity unknown.
 Reference US-EPA, Duluth. QSARdb

2.5 Partition Coefficient

log Pow = 2.95 ..
 Temperature degree C
 Method other (calculated) Year 1979
 GLP no data
 Remark log Pow is estimated by substituent constant method of Hansch C and Leo A (1979): Substituent constants for correlation analysis in chemistry and biology. John Wiley & Sons, New York.
 Reference Moulton MP and Schultz TW (1986): Comparisons of Several Structure-Toxicity Relationships for Chlorophenols. Aquatic Toxicology 8: 121-128

log Pow = 3.13 ..
 Temperature degree C
 Method other (calculated) Year 1988
 GLP no data
 Reference Leo A, Weininger D (1988): CLOGP version 3.34

log Pow = 3.09 ..
 Temperature 25 degree C
 Method OECD Guide-line 107
 Year 1981
 GLP no data
 Reference BASF, Analytisches Labor, 1987

2.6 Water Solubility

Value = 2300 .. mg/l at 20 degree C
 pH ..

Concentration at degree C
 pKa at 25 degree C
 Descr. slightly soluble
 Method OECD Guide-line 105 Year 1981
 GLP yes
 Remark Information from notification form to the Danish-EPA, 1983. The result of the study is 0.23% w/w, recalculated to 2300 mg/l.
 Reference Report from Qvist Laboratory, Denmark. Column elution method

Value = 4000 .. mg/l at degree C
 pH ..
 Concentration at degree C
 pKa at 25 degree C
 Descr. soluble
 Method Year
 GLP
 Reference Woodrow JE, McChesney MM and Seiber JN: Modelling the Volatilization of Pesticides and Their Distribution in the Atmosphere. In: Kurtz DA (Ed.): Long Range Transport of Pesticides. Lewis Publishers, Michigan, 1990.

Value = 3850 .. mg/l at degree C
 pH ..
 Concentration at degree C
 pKa at 25 degree C
 Descr. slightly soluble
 Method Year
 GLP no data
 Reference Callahan HA, Slimak MW, Gabel NW, May IP, Fowler C, Freed JR, Jennings P, Durfee RL, Whitmore FC, Maestri B, Holt BR, Gould C (1979): Water Related Environmental Fate of 129 Priority Pollutants. Vols I and II. EPA-440/4-79-029a and EPA-440/4-79-029b. US-EPA, Washington, D.C.

Value = 7.6 .. g/l at 25 degree C
 pH ..
 Concentration at degree C
 pKa 9.71 at 25 degree C
 Descr.
 Method other Year 1979
 GLP no data
 Reference Weast RC (ed): Handbook of Chemistry and Physics, 60th ed. Boca Raton, Florida, CRC Press 1979.

2.7 Flash Point

Value degree C
 Type open cup
 Method other: DS 345 Year
 GLP no data

===== INDIRECT PHOTOLYSIS =====

Sensitizer		
Conc. of Sensitizer		
Rate Constant	cm ³ /(molecule*sec)	
Degradation	.. % after	
Method	other (measured)	Year 1985
GLP	no data	Testsubstance no data
Remark	The study is performed in closed bottles in sunlight in California, USA. The authors state a half-life of 2.5 days but from the graphic presentation 4 days can be estimated.	
Reference	Crosby DG & Bowers JB (1985): Composition and photochemical reactions of a dimethylamine salt formulation of (4-chloro-2-methylphenoxy)acetic acid (MCPA). J.Agric. Food Chem 33: 569-573.	
Type	air	
Light Source		
Light Spect.	.. nm	
Rel. Intens.	.. based on Intensity of Sunlight	
Spectrum of Substance	lambda (max) [>295nm] nm epsilon (max) epsilon (295)	
Conc. of Substance		
Temperature	degree C	

===== DIRECT PHOTOLYSIS =====

Halflife t1/2	..
Degradation	.. % after
Quantum yield	

===== INDIRECT PHOTOLYSIS =====

Sensitizer	OH	
Conc. of Sensitizer	500000 molecule/cm ³	
Rate Constant =	0.0000000001284 cm ³ /(molecule*sec)	
Degradation =	50 .. % after 1.25 day	
Method	other (calculated)	Year 1991
GLP	no data	Testsubstance
Reference	BASF 1991: Berechnung der reaktionsgeschwindigkeit von PCOC mit OH-radikalen nac Atkinson.	

3.1.3 Stability in Soil

Type	laboratory	Radiolabel no
Concentration	10 mg/kg	
Soil Temperature	25 degree C	
Soil Humidity	other: field capacity	
Soil Classificat.	other: sandy clay	
Year	1989	
Content of Clay	.. %	
Silt	.. %	

Sand	.. %	
Organic Carbon	= 1.1 %	
pH	= 7.1	
Cation Exch. Cap.		
Microbial Biomass		
Dissip. Time DT50	= 21 day	
DT90	..	
Dissipation	= 78 % after 40 day	
Method	other	
Year		
GLP	no data	
Test substance	other TS	
Remark	Remarks to the study is made at record no.4, after presentation of the results.	
Result	Degradation rate for sandy clay followed 1.order rate $K = 0.0378$ /day, equivalent to a half life of 21 days.	
Test condition	Two soil types, sandy clay and silty clay were used. The soil is treated with 0 (control), 10, and 1000 mg/kg 4-chloro-o-cresol. The results are presented in the first 4 records and further test conditions and remarks are made in the last record, no.4.	
Test substance	4-chloro-o-cresol, a commercial sample from Fluka, purified by vacuum distillation.	
Reference	Sattar MA (1989): Fate of Chlorinated Cresols from Environmental Samples. Chemosphere 19(8/9): 1421-1426.	
Type	laboratory	Radiolabel no
Concentration	1000 mg/kg	
Soil Temperature	25 degree C	
Soil Humidity	other: field capacity	
Soil Classificat.	other: sandy clay	
Year	1989	
Content of Clay	.. %	
Silt	.. %	
Sand	.. %	
Organic Carbon	= 1.1 %	
pH	= 7.1	
Cation Exch. Cap.		
Microbial Biomass		
Dissip. Time DT50	= 21 day	
DT90	..	
Dissipation	= 69.5 % after 40 day	
Method	other	Year
GLP	no data	Testsubstance other TS
Remark	Refer to record 4	
Result	Degradation rate for sandy clay at 1000 mg/kg followed 1.order rate $K = 0.0295$ /day, equivalent to a half life of 21 days.	
Test condition	Refer to record 4, this section.	
Test substance	4-chloro-o-cresol, a commercial sample from Fluka, purified by vacuum distillation.	
Reference	Sattar MA (1989): Fate of Chlorinated Cresols from Environmental Samples. Chemosphere 19(8/9): 1421-1426.	

Type	laboratory	Radiolabel no
Concentration	10 mg/kg	
Soil Temperature	25 degree C	
Soil Humidity	other: field capacity	
Soil Classificat.	other: silty clay	
Year		
Content of Clay	.. %	
Silt	.. %	
Sand	.. %	
Organic Carbon	= 3.5 %	
pH	= 5	
Cation Exch. Cap.		
Microbial Biomass		
Dissip. Time	DT50 = 21 day	
	DT90	
Dissipation	= 79 % after 40 day	
Method	other	Year
GLP	no data	Testsubstance other TS
Remark	Refer to record 4 (next record).	
Result	The degradation rate for silty clay at 10 mg/kg followed 1.order rate $K = 0.0378$ /day, equivalent to a half life of 21 days.	
Test condition	Refer to record 4 (next record).	
Test substance	4-chloro-o-cresol, a commercial sample from Fluka, purified by vacuum distillation.	
Reference	Sattar MA (1989): Fate of Chlorinated Cresols from Environmental Samples. Chemosphere 19(8/9): 1421-1426.	

