European Chemicals Bureau

Institute for Health and Consumer Protection

European Chemicals Bureau

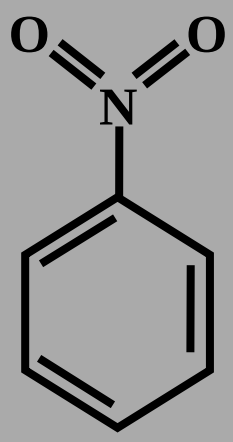
Existing Substances

European Union Risk Assessment Report

CAS No: 98-95-3

EINECS No: 202-716-0

nitrobenzene
Part I - environment



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The mission of the IHCP is to provide scientific support to the development and implementation of EU polices related to health and consumer protection. The IHCP carries out research to improve the understanding of potential health risks posed by chemical, physical and biological agents from various sources to which consumers are exposed.

The Toxicology and Chemical Substances Unit (TCS), commonly known as the European Chemicals Bureau (ECB), provides scientific and technical input and know-how to the conception, development, implementation and monitoring of EU policies on dangerous chemicals including the co-ordination of EU Risk Assessments. The aim of the legislative activity of the ECB is to ensure a high level of protection for workers, consumers and the environment against dangerous chemicals and to ensure the efficient functioning of the internal market on chemicals under the current Community legislation. It plays a major role in the implementation of REACH through development of technical guidance for industry and new chemicals agency and tools for chemical dossier registration (IUCLID5). The TCS Unit ensures the development of methodologies and software tools to support a systematic and harmonised assessment of chemicals addressed in a number of European directives and regulation on chemicals. The research and support activities of the TCS are executed in close co-operation with the relevant authorities of the EU Member States, Commission services (such as DG Environment and DG Enterprise), the chemical industry, the OECD and other international organisations.

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RISK ASSESSMENT

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RISK ASSESSMENT

Final Report, 2007

Germany

The rapporteur for the risk assessment of Nitrobenzene is Germany

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Date of Last Literature Search:	**1998**
Review of report by MS Technical Experts finalised:	**April 2005**
Final report:	**2007**

Foreword

We are pleased to present this Risk Assessment Report which is the result of in-depth work carried out by experts in one Member State, working in co-operation with their counterparts in the other Member States, the Commission Services, Industry and public interest groups.

The Risk Assessment was carried out in accordance with Council Regulation (EEC) 793/93[1] on the evaluation and control of the risks of "existing" substances. "Existing" substances are chemical substances in use within the European Community before September 1981 and listed in the European Inventory of Existing Commercial Chemical Substances. Regulation 793/93 provides a systematic framework for the evaluation of the risks to human health and the environment of these substances if they are produced or imported into the Community in volumes above 10 tonnes per year.

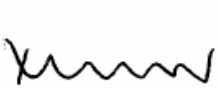
There are four overall stages in the Regulation for reducing the risks: data collection, priority setting, risk assessment and risk reduction. Data provided by Industry are used by Member States and the Commission services to determine the priority of the substances which need to be assessed. For each substance on a priority list, a Member State volunteers to act as "Rapporteur", undertaking the in-depth Risk Assessment and recommending a strategy to limit the risks of exposure to the substance, if necessary.

The methods for carrying out an in-depth Risk Assessment at Community level are laid down in Commission Regulation (EC) 1488/94[2], which is supported by a technical guidance document[3]. Normally, the "Rapporteur" and individual companies producing, importing and/or using the chemicals work closely together to develop a draft Risk Assessment Report, which is then presented at a Meeting of Member State technical experts for endorsement. The Risk Assessment Report is then peer-reviewed by the Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE) which gives its opinion to the European Commission on the quality of the risk assessment.

If a Risk Assessment Report concludes that measures to reduce the risks of exposure to the substances are needed, beyond any measures which may already be in place, the next step in the process is for the "Rapporteur" to develop a proposal for a strategy to limit those risks.

The Risk Assessment Report is also presented to the Organisation for Economic Co-operation and Development as a contribution to the Chapter 19, Agenda 21 goals for evaluating chemicals, agreed at the United Nations Conference on Environment and Development, held in Rio de Janeiro in 1992.

This Risk Assessment improves our knowledge about the risks to human health and the environment from exposure to chemicals. We hope you will agree that the results of this in-depth study and intensive co-operation will make a worthwhile contribution to the Community objective of reducing the overall risks from exposure to chemicals.



Roland Schenkel
Acting Director-General
DG Joint Research Centre

Catherine Day
Director-General
DG Environment

[1] O.J. No L 084, 05/04/1993 p.0001 – 0075

[2] O.J. No L 161, 29/06/1994 p. 0003 – 0011

[3] Technical Guidance Document, Part I – V, ISBN 92-827-801 [1234]

0 OVERALL RESULTS OF THE RISK ASSESSMENT

CAS Number: 98-95-3
EINECS Number: 202-716-0
IUPAC Name: Nitrobenzene

Environment

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

No **conclusion (iii)** was drawn.

Conclusion (i) There is a need for further information and/or testing.

No **conclusion (i)** was drawn

Conclusion (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.

Conclusion (ii) applies to surface water, sediment, the atmosphere and the terrestrial compartment for the production and/or processing of nitrobenzene. All PEC/PNEC ratios are below 1. This conclusion also applies to the industrial WWTPs of all sites.

Human health

(to be added later).

CONTENTS

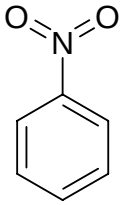
Euses Calculations can be viewed as part of the report at the website of the European Chemicals Bureau: http://ecb.jrc.it

TABLES

1 GENERAL SUBSTANCE INFORMATION

1.1 IDENTIFICATION OF THE SUBSTANCE

CAS No:	98-95-3
EINECS No:	202-716-0
IUPAC-Name:	nitrobenzene
Synonyms:	Nitrobenzol, Benzene, Nitro-Essence of Mirbane; Essence of Myrbane, Mirbane Oil; Myrbane Oil, Mononitrobenzene
Molecular formula:	$C_6 H_5 N O_2$
Molecular weight:	123 g/mol
Structural formula:	



1.2 PURITY/IMPURITIES, ADDITIVES

Purity: > 98.9%

Impurities: Benzene
o-Nitrotoluene
p-Nitrotoluene
p-Dinitrobenzene
m-Dintirobenzene
o-Dinitrobenzene
Toluene
Water