Type	laboratory	Radiolabel no
Concentration	1000 mg/kg	
Soil Temperature	25 degree C	
Soil Humidity	other: field capacity	
Soil Classificat.	other: silty clay	
Year		
Content of Clay	.. %	
Silt	.. %	
Sand	.. %	
Organic Carbon	= 3.5 %	
pH	= 5	
Cation Exch. Cap.		
Microbial Biomass		
Dissip. Time	DT50 = 21 .. day	
	DT90 ..	
Dissipation	= 68.9 % after 40 day	
Method	other	Year
GLP	no data	Testsubstance ther TS
Remark	There is not sufficient data to evaluate the comparativity to guidelines. The soil texture is not characterized. The half life in two soils and 2 concentrations is averaged to a total averaged $T_{1/2}$ of 21 day based on 1.order degradation rate for all results (records 1-4). However, using the calculated rate constants (K-values) the 10 ppm concentrations have a shorter half life than the 1000 ppm in both soils. Calculating $T_{1/2}$ from	

	degradation constants K results in following; Sandy clay 10 ppm: $K = 0.0378/\text{day} \Rightarrow T_{1/2} = 26$ days, 1000 ppm: $K = 0.0295/\text{day} \Rightarrow T_{1/2} = 33$ days. Silty clay, 10 ppm: $K = 0.0378/\text{day} \Rightarrow T_{1/2} = 26$ days, 1000 ppm: $K = 0.0290/\text{day} \Rightarrow T_{1/2} = 34$ days.	
Result	The degradation rate for silty clay followed 1.order rate $K = 0.0290 / \text{day}$, equivalent to a half life of 21 days.	
Test condition	Two soil types; a neutral sandy clay from Bangladesh and a silty clay from Finland were used. 200 g soil from 1-15 cm topsoil is treated with 0 (control), 10 and 1000 mg/kg 4-chloro-o-cresol. The treated soil was incubated for 40 days at 25 degr.Celcius. The soil samples were taken after 0, 10, 20 and 40 days of incubation. The moisture content at field capacity were checked once a week. Ten g of soil sample was extracted with 50 ml hexane-diethylether (1:1) and analysed by GC.	
Test substance	4-chloro-o-cresol, a commercial sample from Fluka, purified by vacuum distillation.	
Reference	Sattar MA (1989): Fate of Chlorinated Cresols from Environmental Samples. Chemosphere 19(8/9): 1421-1426.	
Type	laboratory	Radiolabel no
Concentration	10 ppm	
Soil Temperature	25 degree C	
Soil Humidity	12.1 g water/100g soil dry weight	
Soil Classificat.	other: sandy loam	
Year		
Content of Clay	= 8.81 ..20.76 %	
Silt	= 36.7 ..38.18 %	
Sand	= 51.54 ..55.76 %	
Organic Carbon	= 0.58 ..0.68 %	
pH	= 6.9 ..7.1	
Cation Exch. Cap.		
Microbial Biomass		
Dissip. Time	DT50	ca. 14 .. day
	DT90	ca. 56 .. day
Dissipation		= 96.4 .. % after 84 day
Method	other	Year
GLP	no data	Testsubstance other TS
Remark	The soil texture should have been characterized after the mixing and not before. For further remarks refer to next record	
Result	The dissipation in the sandy loam/clay soil mixture after addition of 10, 200 and 2000 ppm 4-chlor-o-cresol and incubation in 0, 2, 4, 8, and 12 weeks: 10 ppm; 3.0%, 57.5%, 87.2%, 99.4% and > 99%, 200 ppm; 2.4%, 47.37%, 70.62%, 88.92%, and 94.58%, 2000 ppm; 2.5%, 46.25%, 70.47%, 88.50%, and 95.96%.	
Test condition	4-chloro-o-cresol were dissolved in ether and added to 200 g soil. The soil was a non-calcareous dark grey flood-plain soil from Bangladesh collected at five different places in the depths 1-15 cm and 16-30 cm and mixed before use. Distilled water was added to create moisture at field level. The soils were added 10, 200 and 2000 ppm. The soils were incubated at 25 degr.Celcius in closed bottles for 12 weeks. Samples were taken after 0, 2, 4, 8, and 12 weeks of incubation. The residues were	

		analysed by GC after pentafluorobenzylbromide derivatization (detection limit 0.005 ppm).
Test substance		4-chloro-o-cresol, a commercial product from Fluka
Reference		Sattar MA (1981): Persistence of 4-chloro-o-cresol and 5-chloro-3-methylcatechol in soil. Chemosphere 10(9): 1011-1017.
Type		laboratory
Concentration		10 ppm
Soil Temperature		25 degree C
Soil Humidity		15.5 g water/100g soil dry weight
Soil Classificat.		other: clay
Year		
Content of Clay	=	42.36 ..47.14 %
Silt	=	17.74 ..18.9 %
Sand	=	35.12 ..37.74 %
Organic Carbon	=	0.5 ..0.58 %
pH	=	7.15 ..7.23
Cation Exch. Cap.		
Microbial Biomass		
Dissip. Time	DT50	= 14 .. day
	DT90	= 56 .. day
Dissipation		ca. 96 .. % after 84 day
Method		other
GLP		no data
Remark		The dissipation is faster at low concentrations in the soil but was still detectable after 4-8 weeks. The rate of degradation is similar in the two soils (this soil and the soil from the previous record). The methods and analytical results are acceptable, although detailed results are missing in the average calculations. The soil from the two layers, 1-15 and 16-30 cm has been mixed before use, without characterization of the mixture. These two layers are, however, rather similar.
Result		Dissipation of 4-chloro-o-cresol in the clay soil, added 10, 200 and 2000 ppm after 0, 2, 4, 8, and 12 weeks of incubation: 10 ppm; 3.4%, 68.5%, 91.5%, < detection limit (DL), and <DL, 200 ppm; 2.56%, 45.55%, 69.9%, 87.5%, and 93.8%, 2000 ppm; 2.72%, 45.75%, 69.47%, 87.96%, and 94.21%. Average results for both soils (this soil and the preceding record): The dissipation (from results from the recovery analysis in % of added 10, 200 and 2000 ppm 4-chloro-o-cresol after 0, 2, 4, 8, and 12 weeks: 10 ppm; 3.5%, 57.25%, 87.35%, 99.3%, and > 99%, 200 ppm; 2.48%, 46.46%, 70.26%, 88.21%, and 94.61%, 2000 ppm; 2.60%, 46.0%, 69.97%, 88.23%, and 94.59%. The averaged value for all three concentrations; 2.61%, 49.90%, 75.86%, 91.91%, and 96.40%.
Test condition		4-chloro-o-cresol were dissolved in ether and added to 200 g soil. The soil was a Red Brown Terrace soil (clay) from Bangladesh collected at five different places in the depths 1-15 cm and 16-30 cm and mixed before use. Distilled water was added to create moisture at field level. The soils were added 10, 200 and 2000 ppm 4-chloro-o-cresol. The soils were incubated at 25 degr.Celcius in closed bottles for 12 weeks. Samples were taken after 0, 2, 4, 8, and 12 weeks of incubation. The residues were analysed by GC after pentafluorobenzylbromide derivatization (detection limit 0.005 ppm).

Test substance 4-chloro-o-cresol, a commercial product from Fluka
 Reference Sattar MA (1981): Persistence of 4-chloro-o-cresol and 5-chloro-3-methylcatechol in soil. *Chemosphere* 10(9): 1011-1017.

3.2 Monitoring Data (Environment)

Type of Measurement Concentration at contaminated site
 Media other: biota and soil
 Remark The analytical method using capillary GC and EC detector was sensitive enough to show 4-chloro-o-cresol residues from MCPA drifted to the sampling site.

Result After the spraying with a MCPA formulation on railway sides for bush killing in northern Finland in July 1980, complaints were received from nearby garden owners. Fourteen days later 64 vegetable and soil samples were analysed for MCPA and its major metabolites; 4-chloro-o-cresol and 3-methoxy-5-chlorocatechol by GC after pentafluorobenzyl derivation and confirmed by MS. The detection limit was 0.1-1.0 ppb for the three compounds. Results from the 4-chloro-o-cresol analysis; MCPA killed branch 8900 ng/g (ppb, fresh weight), potatoes 0.2 ppb, carrots 2.9 ppb, green salad 52.9 ppb, onions 593.0 ppb, and in a soil sample 337.0 ppb.

Reference Paasivirta J, Sattar MA, Lahtiperä and Paukku R (1983): GC and MS Analysis of MCPA and its Metabolites in the Environment Nearby the Bush Killing Treatment Zone. *Chemosphere* 12 (9/19): 1277-1289.

Type of Measurement concentration at contaminated site
 Media surface water
 Result Fourteen phenolic compounds and phenol derivatives were identified. At the upstream site the mean concentration over the year (n=13) of 4-chloro-2-methylphenol was 2.9 mg/l, the range 0-14.8 mg/l, and the coefficient of variance 153%. Downstream after dilution with unpolluted river the mean concentration was 1.5 mg/l, the range 0-10.6 mg/l and CV 193%. The concentration varied irregularly during the year as seen by range and coefficient of variance. The predominant bacteria were *Pseudomonas*.

Test condition Samples were taken in an English river, Sugden Beck, which receives water from old mine workings contaminated by phenolic wastes and industrial areas in Yorkshire. Samples were taken mid-stream at monthly intervals from April 1981 to April 1982 1300 m above and 300 m below the confluence with an unpolluted river. Concentrations determined by HPLC.

Reference Milner CR and Goulder R (1986): The Abundance, Heterotrophic Activity and Taxonomy of Bacteria in a Stream Subject to Pollution by Chlorophenols, Nitrophenols and Phenoxyalkanoic Acids. *Wat.Res.* 20(1): 85-90.

Type of Measurement other: effluent water from waste water treatment plant
 Media surface water
 Remark The influent and effluent of four municipal waste water treatment plants in Denmark were examined for chlorophenols. Only the effluent from a

	treatment plant receiving waste water from a chlorophenoxyacetic acid production plant contained 4-chloro-2-methylphenol.
Result	Among other chlorphenols, 4-chloro-2-methylphenol was the dominant chlorphenol in the effluent: During holiday was measured 0.5 µg/l (GC-ECD) and 0.28 µg/l (GC-MS) and in the production period 2.9-5.9 µg/l (GC-ECD) and 2.3-5.1 µg/l (GC-MS).
Test condition	Samples taken from the effluent from municipal treatment plants with biological treatment showed the occurrence of 4-chloro-2-methylphenol in the effluent from a plant receiving industrial waste water from a chlorophenoxyacetic acid production. The concentrations were analysed using two methods; gas chromatography with electron capture detection (GC-ECD) and gas chromatographic mass spectrometric method based on selected ion monitoring (GC-MS). Detection limit was 0.02-0.1 µg/l depending on number of chlor substituents.
Reference	Folke J and Lund U (1983): Occurrence of Low- and High-Chlorinated Phenols in Municipal Sewage Before and After Passing Through Biological Treatment Plants. <i>J.Chromatogr.</i> 279: 189-198.
Type of Measurement	concentration at contaminated site
Media	other: leachate from landfill
Remark	The high concentrations of PCOC are a result of the impurities and degradation products from o.a. MCPA (found at 2.5 g/l. The study confirms that PCOC is degradable by adapted <i>Pseudomonas</i> sp.. The information is not sufficient for a mass balance to be performed.
Result	The landfill leachate contained 0.6 g/l para-chloro-ortho-cresol (PCOC). The average removal in the bioreactor was 96.7% of PCOC.
Test condition	The leachate from a landfill in New Zealand containing significant quantities of phenoxy herbicides and the associated chlorophenols were analysed after the relocation of the soil from the original site to a secure landfill. The degradation of the leachate was studied using biological treatment with mixed adapted cultures of <i>Pseudomonas</i> sp. The mixed culture had been operating for 700 days with a fermenter residence time of 14.5 hours (dilution rate 0.07 per hour). The sludge age was 32.6 hours.
Reference	McAllister PJ, Bhamidimarri SMR, Chong R and Manderson GJ (1991): Biological Treatment of a Landfill Leachate Containing Phenoxy Herbicides and Chlorophenols. <i>Water.Sci.Tech.</i> 23: 413-418.
Type of Measurement	other: production site
Media	other: effluents, surface water
Remark	The PCOC concentration was monitored at manufacturing site where production of PCOC, processing into phenoxy acids and formulation of phenoxy herbicides took place.
Result	The PCOC concentration in the manufacturing site effluent before sewage plant treatment was an average of 17 mg/l. The concentration in the sewage treatment effluent was <0.2 to 3.3 µg/l. The concentration in the river just outside the manufacturing site was <0.2 to 3 µg/l. Considering the instrument detection limit was 0.2 µg/l and the limit of detection was 3.6 µg/l, the concentration in surface water was less than 3.6 µg PCOC/l.

Reference	A.H.Marks & Co Ltd. Confidential report. October 1997
Type of Measurement	Other: production site
Media	other: surface water, effluents, sludge
Remark	Monitoring data around manufacturing site where production of PCOC, processing into phenoxy acids and formulation of phenoxy herbicides took place.
Result	The concentration of PCOC in the manufacturing site effluent before sewage treatment during one year from 1996 to 1997 averaged 34 mg/l. And during a week in October 1997 averaged 18 mg/l. The concentration in the effluent from the sewage treatment plant receiving effluent from the manufacturing site ranged 0.13 to 3.1 ug PCOC/l during the same week as above. The detection limit was 0.1 ug/l. The concentration of PCOC in sludge was from below detection limit 1 ug/kg to 2 ug/kg sludge.
Reference	Nufarm UK Ltd. Confidential report. October 1997.

3.3.1 Transport between Environ. Compart.

Type	adsorption
Media	water - soil
Method	other Year 1992
Remark	4-chloro-o-cresol is mobile and has the potential for groundwater contamination. The adsorption/desorption study is not entirely according to guideline; lack of information and results, the desorption time too short etc.
Result	In the adsorption study the Freundlich constant $K = 0.008$. The desorption ranged from 78.9-84.1% depending on the amount of soil. In the degradation study PCOC was adsorbed onto washed (to remove soil organics) soil for 24 hours resulting in the retention of 18 mg PCOC in the soil columns. No traces of PCOC was detectable after 90 hours.
Test condition	The soil was an Ohakea silt loam from New Zealand with 3.6% carbon, CEC 13.2 meq%, and pH 5.2. Soil collected at 1-15 cm depth, air dried and sieved to pass a 1 mm sieve, then washed for 72 hours in distilled water and oven dried. Adsorption study performed at 20 degree C and pH 6.0. One to 10 g of soil, with increment of 1 g soil, added 50-250 ppm para-chlor-o-cresol (PCOC) and shaking until equilibrium. Desorption period 10 hours. Biodegradation was studied in packed columns enriched with adapted bacteria, which was analysed to be predominantly <i>Pseudomonas</i> sp. The column was packed with 85 g soil, and 100 ppm solution of PCOC was recirculated for 24 hours.
Test substance	Test substance was technical grade para-chloro-o-cresol
Reference	Bhamidimarri SMR and Petrie RA (1992): Adsorption and Biodegradation of Herbicide Chemicals in Silt Loam Soil. Proc.Ind.Waste Conf. 46: 591-595.
Type	volatility
Media	water - air
Method	other: Laboratory and field study Year 1986
Remark	4-chloro-o-cresol (PCOC) is a formulation impurity (ca. 0.5%) and a degradation product of MCPA. PCOC was found both in the water and

	<p>air samples. PCOC may form rapidly from MCPA in sun irradiated water solutions or irradiated deposits and also volatilize from water. In the study airsamples around fields treated with MCPA-Dimethylamin salt showed more PCOC than MCPA. Airsamples taken several kilometers from known application sites gave up to 30 ng/m³ of PCOC, which was roughly twice that of MCPA, during the peak of MCPA spraying season. Thus 4-chloro-o-cresol may represent the major MCPA related air residue under environmental conditions. Two references describe the same study with a more specified presentation in Woodrow et al. 1990.</p>
Result	<p>The volatilization potential was evaluated by calculating the Henry's Law constant H. Based on water solubility of 4000 mg/l and a vapour pressure measured in this study to 0.024 Torr = 3.199 Pa, a H was calculated to 1.1 E-06 atm*m³/mole = 0.11 Pa*m³/mole. The highest normalized flux was found on the day of treatment, and then lower values showing the gradual decrease with time; The daily averages for the day 0, 1, 2, and 3 after treatment were, respectively, for volatilization flux: 1.27, 0.43, 0.27, and 0.24 ng/cm²*h, the water concentration was 0.0014, 0.0013, 0.0012, and 0.0013 ppm and the resulting normalized flux: 880, 330, 220, and 180 ng/cm²*h*ppm for 4-chlor-o-cresol.</p>
Test condition	<p>The volatilization of 4-choloro-o-cresol (COC) was calculated, and measured in a field study in a flooded rice field in California. COC was measured by GC and confirmed by GC-MS. The field measurements were performed in June 1983 after application of 0.87 kg a.i./ha MCPA. The air measures were taken 42 cm and 195 cm above water surface and water samples were taken in the field during 3 days after application of MCPA. Aerodynamic method used to calculate flux from air concentration and windspeed data. Daily averages are given.</p>
Test substance	4-chloro-o-cresol from Dow Chemical Co.
Reference	Seiber JN, McChesney MM, Sanders PF and Woodrow JE (1986): Models for Assessing the Volatilization of Herbicides Applied to Flooded Rice Fields. <i>Chemosphere</i> 15(2): 127-138.
Reference	Woodrow JE, McChesney MM and Seiber JN: Modelling the Volatilization of Pesticides and Their Distribution in the Atmosphere. In: Kurtz DA (Ed.): Long Range Transport of Pesticides. Lewis Publishers, Michigan, 1990, p.61-82.