1.3 PHYSICO-CHEMICAL PROPERTIES

Table 1.1 Summary of physico-chemical properties

Property	Value	Reference
Physical state	liquid	
Melting point	5.26°C	BASF AG (1986)
Boiling point	210.8°C	Lide (1991)
Relative density	1.2037	Lide (1991)
Vapour pressure	0.2 hPa at 20°C[1)] 32.6 Pa at 25°C[1)]	Auer (1988) Daubert and Danner, 1989
Water solubility	1,900 mg/l at 20°C [2)]	Bayer AG (1998)
Partition coefficient n-octanol/water (log value)	1.86 at 24.5°C [3)]	BASF AG (1987)
Granulometry		
Conversion factors		
Flash point	88°C	BAM (1997)
Autoflammability	480°C (DIN 51794)	BAM (1997)
Flammability	Not extremely flammable Not highly flammable Not flammable [4)]	BAM (1997)
Explosive properties	No explosive properties	BAM (1997)
Oxidizing properties	Not applicable (liquid)	
Viscosity		
Henry's constant	1.296 Pa·m^3·mol^{-1} at 20°C 2.16 Pa·m^3·mol^{-1} at 25°C [5)]	calculated
Surface tension	43.9 mN/m at 20°C (pure substance)	Lide (1991)

1) The vapour pressure of 0.2 hPa at 20°C was confirmed by entries in safety data sheets of various companies. US EPA confirmed also this value (http://www.who.int/pcs/ehc/full-text/ehc230/part_I.pdf). Daubert and Danner present an experimental vapour pressure as 0.245 mm Hg equivalent to 32.6 Pa at 25ºC (Daubert and Danner 1989).
2) The flask method was used for the determination of the water solubility. In the safety data sheets of Bayer and Hoechst a water solubility of 2.0 g/l at 20°C is cited. No information about the purity of the test substance, the test method and the test conditions are available. Therefore the water solubility of 1.9 g/l at 20°C (pH 6.5) is recommended for the risk assessment.
3) The shaking flask method was used for the determination of the partition coefficient n-octanol/water. The calculation according to Leo and Hansch resulted in a logPow of 1.81. For the risk assessment the experimental value is preferred.
4) The tests according to A.12 and A.13 were not conducted. Due to the properties and the handling of the substance it has not to be assumed that flammable gases format in contact with water or the substance has pyrophoric properties.
5) The Henry law constant is based on the Water solubility-Vapour Pressure Method. Calculation models (both bond and group method) always assume an idealized form of a substance and therefore an experimental determination should be preferred. An experimental Henry's Law constant of $2.4 \cdot 10^{-5}$ atm · m^3/mol at 25ºC exists (Warner et al. 1987) but this value is higher than expected with respect to a temperature difference of 5°C.The data presented in this Draft Risk Assessment Report do not support the current classification as N R51-53. According to this data the current classification should be changed from N R51-53 to R52-53

1.3.1 Current classification

For the environment nitrobenzene is classified with N; R51-53 (had been included in the 22nd ATP).

The current classification is T, N; R 23/24/25-48/23/24-40-62-51/53.

1.3.2 Proposed classification

The data presented in this Draft Risk Assessment Report do not support the current classification as N R51-53. According to this data the current classification should be changed from N R51-53 to R52-53.

2 GENERAL INFORMATION ON EXPOSURE

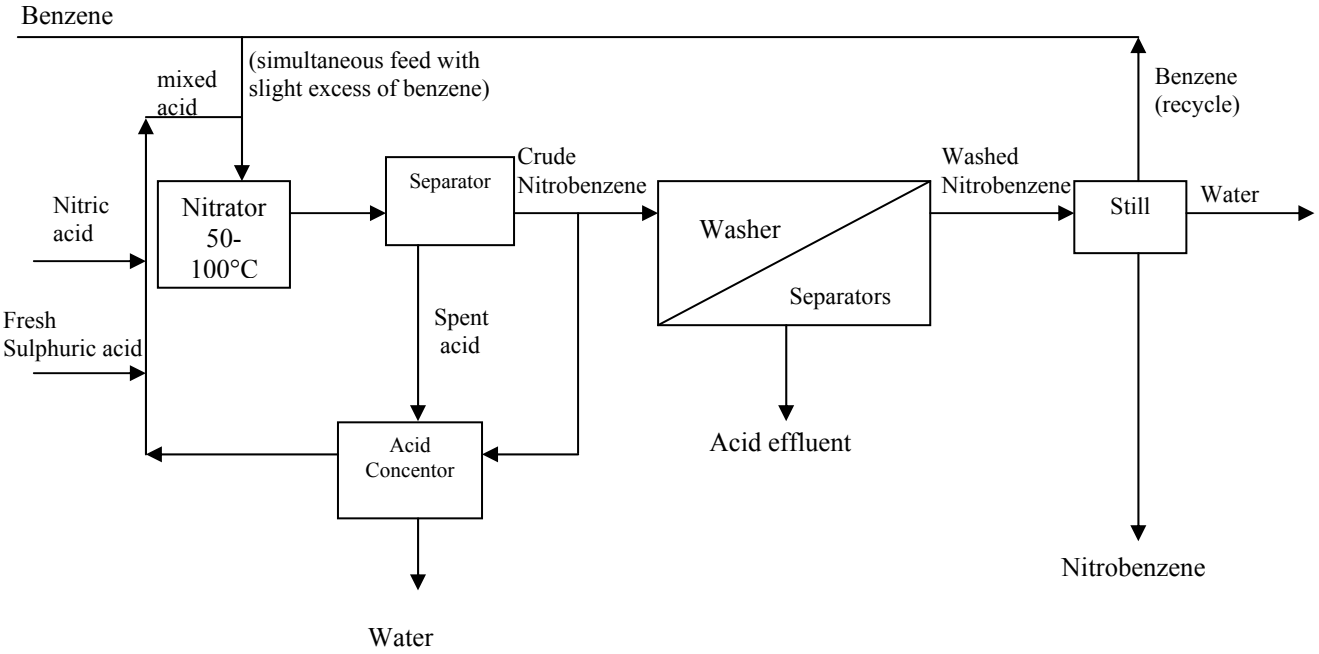
2.1 PRODUCTION

There is no natural source of nitrobenzene known. However, nitrobenzene may be formed by OH-initiated photooxidation of benzene which could theoretically be of natural origin. This possible source is not considered to be significant. Nitrobenzene is almost exclusively produced by nitration of benzene. Nitrobenzene is mainly used as an intermediate in the manufacture of aniline.

2.1.1 Production processes

Nitrobenzene is produced by nitration of benzene with nitrating acid, which is a mixture of nitric acid, sulphuric acid and water. It is usually performed continuously in stirred-vessel cascades or in loop-type reactors. Clean-up of the reaction mixture takes place in static separators or in centrifuges. The organic phase is washed with water, dilute alkali and then with water again to free it from acid and by-products containing hydroxyl groups. The washed nitrobenzene is then freed from un-nitrated components, such as benzene, by steam stripping. Finally, it is dried by azeotropic distillation. Spent acid is continuously concentrated and reintroduced to the cycle. Also fresh acid is added.

Figure 2.1 Production of nitrobenzene – continuous process (Ullmann´s Encyclopedia of Industrial Chemicals, 1995).



2.1.2 Production capacity

According to available data there are 8 production and/or processing sites of nitrobenzene within the EU. The data are based on company information for the year 2000, except for one site which refers to 2002. Taking into account these actual statements, the resultant quantity of nitrobenzene produced in the EU amounts to be $1.18 \cdot 10^6$ tonnes/year.

2.2 USES

2.2.1 Introduction

Almost all nitrobenzene is primarily used for the production of aniline and, to a much lesser extent, for the production of pharmaceuticals and various other chemicals. According to new exposure data from IND nitrobenzene is no longer used as a solvent.

Table 2.1 Use pattern

Type of use	Tonnage [tonnes/annum]	Appr. % in this application*
Processing to aniline	1,162,900	99
Processing to pharmaceuticals	9,300	0.8
Processing to other chemicals	2,800	0.2
Total	1,175,000	100

* These figures refer to the company information given in this report

There is a difference of about 5,000 tonnes/annum between production and processing which amounts only to around 0.42% of the total production volume. It could not be clarified whether this amount is further used at all and if so for which application it might be used. There is no evidence that this missing tonnage in the mass balance is actually further processed and it is hence considered to be due to inaccuracies in estimates rather than due to a missing tonnage as it amounts It is not known that any quantities of nitrobenzene are imported from outside the EU or exported into it.

In Germany nitrobenzene was used for perfuming soaps in the past as the so called Mirbanoil. However, the use of nitrobenzene in cosmetic products has been forbidden in Germany since the 1980s. (Cosmetic Regulation from 19th June 1985). No information is available whether nitrobenzene is or was used in soaps in other EU countries than Germany and whether this possible use has maybe been discontinued in other EU countries.

There are a number of sources that indicate nitrobenzene may be present as a solvent in floor/furniture polishes, shoe polish and some paints[1,2,3]. But these sources seem not to be relevant for Europe.

1 http://www.epa.gov/seahome/housewaste/house/nitroben.htm
2 http://www.arb.ca.gov/toxics/tac/factshts/nitroben.pdf
3 Environmental Hazard Assessment: Nitrobenzene. TSD/24, Toxic Substances Division, Department of the En vironment, 1996

The substance is further subject to annual emissions reporting requirements for the Pollution Inventory in the UK. According to the Pollution Inventory fact sheet, nitrobenzene is also used in small amounts to make explosives, aniline dyes and pesticides.

The content of nitrobenzene in different products is listed in the Danish Product Register. In 2003 nitrobenzene was present in 23 adhesive or binding products and reprographic agents in a range of 0-2% with an approximate quantity of less than 1 tonne/year. These products might be used by professionals or consumers.

The Rapporteur has no information on any of these uses in Europe at present. It can be assumed that they are of historical relevance only and that they can be neglected in the Risk Assessment Report.

This assumption is supported by the SPIN database where in the year 2001 nitrobenzene was only present in 41 products in Denmark (reprographic agents) but with an amount of 0 tonnes/year. In Sweden, Norway or Finland no nitrobenzene containing products were listed at this time.

2.2.2 Scenarios

According to the information given by the companies 99% of the produced nitrobenzene is used for the production of aniline. Another 1% is processed to pharmaceuticals and other chemicals.

Table 2.2 Main, industrial and use category according to the TGD

	Main category	Industry category	Use category	Percentage of total use
Production	Non-dispersive use 1b	Chemical industry: chemicals used in synthesis (3)	Intermediate (33)	100
Processing: Production to aniline and various other chemicals	Non-dispersive use 3	Chemical industry: chemicals used in synthesis (3)	Intermediate (33) Oxidizer (37)	100

2.3 TRENDS

There is no data available.

2.4 LEGISLATIVE CONTROLS

In Germany the use of nitrobenzene in cosmetic products has been forbidden since the 1980s by the Cosmetic Regulation from 19th June 1985.

Industrial releases of nitrobenzene in the UK are controlled under the Pollution Prevention and Control (PPC) Regulation 2000, which implement EC Directive 96/61 on Integrated Pollution Prevention and Control.

Nitrobenzene is on the List of potential Substances of Concern to be considered by HELCOM, but not as a substance for which immediate priority action is necessary. It is on the

Reference List of Substances agreed by the Third and Fourth North Sea Conference (e.g. Annex 1D to The Hague Declaration), for further selection of priority substances.

Nitrobenzene is not on the OSPAR list of substances of possible concern.

Nitrobenzene is a Volatile Organic Compound (VOC) according to the Solvents Emissions Directive 1999/13/EC but its uses do not fall under the categories of activity referred to in Article 1.

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

3.1.1 General discussion

Nitrobenzene is industrially produced on a large scale and primarily manufactured to aniline. Other smaller applications are the use as an intermediate for the production of other various chemicals and pharmaceuticals.

3.1.2 Environmental releases

Releases of nitrobenzene into the environment are to be expected during production and processing with waste water and, to a lesser extend, exhaust gases.

Further emissions to air are expected from waste water treatment plants.

Direct releases to agricultural or natural soil were not identified.

A further source of nitrobenzene may be its formation in the atmosphere by the OH-initiated photooxidation of benzene (Rogozen MB, Rich HE and Guttmann MA, 1987). The quantification of the amount of nitrobenzene formed in the atmosphere is not possible and is not considered within the scope of this risk assessment.

3.1.2.1 Release from production

Nitrobenzene is produced by nitration of benzene with nitrating acid, which is a mixture of nitric acid, sulphuric acid and water.

Within the EU there are 8 sites where production and/or processing takes place. The total production volume is $1.18 \cdot 10^6$ tonnes of nitrobenzene/year. According to the information given by the companies 99% of the produced nitrobenzene is used for the production of aniline and another 1% is processed to pharmaceuticals and other chemicals.

Processing of nitrobenzene takes place on site at 5 production sites, respectively. About 50,000 tonnes/year are processed at external sites.

The highest production volume on a single site is about 380,000 tonnes/year. Companies, where nitrobenzene is processed only, buy it from production companies within the EU. It is not known of any quantities of nitrobenzene imported from outside of the EU or exported to it. All these data refer to the year 2000.

3.1.2.2 Release from formulation

No formulation takes place.

3.1.2.3 Release from private use

No releases of nitrobenzene from private use are to be expected.

3.1.2.4 Release from disposal

As almost all nitrobenzene is used as an intermediate in the production of aniline and various other chemicals no release from disposal is expected.

3.1.2.5 Summary of releases

Releases of nitrobenzene into the environment occur during production and processing via waste water and, to a lesser extend, exhaust gases. Further emissions to air are expected from waste water treatment plants.

Direct releases to agricultural or natural soil are not expected.