3.3.2 Distribution

Media	air - biota - sediment(s) - soil - water
Method	Calculation according Mackay, Level I Year 1993
Result	Estimation of environmental concentrations: log ₁₀ Henry's Law constant = -3.69 atm*m ³ /mole (calculated). Mackay Level 1 Environmental Partitioning at 25 degr.C. Fugacity = 3.539 E-05 Pa: Air = 85.66%, Soil = 1.28%, Water = 11.86%, Suspended solids 0.0%, Aquatic biota 0.0%, Sediments 1.19%.
Reference	US-EPA Aquire, Environmental Research Laboratory, Duluth

3.4 Mode of Degradation in Actual Use

1 22/02/96 RM:1

Remark PCOC is used as an intermediate in the production of the phenoxy acid herbicides MCPA and mecoprop and does not degrade in this use

3.5 Biodegradation

Type	aerobic	
Inoculum	activated sludge	
Concentration	10 µg/l	related to Test substance
Degradation	= 36 ..	% after 54 day
Results	other: biodegradable	
Kinetic	24 day	= 10 ..
	54 day	= 36 ..
Method	other: activated sludge pilot plant	Year
GLP	no data	Testsubstance other TS

Buisson RSK, Kirk PWW, Lester JN (1988): The Behavior of Selected Chlorinated Organic Micropollutants in the Activated Sludge Process: A Pilot Plant Study. *Water Air & Soil Pollution* 37: 419-432.

The mean percentage removal of 4-chloro-2-methylphenol (PCOC) in terms of reduction in the concentration from the influent sewage to the final effluent is calculated for each sludge age: using sludge age of 4 days the removal was 10%, with sludge age 6 days the removal was -20% and with sludge age 9 days removal was 36% in the pilot treatment plant. Sludge age of 4 and 9 day mean cell residence times experiments were run in parallel and therefore comparable and representing the extremes of British waste water treatment. The negative removal at 36 day (6 day sludge age) indicate formation of PCOC from other compounds, degrading faster than PCOC. The temperature was 17.5 +/-1 degr.C.

The degradation of chlorophenols is studied in a pilot plant study using activated sludge with the sludge age of 4, 6, and 9 days. Settled sewage from a full scale treatment plant. Each experimental period lasted six mean cell residence times, a total of 24, 36 and 54 day experiments. Ten different phenols were spiked at 100 mg/l to each replicate. The removal for each sludge age is given.

Type	aerobic	
Inoculum	other: adapted mixed bacteria	
Concentration	80 mg/l	related to Test substance
Degradation	= 63 ..	% after 180 minute
Results	other	
Kinetic	..	
Method	other	Year 1964
GLP	no data	Testsubstance other TS

Tabak HH, Chambers CW, and Kabler PW (1964): Microbial Metabolism of Aromatic Compounds. I Decomposition of Phenolic

Compounds and Aromatic Hydrocarbons by Phenol-Adapted Bacteria. *J.Bacteriology* 87(4): 910-919.

Bacteria from soil or related environments were adapted to metabolize methylphenols and chlorophenols when cultured in media with the specific substrate as the only carbon source. For chlorophenols and cresols the bacteria were identified as *Pseudomonas*, *Achromobacter* and *Flavobacterium*, which were used in mixed culture in the study. The initial concentration was 80 ppm and 50 ppm was lost after 180 minutes of inoculation using 90 µl oxygen. The presence of the chlorine substitute decreased the degradation rate of cresols and phenols.

Type	aerobic	
Inoculum	other: seawater	
Concentration	18 µg/l	related to Test substance
Degradation	> 90 ..	% after 10 day
Results	other: degraded in seawater	
Kinetic	..	
Method	OECD Guide-line 301 A (old version)	Year 1981
GLP	no data	Testsubstance other TS

Lindgaard-Jørgensen P (1989): Biodegradability of Chlorophenols and mixtures of Chlorophenols in Seawater. *Ecotoxicol.Environ.safety* 17(2): 216-220.

A shake flask die away test performed in climate rooms at 15 degr.C in diffuse light. The seawater was taken 10 cm below the surface. The initial biomass measured as plate count on marine agar modified to seawater: 35000 viable cells/ml. The degradation was measured as DOC. The initial test concentration was 18 µg/l 4-chloro-o-methylphenol. Chemical analysis by GC-ECD.

The degradation rate is calculated to 2.8 µg/liter/day. However, adding complex wastewater to seawater (1:39), which is assumed to be realistic levels, reduced the initial concentration to 3.6 µg/l and reduced the rate of degradation 70 times to 0.04 µg/liter/day.

Type	aerobic	
Inoculum	activated sludge	
Concentration	100 mg/l	related to Test substance
Degradation	= 0 ..	% after 28 day
Results	under test conditions no biodegradation observed	
Kinetic	..	
Method	OECD Guide-line 301 C	Year 1981
GLP	no data	Testsubstance other TS

MITI (1992): Biodegradation and Bioaccumulation Data on Existing Chemicals based on the CSCL Japan. Ministry of International Trade and Industry Japan.

The high concentration may be inhibitory to bacteria. As only studies on lower concentrations have shown degradation a lower concentration should have been used.

Type	anaerobic	
Inoculum	activated sludge	
Concentration	10 µg/l	related to Test substance
Degradation	< 0 ..	% after 32 day
Results	under test conditions no biodegradation observed	
Kinetic	..	
Method	other: batch anaerobic digestion	Year 1988
GLP	no data	Testsubstance other TS

Kirk PWW, Lester JN (1988): The behaviour of Chlorinated Organics During Activated Sludge Treatment and Anaerobic Digestion. *Wat.Sci.Tech.* 20(11/12): 353-359.

4-chloro-2-methylphenol did not show market changes during the test period. Either there was no anaerobic degradation or degradation products from other compounds, e.g. MCPA, was added to the concentration. The result was that after 32 days the degradation of 4-chloro-2-methylphenol was - 15% (115% of initial concentration). The results are presented graphically in another reference on the study; Buisson RSK, Kirk PWW, Lester JN, Campbell JA (1986): Behaviour of Selected Chlorinated Organic Micropollutants During Batch Anaerobic Digestion. *Water Pollut.Control* 85:387-394. The results suggest that 4-chloro-2-methylphenol was resistant to chemical or biologically-mediated changes during anaerobic digestion. However, batch studies do not give sufficient information on the individual compounds. The potential degradation is superseded by the degradation products.

The same study as Record 2 (Buisson et al. 1988), but with the addition of a Batch Anaerobic Digestion study. Digested sludge was flushed with oxygen-free nitrogen and spiked with 12 chlorinated compounds at 10-125 µg/l (e.g. MCPA 125 µg/l and 4-chlor-2-methylphenol 10 µg/l). Another series of experiments was done using 15 compounds spiked at 25-1250 µg/l (MCPA 1250 µg/l, MCPP 1250 µg/l and 4-chloro-2-methylphenol 25 µg/l). The incubation period was 32 days at 37 degr.C.

3.7 Bioaccumulation

Species	Salmo trutta	
Exposure Period	28 day	Temperature 10 degree C
Concentration	0.5 mg/l	
BCF	= 6.9 ..	
Elimination	no data	
Method	other	Year

GLP	no data	Testsubstance other TS
Remark	Bioaccumulation values calculated from the results given in the reference: Concentration of 4-chloro-o-cresol in the wet weight of the fish / concentration in water. Average values from ten specimens: 28 day study; 3.45/0.5 = 6.9, 5.18/1.0 = 5.2. Results from 21 day study; 3.15/0.5 = 6.3, 4.19/1.0 = 4.2, 6.39/1.5 = 4.3.	
Test condition	The trouts, less than one year old, had the average weight of 5.0 g. Twenty fish per aquarium were used. Two subchronic experiments were performed. In the first study the fish were exposed to 0, 0.5 and 1.0 ppm 4-chloro-o-cresol for 28 days. In the second study the fish were exposed to 0, 0.5, 1.0 and 1.5 ppm for 21 days. The solutions were renewed daily.	
Test substance	4-chloro-o-cresol purified to > 99% product from the commercial product of Fluka. The purity controlled by IR, NMR and mass spectrometry. The substance was dissolved in ethanol	
Reference	Buccafusco RJ, Ells SJ, Leblanc GA (1981): Acute Toxicity of Priority Pollutants to Bluegill (<i>Lepomis macrochirus</i>). Bull. Environm.Contam.Toxicol 25: 446-453.	
Species	Cyprinus carpio	
Exposure Period	42 day	Temperature 25 degree C
Concentration	20 µg/l	
BCF	= 8.2	..28
Elimination	no data	
Method	other: Japanese industrial standard	Year 1981
GLP	no data	Testsubstance other TS
Remark	In a second study using 2 µg/l 4-chloro-o-cresol the BCF ranged from 6.4 to 14. 4-chloro-o-cresol is a low accumulating substance.	
Reference	MITI (1992): Data on Existing Chemicals Based on the CSCL Japan. Ministry of International Trade and Industry, Japan	

3.8 Additional Remarks

1 23/06/94 RM:1 RE:1

Remark	Aqueous solutions of MCPA with initial concentrations 50 mg/l were treated in a photoreactor that allowed simultaneous action of light and ozonized air. The degradation product 4-chloro-2-methylphenol (PCOC) was found in all cases; ozone with and without light and light without ozone. Under acidic conditions, pH 3.5, PCOC was only formed under light regimes at 565 µg/l after 6 and at 1160 µg/l after 12 hours of ozonation. At neutral to low pH (7-3.5), 4-chloro-2-methylphenol was formed as a degradation product during light regimes (370 µg/l after 6 hours of ozonation and 920 µg/l after 12 hours of ozonation). In the dark the PCOC was not detected after 6 hours and 15 µg/l after 12 hours of ozonation. At pH 8 only 11 µg/l was formed in the dark and 280 µg/l in light after 6 hours of ozonation. After 12 hours of ozonation the 4-chloro-o-methylphenol was formed in the dark at 45 µg/l, up to 2%, and 70 µg/l in light. Thus MCPA irradiated by sunlight or UV light is degraded to 4-chloro-o-methylphenol and other compounds.
--------	---

Reference	Benoit-Guyod JL, Crocby DG and Bowers JB (1986): Degradation of MCPA by Ozone and Light. <i>Water Res.</i> 20(1): 67-72.		
	2	23/06/94	RM:1 RE:1
Remark	MCPA photodegradation was studied by UV radiation and the degradation products identified by GC-MS. The study was performed by a photoreactor using a Hg-lamp. The study confirmed the formation of 4-chloro-o-cresol from MCPA as the major photoproduct and that its relative concentration increased along the time reaction.		
Reference	Clapés P, Soley J, Vicente M, Rivera J, Caixach J, Ventura F (1986): Degradation of MCPA by Photochemical Methods. <i>Chemosphere</i> 15(4): 395-401.		
	3	17/06/94	RM:1 RE:1
Remark	4-chloro-o-cresol is degraded by radiation oxidation by a Co-60-gamma radiation, which dechlorinated the compound. The initial concentration of 0.0037 mole/l (25.9 µg/l) was totally degraded (dechlorinated) after an adsorbed dosis of 6 Mrad under oxidated conditions. The organic bound chlorine was replaced by oxygen. The analysis of a solution of industrial waste water containing more than 90% 2,4-D and 4-chloro-o-cresol in concentrations 0.0033 mole/l and 0.0037 mole/l respectively showed following analytical data: Initial solution: TOC 530 mg C/l, COD 1600 mg O ₂ /l, BOD-5 355 mg O ₂ /l, and BOD-5/COD 0.22. After absorption of 4.5 Mrad: TOC 530 mg C/l, COD 700 mg O ₂ /l, BOD-5 249 mg O ₂ /l, and BOD-5/COD 0.36. Since TOC remains constant after degradation CO ₂ is not developed but rather a product with a higher oxidation level. This is confirmed by the increase in BOD-5/COD relation which indicate binding of oxygen instead of chlorine which was detected as chloride in the solution.		
Reference	Gilbert E, Güsten H (1977): Die strahlenchemische Oxidation biologisch resistenter organischer Schadstoffe in Industrieabwässern. <i>Chemiker-Zeitung</i> 101(1): 22-27.		

4. Ecotoxicity

4.1 Acute/Prolonged Toxicity to Fish

Type	static		
Species	Lepomis macrochirus		
Unit mg/l	Exposure Period	96	hour
NOEC	..		
LC0	..		
LC50	=	2.3	..
LC100	..		
	..		
Analyt. Monitoring Method	no other: US-EPA Methods for acute tests with fish, macroinvertebrates and amphibians (EPA-660/3-75-009) Year 1975		

GLP	no data	Testsubstance other TS
Remark	LC50 (24 hours) 3.8 mg/l. Data reported based on nominal values. LC50 and 95% Confidence Limits calculated by moving average angle method (Harris 1959) or log probit (Litchfield and Wilcoxon 1949). LC50 (96 hour) 2.3 mg/l (95% C.L. 1.9-2.9). The method seems very similar to the OECD guideline and the results are considered acceptable.	
Test condition	The water was reconstituted deionized water with a hardness 32-48 mg/l CaCO ₃ , pH 6.7-7.8, temperature 22 degr.Celcius, dissolved oxygen 7.0-8.8 mg/l. The bluegills were less than one year old. Ten fish with wet weight ranging from 0.32-1.2 g were exposed in each jar containing 15 l.	
Test substance	4-chloro-6-methylphenol	
Reference	Buccafusco RJ, Ells SJ, Leblanc GA (1981): Acute Toxicity of Priority Pollutants to Bluegill (<i>Lepomis macrochirus</i>). Bull. Environm.Contam.Toxicol 25: 446-453.	
Type	static	
Species	Salmo trutta	
Unit mg/l	Exposure Period 24	hour
NOEC	..	
LC0	..	
LC50	= 2.12	..
LC100	..	
Analyt. Monitoring	no	
Method	other	Year 1979
GLP	no data	Testsubstance other TS
Test condition	The trout which were less than one year old had the average weight of 2.5 g. Ten fish were placed in 20 liter aquaria. The temperature was 10 degr.Celcius.	
Test substance	4-chloro-o-cresol purified to > 99% product from the commercial product of Fluka, purity controlled by IR, NMR and mass spectrometry.	
Reference	Hattula ML, Reunanen H, Wasenius V-M, Krees R, Arstila AU (1979): Toxicity of 4-Chloro-o-Cresol to Fish. Light Microscopy and Chemical Analysis to the Tissue. Bull.Environm.Contam.Toxicol 22: 508-511.	
Type	static	
Species	Oryzias latipes	
Unit mg/l	Exposure Period 48	hour
NOEC	..	
LC0	..	
LC50	= 6.3	..
LC100	..	
Analyt. Monitoring	no data	
Method	other: Japanese industrial standard	Year 1981
GLP	no data	Testsubstance other TS
Reference	MITI (1992): Data on Existing Chemicals Based on the CSCL Japan. Ministry of International Trade and Industry, Japan.	
Type	static	
Species	Brachydanio rerio	
Unit mg/l	Exposure Period 96	hour

NOEC	..	
LC0	..	
LC50	= 3	..6
LC100	..	
	..	
Analyt. Monitoring	no data	
Method	OECD Guide-line 203	Year 1981
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4
Reference	Test report from the water Quality Institute (VKI), Denmark 1983.	