3.1.3 Environmental fate

Using the distribution model according to Mackay (level 1) results in the following theoretical distribution figures:

Table 3.1 Level I environmental partitioning of nitrobenzene

Compartment	Percentage
Air	30.7
Water	68.5
Soil	0.39
Sediment	0.40

The hydrosphere, followed by the atmosphere is therefore the target compartments for nitrobenzene in the environment.

3.1.3.1 Degradation in the environment

3.1.3.1.1 Atmospheric degradation

Direct Photolysis

The direct photolysis behaviour of nitrobenzene in air was examined by Freitag et al. (1982). Nitrobenzene, which is adsorbed on silica gel (60 ng/g silica gel), was irradiated with a high pressure mercury lamp at 290 nm, which can be considered as environmentally relevant. After 17 hours 6.7% were mineralised to carbon dioxide. This result indicates that direct photolysis is not an important degradation pathway for nitrobenzene.

Nitrobenzene shows a broad absorption maximum at 260 nm and absorbs UV-light up to 400 nm. When nitrobenzene is irradiated with light in the wavelength of 260 nm the primary reaction products are nitrosobenzene and p-nitrophenol (Hastings and Matsen, 1948). Since the sunlight on earth contains only a very small amount of irradiation with a wavelength of 260 nm this reaction has no relevance for the environment.

Both o-and p-nitrophenol were found when irradiating nitrobenzene for 5 hours at 25-30°C with a xenon lamp ($\lambda > 300$ nm) in the presence of O_2, whereas phenol was also found when O_2 was absent (Nojima and Kanno, 1977). The authors state that 38% of the initial nitrobenzene was degraded within 5 hours. But these figure was obtained by extracting the residue in the reaction vessel with methanol after the reaction and subsequent analysis of the extract. So only the residue which was adsorbed to the vessel sides was recorded. This result is therefore not considered to be valid.

Photooxidation in the Troposphere

The photo-reaction of nitrobenzene with hydroxyl radicals or ozone in the troposphere was also examined by Atkinson et al. (1987). In order to investigate the reaction with OH-radicals nitrobenzene (0.005 mg/l at 23°C) was irradiated in a Teflon-chamber with a Xenon lamp (λ>290 nm). No information is given about the reaction time. In this experimental system no decay of nitrobenzene was observed outside of the analytical uncertainties. Hence, the upper limit of the reaction rate constant was determined to be $7 \cdot 10^{-13}$ $cm^3/(molecules \cdot sec)$. Given an OH-concentration of $5 \cdot 10^5$ $molecules \cdot cm^{-3}$ this leads to an atmospheric half-life of more than 23 days.

Further investigations resulted in half-lives of 62 to 100 days (Zetzsch, 1982) based on a rate constant of $(0.21 \pm 0.05) \cdot 10^{-12}$ $cm^3/(molecules \cdot sec)$, 115-125 days (Witte et al., 1986) based on a rate constant of $(1.32 \pm 0.07) \cdot 10^{-13}$ $cm^3/(molecules \cdot sec)$ and 107 days (Becker et al., 1984) based on a rate constant of $0.15 \cdot 10^{-12}$ $cm^3/(molecules \cdot sec)$. An OH-concentration of $5 \cdot 10^5$ $molecules \cdot cm^{-3}$ was used to calculate these half-lives.

Calculation of the reaction rate constant and the half-life of nitrobenzene in air with the AOP v.1.9-model, using a hydroxyl radical concentration of $5 \cdot 10^5$ $molecules \cdot cm^{-3}$, results in a reaction rate constant of $2.44 \cdot 10^{-13}$ $cm^3 \cdot molec.^{-1} \cdot s^{-1}$ and a half-life of 65.8 days ($kdeg_{air}=1.06 \cdot 10^{-2}$ d^{-1}). For calculation see **Appendix F**. This value is within the range of the experimentally determined half-lives and is used in the further calculations.

3.1.3.1.2 Aquatic degradation (incl. sediment)

Aerobic biodegradation in waste water treatment plants

The biodegradability of nitrobenzene has been investigated in some standard tests on ready biogradability and in similar test configurations as well.

In a MITI I test (OECD 301C) (CITI, 1992) nitrobenzene at a concentration of 100 mg/l was tested with an inoculum (30 mg/l) containing activated sludge from a municipal sewage plant and 10 samples from 10 different sites in Japan. A degradation of 3.3% related to BOD after an incubation of 14 days has been measured.

In another standard test the biodegradability of nitrobenzene was studied according to the modified OECD screening test (OECD 301E) (BASF AG, 1989a). At a nitrobenzene concentration of 38.5 mg/l an elimination of 100% related to DOC after 21 days was measured, but in the physico-chemical batch an elimination of 88% has also been determined. Because nitrobenzene is not likely to adsorb to organic matter it can be assumed that it evaporated in this test system and that this test is consequently not appropriate for testing semi-volatile substances.

In a manometric respirometry test (similar to OECD 301F) (BASF AG, 1989c) two test concentrations were tested, 60 and 120 mg/l. Concerning the test concentration of 120 mg/l there is conflicting information. The text of the test description stated that the concentration is 120 mg/l whereas the marking of the diagram says 100 mg/l. At a concentration of 60 mg/l a biodegradation rate of 48% related to BOD after an incubation of 35 days has been determined. The lag phase was 25 days. At the higher test concentration 5 parallel assays were run and the biodegradation rate varied between 0 and 16% related to BOD. Only few experimental details are given in the report. Due to the long lag phase it can be concluded that adaptation has taken place. In fact this study cannot be considered valid but it confirms the prediction from the other studies that nitrobenzene is not readily biodegradable.

In a study on ready biodegradability (Gomólka and Gomólka, 1979) using a Warburg respirometry test system, it was shown that at initial concentrations up to 300 mg/l, nitrobenzene was degraded slowly. 33% related to BOD were degraded by day 14 at an initial concentration of 100 mg/l test substance with biodegradation starting after 90 hours lag time. At an initial dosage of 300 mg/l 30% were degraded after 10 days. At this concentration nitrobenzene slowly dissolves in water so nitrobenzene concentration increases during the first 80 hours. After that the concentration declines. At an initial concentration of 1,400 mg/l the nitrobenzene concentration increased at first due to slow solution in water. No decrease and no elimination of nitrobenzene were reported. The authors state that at concentrations above 1,000 mg/l micro-organisms are inhibited.

Nitrobenzene at a concentration of 100 mg/l was only degraded to 10% related to BOD after 10 days of incubation with domestic activated sludge in an electrolytic respirometer system similar to the MITI procedures (Urano and Kato, 1986). BOD, DOC and biomass were monitored, whereas no substance-specific analytic procedure was performed.

It can be concluded that nitrobenzene is not readily biodegradable.

A test on inherent biodegradation according to a modified Zahn-Wellens test system (OECD 302B), (BASF AG, 1989b) was conducted using activated sludge from an industrial waste water treatment plant (WWTP), that has to be regarded as adapted to nitrobenzene. The test batch with a nitrobenzene concentration of 221 mg/l shows 86% elimination after 10 days whereas in the physico-chemical control (without inoculum) using the same nitrobenzene concentration, 79% were eliminated by day 10. It can be assumed that a removal through evaporation may have taken place. The test system has not to be considered valid because of the high removal rate in the physico-chemical batch. Nitrobenzene is therefore not biodegradable in this test.

In a Sapromat respirometric test system with an inoculum originating from industrial adapted activated sludge nitrobenzene concentrations between 5.4 mg/l to 541.5 mg/l were tested. The test period lasted for 28 days and nitrobenzene was the only carbon source. The inoculum concentration was 200 mg/l (BASF AG, 1985). The biodegradation ranged between 34% at a

concentration of 54 mg/l and 1,600% at 5.4 mg/l. At 180 mg/l nitrobenzene was degraded to approximately 50% after 12 days. No further degradation was observed after that day. At concentrations 18 mg/l and 541 mg/l no biodegradation was observed. All biodegradation data are related to BOD. No explanations are given for these inconsistencies. As the results are so extremely contradictory they have only a restricted reliability.

In a modified OECD-Confirmatory test (OECD 303 A) (BASF AG, 1984) nitrobenzene concentrations between 0.1 and 10.5 mg/l have been added to a bench scale WWTP with sewage cultivated in bench scale treatment systems over a period of 4 months. The system was designed to simulate conditions in waste water treatment plants featuring activation basins and sludge recycled from clarifiers. During the first phase (35 days) a nitrobenzene concentration of 3 mg/l had been maintained in the influent of the bench scale WWTP. In the second phase which lasted for 7 days it was maintained at 10 mg/l. The authors stated that 23 days elapsed between starting the test and complete elimination of nitrobenzene in the effluent. However, elimination rates of 72-93% were already recorded during this period of adaptation. After the adaptation period a feed concentration of 3.5 mg nitrobenzene/l was totally eliminated in one day and 10 mg/l within 3 days. Inhibitors in the form of 1 to 3 mg/l hydroxylamine and 3 to 6 mg/l potassium cyanide did not impair the elimination efficiency. Interrupting the addition of nitrobenzene for seven to nine days and then restarting it, showed that the activated sludge was still able to totally eliminate nitrobenzene after a lag phase of two days after this pause. It can be recorded that even if nitrobenzene was mostly eliminated by 100% there are considerable fluctuations in the elimination behaviour (20-100%) independent of the tested concentration. Mere primary degradation has taken place as only nitrobenzene concentrations were measured in the effluent. It is unclear whether the losses are due to real biodegradation or to volatilisation and/or adsorption, so the biodegradation rates cannot be explicitly determined. Evaporation might play an important role. The fact that the inhibitors did not affect adversely the elimination of nitrobenzene confirms this.

The biodegradation rates are more or less in accordance with monitoring results from an adapted industrial activated sludge treatment plant. Within a period of 7 months over 90% of nitrobenzene were eliminated most of the time. However, at some sampling days the elimination rate was significantly lower, sometimes only 34% (BASF AG, 1983). Reasons for these fluctuations are not known. Maybe they were due to toxic effects of nitrobenzene to microorganisms.

Gomólka (1979) investigated the biological degradation of nitrobenzene in a two stage bench-scale waste water treatment plant. In this pilot plant nitrobenzene concentrations were determined by spectrophotometry at 252 nm and hence the elimination rates are based on the parent substance. The first stage of the WWTP (activated sludge was prior adapted to pyridine) received increasing nitrobenzene concentrations from 5 to 60 mg/l during a first step. The elimination ranged from 98.6–100% after 22 days. At a concentration of 60 mg/l, the elimination was 89.4%. The influent concentrations of the secondary reactor were lower (2.5-33.5 mg/l) and elimination rates of 88.8% (at 60 mg/l) to 98.1% (at 10 mg/l) were found. In these tests it could not be clarified, whether the high removal rates of nitrobenzene were due to its biodegradation or to evaporation resulting from the intensive aeration of the wastewater in a system open to the atmosphere.

An increasing degradation capacity after a stepwise adaptation to increasing nitrobenzene concentrations was also observed by the same authors (Gomólka and Gomólka, 1979) in a Warburg respirometry test system. The maximum concentration of 300 mg was decomposed

to < 0.1 mg/l within 3 days. The sludge inoculum originated from the above mentioned two stage bench-scale pilot plant system.

Nitrobenzene removal and fate has been furthermore determined in pilot-scale activated sludge systems in two separate studies, one with nitrobenzene concentrations of about 0.13 mg/l and the other with about 0.45 mg/l (Bhattacharya et al., 1989). These treatment systems both consisted of primary clarification followed by conventional plug flow activated sludge treatment and sedimentation. In each study two pilot-scale activated sludge systems (sludge retention time was 4 days for 0.4473 mg/l and 8 days for 0.129 mg/l) were operated in parallel. One system was continuously fed with sewage spiked by nitrobenzene at concentrations of 0.129 mg/l and 0.4473 mg/l, respectively ("acclimated biomass"), the other one was fed intermittently 24 hours with sewage spiked by nitrobenzene (at the same nominal concentration as in the continuously fed assay) followed by 24 days without nitrobenzene spiking („unacclimated biomass"). Mass balances were carried out. However, special problems have been encountered with the analytical procedures, so recovery rates could not be determined and variations in results are high. Nitrobenzene concentrations were detected with GC/MS, so only primary biodegradation was measured. Air emission sampling was reported to be performed in the study with 0.13 mg nitrobenzene/l but no results on air concentrations are listed in the study report. In the study with 0.45 mg /l no air emissions were measured.

Table 3.2 Nitrobenzene elimination in two bench scale pilot plants (Bhattacharya et al., 1989)

	Continuous feed system		Intermittent feed system	
initial concentration [mg/l]	0.129	0.4473	0.129	0.4473
elimination [%]	93 ± 6	91.3 ± 3.4	73 ± 13	50 ±18

It can be seen, that the elimination in the acclimated system was significantly higher. This result is in good accordance with the outcomes of the other studies which show that adapted microorganisms have the ability to biodegrade nitrobenzene. Although nitrobenzene is only a semi-volatile substance, evaporation seems to have taken place in several of the biodegradation studies. As in this study no results on air emissions are available, it is unclear how much of the nitrobenzene evaporated. Results can therefore only be declared as elimination and not primary degradation. Adsorption to sludge turned out only to be 1-2% in both studies.