4.2 Acute Tox. to Aquatic Invertebrates

Species	Daphnia magna		
Unit mg/l	Exposure Period	48	hour
NOEC	=	0.028	..
EC0			..
EC50	=	0.29	..
EC100			..
Analyt. Monitoring	no		
Method	other: US-EPA (1975), Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians, EPA-660/3-75-009 Year 1975		
GLP	no data Testsubstance other TS		
Remark	Static test: LC50 (24 hours) 1.9 mg/l (95% confidence limits: 1.5-2.3). LC50 (48 hours) 0.29 mg/l (95% confidence limits 0.19-0.40). The method resembles the OECD guideline and the results are considered acceptable		
Test condition	Daphnia magna < 24 hours old used in the test. The water used in the tests was reconstituted well water with a hardness of 173 +/-13 mg/l CaCO ₃ , pH 8.0 +/-0.2, temperature 22 +/-1 degree Celcius, oxygen concentration > 60% of saturation. Five nominal concentrations used in triplicate with five Daphnia in each (a total of 15 Daphnia per concentration)		
Test substance	4-chloro-6-methylphenol		
Reference	LeBlanc GA (1980): Acute Toxicity of Priority Pollutants to Water Flea (Daphnia magna). Bull. Environm. Contam. Toxicol. 24: 684-691.		
Species	Daphnia magna		
Unit mg/l	Exposure Period	48	hour
NOEC			..
EC0			..
EC50	=	0.63	..
EC100			..
Analyt. Monitoring	no data		
Method	OECD Guide-line 202, part 1 Year 1981		
GLP	yes Testsubstance as prescribed by 1.1 - 1.4		
Remark	No further comments. The result is slightly differing from the preceding reference where LC50 (48 h) were 0.29, but minor differences in methods may have caused this small difference in results.		
Test substance	4-chloro-2-methylphenol, 97.09% pure		
Reference	Water Quality Institute, Denmark, for the Danish EPA		

Species	Daphnia magna
Unit	mg/l
Exposure Period	48 hour
NOEC	..
EC0	= 0.32 ..
EC50	= 1 ..
EC100	= 1.8 ..
Analyt. Monitoring	no data
Method	other Year 1988
GLP	no data Testsubstance as prescribed by 1.1 - 1.4
Reference	BASF, unpublished study (0299/88). Performed according to DIN 38412 L11

4.3 Toxicity to Aquatic Plants e.g. Algae

Species	other aquatic plant: Lemna minor
Endpoint	other: mortality (degree of chlorosis)
Unit	mol/l
Exposure Period	48 hour
NOEC	..
LOEC	..
EC0	..
EC10	..
EC50	= 0.00065 ..
Analyt. Monitoring	no data
Method	other Year 1955
GLP	no data Testsubstance other TS
Remark	LC50 (48 h) of 0.00065 moles/l is equivalent to 92.7 mg/l. It was found that the degree of chlorosis is sensitive to small changes in phenol concentrations and for a single chlorine substitution the relative positions of the methyl and chlorine groups were of importance. The study is an older study and not according to guideline. The method seems acceptable but the temperature too high. 4-chloro-o-cresol is able to volatilize and is degradable in light and the resulting LD50 therefore too high.
Test condition	Preliminary experiments were undertaken to establish the approximate level of 50% mortality, i.e. chlorosis in half the fronds of duckweed. Five different concentrations with fourfold replication were used in the final experiment. Beakers were filled with the phenol culture solutions, pH was adjusted to 5.1, which is optimal for growth, and 50 fronds were placed in each beaker for 48 hours at 25 +/-1 degr.Celcius. The light was 320 +/- 20 foot-candles at the level of the floating fronds. The fronds were transferred to nutrient solutions, after washing in distilled water, for 24 hours. Then the degree of chlorosis was recorded for each beaker
Test substance	2-methyl-4-chloro-phenol
Reference	Blackman GE, Parke MH, and Garton G (1955): The Physiological Activity of Substituted Phenols. I. Relationships between Chemical Structure and Physiological Activity. Arch.Biochem.Biophys. 54: 45-54
Species	Scenedesmus subspicatus
Endpoint	biomass
Unit	mg/l
Exposure Period	96 hour
NOEC	..

LOEC		..
EC0		..
EC10	= 0.89	..
EC50	= 8.2	..
Analyt. Monitoring	no data	
Method	other	Year 1988
GLP	no data	Testsubstance as prescribed by 1.1 - 1.4
Reference	BASF 1988: unpublished data, Study performed according to DIN 318412 Part 9, inhibition of algae growth	

4.4 Tox. to Microorganisms e.g. Bacteria

Type		aquatic
Species		other bacteria
Unit		Exposure Period 18 hour
EC0		..
EC10		..
EC50		..
mm	= 20.2	..
Analyt. Monitoring	no	
Method	other: diameter of inhibition zone	Year 1981
GLP	no data	Testsubstance other: 4-chloro-2-methylphenol
Remark	The toxicity of chlorophenols increased with increase in degree of chloronation, but was also related to the position of the chlorine substitution on the phenol molecule. 4-chloro-2-methylphenol was more toxic than monochlorophenols, MCPA and 2,4-D. The mean inhibition zone was presented as the mean diameter = 20.2 mm, n= 180 (6 isolates times 30 replicates). The controls had no inhibition zone. Pseudomonas was the most resistant genera amongst the freshwater bacteria isolates and also the most dominant in the polluted river.	
Test condition	Toxicity toward bacteria was determined by measuring inhibition of growth on agar plates using the method of Liu and Kwasniewska 1981 (An improved agar plate method for rapid assessment of chemical inhibition to microbial populations. Bull.Environ.Contam.Toxicol. 27:289-294). The used bacteria was isolated from a polluted river; Pseudomonas (3 isolates), Aeromonas (1 isolate), Flavobacterium (1 isolate) and Gram-positive bacteria (1 isolate). A volume of 0.01 ml 4-chloro-2-methylphenol (250 mmol/l) was spotted onto the seeded agar surface together with a control spot, 30 times against each of the 6 bacterial isolates. The diameter of inhibition zones were measured after incubation at 20 degr.C for 18 hours.	
Reference	Milner CR and Goulder R (1986): Comparative Toxicity of Chlorophenols, Nitrophenols, and Phenoxyalkanoic Acids to Freshwater Bacteria. Bull.Environ.Contam.Toxicol 37: 714-718.	
Type		other: laboratory
Species		Tetrahymena pyriformis
Unit mg/l		Exposure Period 48 hour
EC0		..
EC10		..

EC50			..
IGC50	=	1.02	..
Analyt. Monitoring	yes		
Method	other: bioassay		Year 1983
GLP	no data	Testsubstance	other TS
Remark	The result is given as the logarithm of the inverse of the IGC50 value in mmol/l (log BR). Log BR = 0.700, Recalculated to 1.02 mg/l		
Test condition	A sublethal static bioassay test using the population densities of axenic cultures as end point, where 50% growth inhibitory concentration, IGC50 is determined. The cell population is determined spectrophotometrically.		
Reference	Schultz TW, Wesley SK, Baker LL (1989): Structure-Activity Relationships for Di and Tri Alkyl and/or Halogen Substituted Phenols. Bull.Environ.Contam.Toxicol 43:192-198.		
Type	other		
Species	activated sludge		
Unit mg/l	Exposure Period	30	minute
EC0			..
EC10			..
EC50	=	55	..
EC20	=	30	..
Analyt. Monitoring	no data		
Method	ISO 8192		Year 1988
GLP	no data	Testsubstance	as prescribed by 1.1 - 1.4
Reference	BASF, unpublished data, 1988		

4.5.1 Chronic Toxicity to Fish

Species	Salmo trutta		
Endpoint	other: Histopathological changes		
Unit mg/l	Exposure Period	21	day
LLC			..
NOEC	>=	0.5	..
LOEC	=	1	..
Analyt. Monitoring	no		
Method	other		Year 1979
GLP	no data	Testsubstance	other TS
Result	No fish exposed at 0.5 ppm 4-chloro-o-cresol had histological changes in examined organs. Some species from 1.0 ppm had histopathological changes; One had cytoplasmic vacuolar changes in liver cells, one specimen had changes in the kidney (epithelium degenerated, cytoplasm was eosinophilic, nuclei pycnotic, inside the tubuli there were necrotic cells). In fish from 1.5 ppm cresol some changes were observed in kidneys and gills. In the kidney as mentioned above. In gills changes were observed in all but one; lamellar teleangiectasic changes in the secondary filaments, the globes in the filaments were of different size with increasing size and number in increasing exposure concentrations.		
Test condition	The trouts, less than one year old, had the average weight of 5.0 g. Twenty fish per aquarium were used. Two subchronic experiments were performed. The first study the fish were exposed to 0, 0.5 and 1.0 ppm		

	4-chloro-o-cresol for 28 days. In the second study the fish were exposed to 0, 0.5, 1.0 and 1.5 ppm for 21 days. The solutions were renewed daily. For pathological analysis samples were taken from liver, kidney and gills from 10 specimens.
Test substance	4-chloro-o-cresol purified to > 99% product from the commercial product of Fluka. The purity controlled by IR, NMR and mass spectrometry. The substance was dissolved in ethanol
Reference	Hattula ML, Reunanen H, Wasenius V-M, Krees R, Arstila AU (1979): Toxicity of 4-Chloro-o-Cresol to Fish. Light Microscopy and Chemical Analysis of the Tissue. Bull.Environm.Contam.Toxicol 22: 508-511.