The elimination of nitrobenzene in a complete-mix, bench-scale, continuous-flow activated sludge reactor was also examined (Stover and Kincannon, 1982). The reactor was fitted with stainless steel covers to facilitate off-gas analysis. Nitrobenzene was added to synthetic waste water containing ethylene glycol, ethyl alcohol, glucose, glutamic acid, acetic acid, phenol, ammonium sulphate, phosphoric acid and salts. Activated sludge from a municipal activated sludge sewage treatment plant was acclimated to the nitrobenzene-containing waste water and then used as inoculum. The hydraulic retention time was 8 hours. Mean cell residence times of the activated sludge system were 2, 4 and 6 days. Over a period of 60 days elimination of nitrobenzene was measured by GC analysis. With an influent concentration of 100 mg/l the nitrobenzene concentration was reduced by 76% (sludge age: 2 days) and by 97.8% (sludge age: 6 days). 0% of nitrobenzene were found to be stripped from the test system. BOD_5, COD and TOC of the synthetic waste water were also measured over a period of 60 days. With a sludge age of 6 days the BOD_5 was reduced by 99.6%, COD by 95.7% and TOC by 90%.

Biodegradation in surface water

Biodegradability of several organic compounds in river and sea water was tested by Kondo et al. (1988b). The test chemical was added to a mixture of river or sea water from an unpolluted area and an autoclaved solution of 0.2% peptone (and 3% NaCl for sea water) in a test tube with a tight plug. The test tubes were incubated in the dark at 30°C. After 3 days of incubation a primary degradation of nitrobenzene of 0% were found in river water and of 13% in sea water (Kondo et al., 1988a). According to the classification of Kondo nitrobenzene has to be considered as to be of "hard degradability". No information was given on the analytical method.

Anaerobic Biodegradation

The anaerobic biodegradation behaviour of nitrobenzene was examined (Kameya et al., 1995). Nitrobenzene (30 mg C/l) with glucose and glutamic acid as a coexistent organic medium (15 mg C/l each) had been incubated for 28 days. After every week a sample was analysed. DOC-decrease is taken as parameter for biodegradation and 33% nitrobenzene were degraded after 28 days.

The anaerobic degradation rates and toxic effects of nitrobenzene on acetate utilizing methanogens were investigated (Bhattacharya et al., 1996). An acetate enrichment culture in combination with a nutrient solution and yeast extract with stable gas production was spiked with nitrobenzene. Acetic acid was added daily. 10 mg/l of nitrobenzene did not inhibit total gas production in the acetate enrichment methanogenic culture. 20 and 30 mg/l both caused reversible inhibition of methanogenesis. Nitrobenzene was analysed by HPLC. As a result of the anaerobic degradation study 90% of the nitrobenzene in the presence of the acetate enrichment culture was eliminated within 6 days. The initial nitrobenzene concentration was 20 mg/l. But control samples showed that 45% of the elimination was due to abiotic processes. No nitrobenzene was detected in the extracted samples from solids in the methanogenic systems. This indicates that primarily biodegradation of nitrobenzene (45%) in the methanogenic system has taken place.

In another study (Dickel et al., 1993) biodegradation of nitrobenzene by a sequential anaerobic-aerobic process was investigated. Increasing nitrobenzene concentrations (98-678 mg/l) in a 20 mmol/l glucose solution were pumped through a closed fixed–bed column filled with glass beads which were inoculated with anaerobic sewage sludge. Adaptation to the increasing nitrobenzene concentrations took place in 4 weeks during which the concentration was steadily raised. Nitrobenzene and its reduction product aniline were monitored analytically. At concentrations up to 344 mg/l nitrobenzene was completely converted to aniline and no nitrobenzene was detected in the effluent of the column (retention time: 2 days). At the highest concentration tested 7% nitrobenzene were found in the effluent of the column and 78% were recovered as aniline. A control experiment without inoculum under the same conditions, however, showed no chemical reduction of nitrobenzene. After the anaerobic treatment of nitrobenzene the formed aniline was metabolised by aerobic microorganisms in a subsequent aeration tank.

Bacterial strains of *Methanococcus* sp. were tested under anaerobic conditions during static incubation at a nitrobenzene concentration of 61.6 mg/l (Boopathy, 1994). An elimination of 65% was achieved after 20 days under formation of aniline. This elimination may be biologically mediated as without inoculum or after inactivation by heating, no elimination of nitrobenzene occurred.

Hydrolysis

No investigations are available with regard to the hydrolytic degradation behaviour of nitrobenzene. However, the substance category of the aromatic nitro compounds is generally resistant to hydrolysis (Harris JC, 1990), so that nitrobenzene is not expected to hydrolyse under environmental conditions.

Photodegradation

In principle there are two pathways of nitrobenzene degradation in the hydrosphere, the direct photolysis and the photo oxidation by hydroxyl radicals.

In view of the poor biodegradability and the stability to hydrolysis, photolysis may be the only relevant degradation pathway for nitrobenzene in the hydrosphere even if it only occurs in the upper layer of the water.

Direct photolysis in water was studied both in distilled water and in the presence of humic substances (Simmons and Zepp, 1986). Firstly, a very diluted aqueous nitrobenzene solution (0.00001 mol/l distilled water) at pH 5.5 was exposed to irradiation with a wavelength of 313 nm. No specific information on exposure time is available. It is only stated that the exposure times varied depending on which nitroaromatic was tested, but achieving approximately 30% reaction for each exposure. For nitrobenzene a half-life of 133 days was calculated from the direct photolysis constant of $5.2 \cdot 10^{-3}$ d^{-1}. Then the influence of humic substances on photoreactions were determined by comparing results in humus-containing water (13.6 mg C/l) with those in distilled water. In contrast to most of the examined nitroaromatic compounds, which showed enhanced photolysis rates, nitrobenzene was hardly affected by the presence of humic substances.

Nitrobenzene in the upper layers of the water can also undergo photochemical reactions with OH-radicals (Anbar et al., 1966). A rate constant of $2.0 \cdot 10^{9}$ l/(mol·sec) was experimentally determined and a half-life of 40-400 days was calculated depending on the concentration of OH-radicals which is given as 10^{-16}-10^{-17} mol/l in this study. Only few data are given, so that the result has to be treated with caution.

A rate constant of $3.2 \cdot 10^{9}$ l/(mol·sec) was determined (Neta and Dorfman, 1968) and half-lives of 25-250 days were calculated, again depending on the varying concentrations of OH-radicals (10^{-16}-10^{-17} mol/l). The nitrobenzene concentration tested was 0.0005 mol/l, the pH was 7.

The nitrate-induced photooxidation of trace organic chemicals in water was examined (Zepp et al., 1987). 1 µmol/l nitrobenzene, 4,000 µmol/l nitrate and 1-octanol in an aqueous phosphate buffer at pH 6.2 were irradiated in a merry-go-round reactor at 313 nm for about 5-6 hours. After irradiation the solution was analysed by HPLC and it was found that 63% nitrobenzene were degraded. The OH-radical concentration was not reported.

Biodegradation in sediment (aquifer microcosms)

During incubation of nitrobenzene in an aquifer system (groundwater plus fine material of sediment) no biodegradation was observed during the exposure period of 150 days. The incubation was performed at 10°C in the dark in a slowly rotating box with aeration taking place (minimum oxygen concentration 9 mg/l). The test substance was monitored by GC-FID and GC-ECD, the initial concentration was 0.15 mg/l (Nielsen et al., 1996).

In an earlier study performed by the same author (Nielsen and Christensen, 1994) sediment and groundwater were incubated with a mixture of organic compounds containing nitrobenzene at a concentration of 0.15 mg/l. After a lag phase of 70 days nitrobenzene was primarily degraded by 100% within 20 days in only 2 out of 16 experiments. No degradation took place in the other experiments. No explanation for this inconsistency is given. These results are considered not valid, however they confirm that nitrobenzene is persistent under environmental conditions.

20% primary degradation of nitrobenzene in an aquifer test system with an initial concentration of 0.1 mg/l were found after 50 days (Albrechtsen et al., 1997). Again a mixture of chemicals was tested. This time a control sample was examined. The decrease of nitrobenzene in this control was 15%. Hence the loss of nitrobenzene was mainly due to abiotic elimination processes such as evaporation.

It is not possible to derive a degradation rate constant for the sediment. All that can be said is that nitrobenzene in sediment is not biodegradable in the tests described above.

3.1.3.1.3 Degradation in soil

Aerobic soil micro-organisms have been tested for their potency to degrade nitrobenzene during incubation in soil columns (Kincannon and Lin, 1985). Nitrobenzene as a component of different types of waste sludge was given to different types of soil. The origin and composition of these different types of sludge were not further specified. A column filled with sandy loam soil was loaded with DAF sludge (an industrial waste not further described). The nitrobenzene concentration dropped from 2,400 mg/kg soil to 800 mg/kg within 97 days (67% elimination). Another sandy loam soil column was loaded with slop oil sludge and the nitrobenzene concentration dropped by 98% within 76 days (from 2,746 mg/kg to 54 mg/kg). In silt loam soil, loaded with wood preserving sludge the nitrobenzene degradation was 87% (from 393 mg/kg to 54 mg/kg) within 78 days and started at day 151. Nitrobenzene was monitored by gas chromatography of extracts of treated soils. In a sterilised control assay a nitrobenzene concentration of 122 mg/kg soil dropped to 19 mg/kg within 21 days (84% removal). It can be assumed that the loss is due to volatilisation.

To simulate a rapid infiltration land treatment system for wastewater microcosms were used (Piwoni et al., 1986). The microcosms consisted of 1.5 metre soil columns filled with a fine sandy soil with sampling ports at various depths. The top of the column was closed in a ‘green house’ and air was replaced every 8 minutes. Nitrobenzene containing wastewater was added to the soil during a 12 week acclimatisation period. After that the columns received wastewater containing nitrobenzene at a concentration of 271 µg/litre each day (every 4 hours at a dosage of 4.4 ± 0.17 cm^3/day). The water samples were analysed by extraction and GC-analysis. As a result, only less than 0.1% of the nitrobenzene volatilised from the column and less than 0.1% were found in the final effluent which means that more than 99.9% were degraded. As only primarily biodegradation was determined in adapted soil samples, results cannot be taken for the derivations of kinetic biodegradation rates in soil.

There are contradictory results on the volatilisation behaviour and biodegradability of nitrobenzene in soil. In one study the elimination of nitrobenzene was due to volatilisation and the other study shows that more than 99% of the nitrobenzene was primarily degraded and almost no nitrobenzene evaporated. No explanation for this inconsistency can be given.

3.1.3.1.4 Summary of environmental degradation

Summary Photodegradation in water and air

In summary photodegradation of nitrobenzene both in the hydrosphere and in the atmosphere seems to be a slow process. Nitrobenzene is expected to be a long lived contaminant in urban air. It is expected to be slowly removed from the atmosphere by physical processes, including dry deposition ($t_{1/2}$ > 2 months) (Grosjean, 1991). But this reaction mechanism is considered to be speculative and the study of Grosjean is therefore not considered valid.

The nitrate-induced photooxidation maybe a significant transformation mechanism for nitrobenzene in shallow, clear water bodies with high ratios of nitrate to DOC concentrations (Zepp et al., 1987). But in deep water bodies oxidation of organic chemicals by this process is much slower because of the strong attenuation of the UV light required to initiate nitrate photolysis.

The half-life of nitrobenzene in water due to photo-oxidation with OH-radicals can vary in a rather wide range depending on the hydroxyl radical concentration in water and the second order rate constant.

Besides the poor biodegradability and the stability to hydrolysis, photolysis of nitrobenzene also does not play an important role under environmental conditions.

Both direct photolysis and the photochemical reaction with OH-radicals only take place in the upper layers of surface water. Experimentally determined photodegradation half-lives of nitrobenzene range from 25-400 days. These laboratory results, carried out with distilled or tap water, do not represent environmental conditions, where the surface water is normally deeper and muddier. Considering the total water body, the environmental half-lives are expected to be significantly higher than the results from laboratory studies.

Table 3.3 Summary of photodegradation

Compartment	Degradation process	Half-life period [d]
Air	Photo-oxidation with OH radicals (calculation)	65.8
Water	Direct photoysis	133
Water	Photo-oxidation with OH radicals	25-400 (∞)

Summary of biodegradation results

The available biodegradation tests show a great variation of the results.

It can be stated that nitrobenzene is not biodegradable with unadapted inoculum. Regarding the various non-standard biodegradation tests there are contradictory results. Some tests show high elimination rates without stripping of nitrobenzene while in other tests the elimination appears almost completely to be due to evaporation.

The Zahn-Wellens test conducted with industrial inoculum showed no biodegradation within 10 days but volatilisation of nitrobenzene from the physico-chemical batch. Hence for reasons of precaution a rate constant of 0 h^{-1} is derived according to the TGD as an input parameter for Simple Treat calculations.

However, the tests and the monitoring data show clearly that adapted microorganisms in industrial WWTP have the ability to biodegrade nitrobenzene at high levels (over 90%). But occasionally there are significant fluctuations in the degradation behaviour and then nitrobenzene is partly degraded at only 34%. The reason for this has not yet been found out so far. Toxic effects to microorganisms may play a role.