4.5.2 Chronic Tox. to Aquatic Invertebrates

Species	Daphnia magna		
Endpoint	other: reproduction		
	Unit mg/l	Exposure Period 21	day
NOEC	=	0.55	..
LOEC	>	0.55	..
EC50	>	0.55	..
Analyt. Monitoring	yes		
Method	OECD Guide-line 202, part 2		Year 1984
GLP	yes Tests substance as prescribed by 1.1 - 1.4		
Remark	In the daphnia reproduction test, no significant effects were observed in mortality, length or reproduction at the highest concentration used. The concentrations were measured and were between 88% to 106% of nominal in the two highest concentrations (0.32 and 0.56 mg/l). The NOEC (21d) is 0.55 mg/l based on average measured concentrations.		
Reference	PCOC Task Force (1997): PCOC: Chronic toxicity to Daphnia magna. Brixham Environmental Laboratory Zeneca Ltd.Report No.BL6032/B, Sept 1997 to AHMarks and Nufarm UK.		

4.9 Additional Remarks

	1	17/06/94	RM:1 RE:1
Remark	Flavour impairment of fish from odorous compounds. For 2-methyl-4-chlorophenol the estimated threshold concentration for flavour impairment of fish (ETC) is lower than the corresponding threshold odour concentration in water (TOC). ETC is the lowest concentration in water that impairs the flavour of fish. TOC is the concentration in water detectable by a group of observers at a probability of 0.5. In <i>Oncorhynchus mykiss</i> , Rainbow trout, the geometric mean ETC = 0.047 mg/l (range 0.03-0.075 mg/l) and TOC = 1.8 mg/l. Exposure time was 48 hours, but the concentration is not mentioned. If a low bioaccumulation is considered as found earlier (Record 3.7), a concentration of about 0.01 mg/l is sufficient to impair taste in fish.		
Reference	Persson P-E (1984): Uptake and Release of Environmentally Occurring Odorous Compounds by Fish. Water Res. 18(19): 1263-1271.		

2 17/06/94
3 18/12/97 RM:1 RE:1

Remark In an in-vitro assay for oestrogenic effects using human breast cancer cells, PCOC was observed to have an oestrogenic activity with a potency 1×10^{-6} of the potency of 17-beta-estradiol. The possible influence on reproductive parameters is difficult to evaluate.

Reference Körner W, Hanf V, Schuller W, Batsch H, Kreienberg R, Hagenmaier H (1997): Validation and application of a rapid in-vitro assay for assessing the estrogenic potency of halogenated phenolic chemicals. Chemosphere (accepted 12 Nov. 1997)

5. Toxicity

5.1.1 Acute Oral Toxicity

Type LD50
Species rat
Value = 3195 .. mg/kg
Method OECD Guide-line 401 Year 1981
GLP yes Testsubstance as prescribed by 1.1 - 1.4
Remark Dosing was carried out by gavage using the doses 1728, 2488, 3583, and 5160 mg/kg. Symptoms observed just after dosing were paresis and depressions. These changed to ruffled fur on the second day which lasted to day 5 in the 3583 mg/kg group. In the 5160 mg/kg group all animals died within one hour after dosing. Animals which died during the observation period showed at autopsy bleedings of the ventricle wall. Animals sacrificed after the 14 day observation period showed no dose related macroscopic changes

Reference Scantox report No. 10150, 24th November 1982. Scantox, Denmark.

Type LD50
Species mouse
Value ..
Method .. Year
GLP .. Testsubstance
Remark Sax & Lewis 1987 reports a LD50 for mouse at 1320 mg/kg, however, checking the original reference shows that the substance tested is not 4-chloro-2-methylphenol but 4-chloro-2-methyl-6-ethylphenol (Schrötter et al., 1975)

Reference Schrötter E, Högel E, Tschäpe M. Organische Synthetica und ihre vermiziden Eigenschaften. 4.Mitteilung: 2-Äethylphenole. Pharmazie 1975; 30: 147-51.

Type LD50
Species rat
Value = 1190 .. mg/kg
Method other Year 1979
GLP no data Testsubstance other TS
Remark It is uncertain how the test substance was applied as both intraperitoneal and oral administration is mentioned under experimental. The animals

were all killed 24 hours after dosing, which renders the LD50-figure given of little value, as the test was not carried out according to OECD or other guide-lines.

Reference Hattula ML, Reunanen H, Arstilla AU. Toxicity of 4-chloro-o-cresol to rat: I. Light microscopy and chemical observations. Bull Environm Contam Toxicol 1979; 21: 492-7.

5.1.2 Acute Inhalation Toxicity

Type	LC50	
Species	rat	
Exposure Time	4 hour	
Value	= 0.9 .. mg/l	
Method	OECD Guide-line 403	Year 1981
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4
Remark	A liquid containing 50% alcohol/water (v/v) was used for the generation of the exposure mixture. It was not possible to generate dust aerosols for the exposure, because of the tendency of the test substance to clump. The symptoms observed during and after exposure were respiration difficulties, depressions, ruffled fur, and bleeding from the nose. These symptoms occurred in a dose related manner.	
Reference	Scantox report No. 10153 of February 28th 1983. Scantox, Denmark.	

5.1.3 Acute Dermal Toxicity

Type	LD50	
Species	rat	
Value	= 2240 .. mg/kg	
Method	OECD Guide-line 402	Year 1981
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4
Remark	During the first 24 hours after treatment blood was observed in the urine of all rats. From the day after treatment the application sites showed erythema and oedema. Clinical signs observed. Paresis occurred in nearly all animals for 1 to 6 hours after the treatment. Depressions occurred for up to 2 days after treatment, and ruffled fur for up to 3 days after treatment. Autopsy findings. In all animals found dead, bleedings of the lungs and intestine, and enlarged kidneys were observed. Animals sacrificed on day 14 showed in five rats weak bleedings of the intestine (jejunum).	
Reference	Scantox Report No. 10152 of 26th November 1982. Scantox, Denmark.	

5.2.1 Skin Irritation

Species	Rabbit	
Result	highly irritating	
Classification	irritating	
Method	OECD Guide-line 404	Year 1981
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4

Remark	The primary irritation index was calculated to 8.0, the maximum value obtainable.
Reference	Scantox Report No. 10154 of November 17th 1982, Scantox, Denmark.

5.2.2 Eye Irritation

Species			
Result			
Classification			
Method			Year
GLP		Testsubstance	
Remark	This test has not been performed, probably due to the highly skin irritating properties of the test substance.		

5.3 Sensitization

Type	Guinea pig maximation test		
Species	guinea pig		
Result	not sensitizing		
Classification	not sensitizing		
Method	OECD Guide-line 406		Year 1981
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4	
Remark	As the provocation test with 30% solution of the testsubstance caused erythema, a further provocation test with 10% and 20% of the testsubstance applied on the left and right flank, respectively, was carried out a week later. There were no clear differences between the control group and the test group at this occasion.		
Reference	Scantox Report No. 10155 of 28th December 1982. Scantox, Denmark.		

5.4 Repeated Dose Toxicity

Species	rat		
Strain	Wistar		Sex male/female
Route of Administration	gavage		
Exposure Period	28 days		
Frequency of Treatment	daily		
Post Exposure			
Observ. Period	none		
Doses	0, 50, 200, and 800 mg/kg/day		
Control Group	yes, concurrent vehicle		
NOEL	= 200	..	mg/kg bw d
LOEL	= 800	..	mg/kg bw d
Method	OECD Guide-line 407		Year 1982
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4	
Remark	During the last three days of the dosing period three rats of the high dose group showed salivation after dosing, and the last day of dosing three rats of the high dose group had ruffled fur. Body weight gain and feed consumption did not differ between groups. In blood parameters the		

thromboplastin time and the number of leucocytes were statistically lower in females of the 800 mg/kg group, in males of the same group the erythrocyte count was statistically significant reduced. Serum alanine-aminotransferase (ALAT) was marginally increased in both sexes of the 800 mg/kg group, but only statistically significant in males. In females of the 800 mg/kg group liver weights were significantly increased both absolutely and relatively to body weight. The changes of ALAT and liver weights in the 800 mg/kg group might indicate that this dose is marginally toxic to the liver.

Reference	Scantox report No. 10149 of 27th December 1982. Scantox, Denmark.		
Species	Rat		
Strain	Wistar	Sex male/female	
Route of Administration	gavage		
Exposure Period	Up to 43 days		
Frequency of Treatment	daily		
Post Exposure			
Observ. Period	none		
Doses	0, 50, 200, and 600 mg/kg bw		
Control Group	yes, concurrent vehicle		
NOEL	= 200	..	mg/kg bw d
LOEL	= 600	..	mg/kg bw d
Method	other: OECD 422 (draft)		Year 1993
GLP	yes	Testsubstance other TS	
Result	No effect was seen of 4-chloro-2-methylphenol on the reproductive and developmental parameters. 4-chloro-2-methylphenol was not found to cause any changes in the behaviour observed by the functional observational battery, or in motor activity. No effect was seen in the macroscopic and histological examination of the organs from animals dosed with 4-chloro-2-methylphenol. Males in the high dose group given 4-chloro-2-methylphenol showed a decrease in haemoglobin concentration ($P < 0.01$) and in the middle dose group a decrease in plasma creatinine ($P < 0.05$).		
Reference	4-chloro-2-methylphenol. Combined repeated dose and toxicity study with the reproductive/developmental toxicity screening test on 1-chloro-2-methylphenol in rats. Ernst Hansen, study No. IT931111, Institute of Toxicology, National Food Agency, Denmark, 1996.		

5.5 Genetic Toxicity in Vitro

Type	Ames test		
System of Testing	Salmonella typhimurium strains TA1537, TA1535, TA100, and TA98		
Concentr.	0, 1, 5, 10, 50, 100, and 500 microg/plate		
Metabolic Activation	with and without		
Result	negative		
Method	OECD Guide-line 471		Year 1982
GLP	no data	Testsubstance as prescribed by 1.1 - 1.4	
Reference	Test Report No. 2254851/60 of December 1982 by Teknologisk Institute, Microbiologi, Taastrup, Denmark.		

Type	Ames test	
System of Testing	Salmonella typhimurium strains TA98 and TA97	
Concentr.	0, 10, 25, 50, 100, 250, and 500 microgram/plate	
Metabolic Activation	with and without	
Result	negative	
Method	OECD Guide-line 471	Year 1983
GLP	no	Testsubstance other TS
Remark	The study was carried out and reported with quality assurance and according to principles of GLP.	
Reference	4-chloro-2-methylphenol: Assessment of mutagenic potential in histidine auxotrophs of Salmonella typhimurium (the Ames Test). Mona-Lise Binderup, Institute of Toxicology report No. 08-3751-22, National Food Agency of Denmark, 1996.	

5.6 Genetic Toxicity in Vivo

Type	Micronucleus assay	
Species	mouse	
Strain	NMRI	Sex male/female
Route of Administration	gavage	
Exposure Period	24, 48, and 72 hours	
Doses	0 and 1600 mg/kg	
Method	OECD Guide-line 474	Year 1982
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4
Result	It is shown that the positive control increased the number of micronuclei significantly. In the 1600 mg/kg testsubstance groups sacrificed 24, 48, and 72 hours after dosing the number of micronuclei was significantly ($p < 0.0007$) increased over the negative control groups. Thus the results indicate that 4-chloro-o-methylphenol has some capacity to damage chromosomes.	
Reference	Scantox Report No. 10156 of 23th December 1982. Scantox, Denmark.	
Type	Micronucleus assay	
Species	mouse	
Strain		Sex male/female
Route of Administration	gavage	
Exposure Period	24 and 48 hours	
Doses	0, 100, 200 and 400 mg/kg bw	
Method	other: EEC B.12 (29 Dec.1992) and OECD 1996 guideline rev.	Year 1997
GLP	yes	Testsubstance as prescribed by 1.1 - 1.4
Result	Bone marrow samples were examined (1000 erythrocytes per smear) after 24 and 48 hours and did not show any substantial increase in the incidence of micronucleated immature erythrocytes or decrease in the proportion of immature erythrocytes. It was concluded that PCOC did not show any evidence of causing chromosome damage or bone marrow cell toxicity in this test.	

The positive control caused highly significant ($P < 0.001$) increase in the number of micronucleated immature erythrocytes at both 24 and 48 hours. Results for PCOC treated and control animals were within the

	expected range for unaffected mice based on published information and laboratory control data.
Test substance	The test substance 99.3% pure PCOC consisting of 50% of current production lots from each of the two UK producers was suspended in aqueous 0.5% gum tragacanth. OECD guideline revision (OECD1996) recommended use of aqueous suspending agents for poorly soluble substances.
Reference	Huntingdon 1997: PCOC mouse micronucleus test. Confidential report. Huntingdon Lab. England.

5.10 Other Relevant Information

Type	Metabolism
Remark	A rat metabolism study with MCPA performed at Hazleton lab. showed that PCOC was not a metabolite. It is therefore possible that the PCOC found in the Hattula et al. (1977) study (where a concentration of 47 to 31 ug/g in the liver of rats receiving 2-3 g/l MCPA in drinking water for three months was observed) was a contaminant of MCPA.
Reference	Jahanshahi J, Stow RA (1995): (14-C)-MCPA: Absorption, distribution, metabolism and excretion in the rat. Final report. Corning Hazleton, June 1995.

EXTRACT FROM IRPTC LEGAL FILES

file: 17.01 LEGAL rn : 522523

!!! WARNING - not original IRPTC record - WARNING !!!

systematic name: Phenol, 4-chloro-2-methyl-

common name : 4-chloro-O-cresol

reported name : 4-Chloro-2-methylphenol

cas no : 1570-64-5

rtecs no : G07120000

area : DEU

type : REG

```

-----
|subject|specification|descriptor|
|-----+-----+-----|
| AQ    |          | CLASS |
| USE   |  INDST  |  RQR  |
|-----+-----+-----|

```

This substance is classified as hazardous to water (Water Hazard Class: WHC 2). (There are 3 water hazard classes: WHC 3 = severely hazardous; WHC 2 = hazardous; WHC 1 = moderately hazardous; and the classification as "not hazardous to water"). The purpose of the classification is to identify the technical requirements of industrial plants which handle substances hazardous to water.

entry date: SEP 2001

effective date: 01JUN1999

title: Administrative Order relating to Substances Hazardous to Water
(Verwaltungsvorschrift wassergefahrdende Stoffe)

original : BUANZ*, Bundesanzeiger, 51 , 98a , 1 , 1999

file: 17.01 LEGAL rn : 600176

systematic name: Phenol, 4-chloro-2-methyl-

common name : 4-chloro-O-cresol

reported name : 4-Chloro-2-methyl phenol

cas no : 1570-64-5

rtecs no : G07120000

area : GBR

type : REC

```

-----
|subject|specification|descriptor|
|-----+-----+-----|
| AQ    |  METHD  |  RQR  |
|       |  DRINK  |       |
|-----+-----+-----|

```

Determines this substance in rivers, waters, sewage effluents and industrial effluents using the trimethyl-silylethers and gas chromatography.

entry date: MCH 1995

effective date: 1981

title: Phenols in Waters and Effluents by Gas Liquid Chromatography or 3-Methyl-2-benzothiazoline Hydrazone.

original : SCAA**, , , , , 1983

file: 17.01 LEGAL rn : 1403920

systematic name: Phenol, 4-chloro-2-methyl-

common name : 4-chloro-O-cresol

reported name : 4-Chloro-o-cresol

cas no : 1570-64-5

rtecs no : G07120000

area : EEC

type : REG

Classification: T; R23. C; R35. N; R50. - Labelling: T: Toxic; C: Corrosive; N: Dangerous for the environment. Risk phrases (R): 23-35-50. Toxic by inhalation (R23). - Causes severe burns (R35). - Very toxic to aquatic organisms (R50). Safety advice phrases (S): (1/2-)26-36/37/39-45-61. (Keep locked up and out of the reach of children (S1/2).) - In case of contact with eyes, rinse immediately with plenty of water and seek medical advice (S26). - Wear suitable protective clothing, gloves and eye/face protection (S36/37/39). - In case of accident or if you fell unwell, seek medical advice immediately (show label where possible) (S45). - Avoid release to the environment. Refer to special instructions/safety data sheets (S61). - For the classification of dangerous preparations special concentration limits are given for this substance.

entry date: OCT 2001

effective date: 24AUG2001

title: Council Directive of 27 June 1967 on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances (67/548/EEC)

original : OJECFC, Official Journal of the European Communities, 196 , ,
1 , 1967

amendment: OJECFC, Official Journal of the European Communities, L225 ,
, 1 , 2001