Anaerobic biodegradation seems to be a more efficient way of eliminating nitrobenzene from wastewater. Even with unadapted microorganisms relatively high elimination rates are achieved. With adapted microorganisms the elimination rate is still higher. But as only primary degradation takes place, aniline as a reduction product is formed. This is not further anaerobically biodegradable and has to undergo subsequent aerobic biodegradation. Under aerobic conditions aniline is readily biodegradable. This substance has been subject to a recent risk assessment under the Existing Substances Regulation (see EU Risk Assessment Report on Aniline).

Nitrobenzene is considered to be not inherently biodegradable. Hence the rate constants $kbio_{wwtp}$, $kbio_{water}$, $kbio_{soil}$ and $kbio_{sed}$ *) are set to be 0 d^{-1}.

*) As the sediment in general consists of a relatively thin oxic top layer (10%) and anoxic deeper layers (90%), anaerobic conditions dominate there. Nitrobenzene can be primarily degraded to aniline under anaerobic conditions. Aniline again forms covalent bonds to humic acids under anaerobic conditions and can therefore accumulate in the sediment. But as the sediment is not the targeted compartment for nitrobenzene, this mechanism has only limited relevance for the environment. So the approach to allocate a rate constant of 0 d^{-1} to the sediment seems to be fully justified.

3.1.3.2 Distribution

3.1.3.2.1 Adsorption

A chemical's ability to bind or adsorb to soils is characterised by its organic-carbon partition coefficient Koc. On the basis of the log Pow value (1.86) and according to the TGD equation for phenols, anilines, benzonitriles and nitrobenzenes ($\log Koc = 0.63 \log Kow + 0.90$) the Koc value is calculated as 118 l/kg (for calculation see **Appendix D**). This calculated Koc value is located within the range of the experimentally determined values and is taken in all model calculations of this report. The value of 118 l/kg does not indicate a significant potential for geoaccumulation. If nitrobenzene is released or deposited to soil most of the substance is expected to leach through the soil into the groundwater. To a smaller extend nitrobenzene is likely to volatilise to the atmosphere.

The adsorption of nitrobenzene to 2 different soils (organic carbon content of 2.58% for soil 1 and 1.82% for soil 2) at a initial concentration range from 2-100 mg/l was tested (Loekke, 1984). The adsorption behaviour could sufficiently be described by a Freundlich isotherm and Koc-values of 170-370 l/kg were calculated. The tests were carried out at two different temperatures (5°C and 21°C). At the lower temperature the experiments were performed for 72 hours, the test duration at the higher temperature was 48 hours. The results are as follows:

Soil 1: 5°C: 210 l/kg
21°C: 170 l/kg

Soil 2: 5°C: 170 l/kg
21°C: 370 l/kg

The results show a broad distribution and no temperature dependence. It seemed not justified to calculate a mean value out of these 4 results.

The soil sorption capacity of three different types of soils was examined (Seip et al., 1986). The three soil columns were supplied with water containing nitrobenzene (1.0 mg/l) and eluted with tap water, respectively. For the sandy forest soil with 0.2% organic carbon a Koc of 30.6 was calculated. The silty agriculture soil (2.2% organic carbon) and the silty forest soil (3.7% organic carbon) result in Koc values of 88.8 and 103 l/kg, respectively.

In another test soil columns (sandy soil, 0.087% organic C) were fed with aqueous solutions of nitrobenzene (Wilson et al., 1981). With the concentration in the effluent the migration velocity of nitrobenzene relative to water was obtained. The retardation factor experimentally determined was 1.5–2.3 (calculated value 1.4). This leads to the conclusion that nitrobenzene is mobile in soil which is in accordance with the conclusion drawn from the calculated and measured Koc-values.

The Koc-value was also calculated from the water solubility and from the Kow (Roy and Griffin, 1985). The resulting Koc-values are 79 and 62 l/kg, respectively. Although the equations used for calculations are not specifically designed for substituted benzenes, the calculated Koc-values lie in the same order of magnitude as the other calculated and experimentally determined values.

The solid-specific partition coefficients Kp were estimated for soils, sediments, suspended matter based on the Koc value of 118 l/kg.

Table 3.4 presents the calculated soil/water partition coefficients of these compartments based on the Koc value.

Table 3.4 Calculated partition coefficients for nitrobenzene

Compartment	Partition coefficient*)	
Soil-water	Kp_{soil} = 2.36 l/kg	$Kp_{soil\text{-}water}$ = 3.74
Sediment-water	Kp_{sed} = 5.90 l/kg	$Kp_{sediment\text{-}water}$ = 3.75
Suspended matter-water	Kp_{susp}= 11.8 l/kg	$Kp_{suspension\text{-}water}$= 3.85
Sewage sludge-water, calculated	Kp_{sludge}= 43.7l/kg	

*) For the calculation see Appendix G

3.1.3.2.2 Volatilisation

With a vapour pressure of 20 Pa and a water solubility of 1,900 mg/l a Henry´s law constant of 1.296 $Pa \cdot m^3 \cdot mol^{-1}$ at 20°C was calculated. This value is used for all model calculations in this report. A Henry constant of 2.23 $Pa \cdot m^3 \cdot mol^{-1}$ is estimated by Thomas (1990), who stated that in the range of $1.013 < H < 101.3$ $Pa \cdot m^3 \cdot mol^{-1}$, liquid phase and gas phase resistances are both important. Volatilisation for compounds in this range is less rapid than for compounds in

a higher range of H but is still a significant transfer mechanism. The substance therefore remains preferably in water, but it can also be assumed that a slight volatilisation from an aqueous solution takes place.

The volatilisation rate constant and half life of nitrobenzene due to evaporation from two lakes near Istanbul were predicted (Ince, 1992). For lake 1 a half life of 8 days (rate constant was 0.0036 h^{-1}) and for lake 2 a half life of 20 days (rate constant = 0.00147 h^{-1}) were predicted. The differences were due to the different depths of the lakes (lake 2 is 2.5 times deeper than lake 1) and due to different water evaporation rates (in lake 2 the evaporation rate is about two times lower than in lake 1).

Table 3.5 Air/Water Partition Coefficients

Compartments	Partition Coefficient	Value	Source
Henry's law constant	H	1.296 Pa m^3 mol^{-1}	calculated
Henry's law constant	log H	0.1126	calculated
Air/Water partitioning	K_{air_water}	$5.32 \cdot 10^{-4}$	calculated

3.1.3.2.3 Distribution in wastewater treatment plants

Based on the physico-chemical properties of nitrobenzene and the rate constant for biodegradation of 0 h^{-1} the elimination of nitrobenzene in municipal WWTPs is calculated with the SIMPLETREAT 3.0 model (debugged version, February 1997) in accordance with the TGD (see **Appendix G**).

Table 3.6 Behaviour of Nitrobenzene in WWTP according to the Simple Treat Model

	$kbio_{stp}$ = 0 h^{-1}
Evaporation to air [%]	2.5
Release (dissolved) to water [%]	96.7
Adsorption to sewage sludge [%]	0.8
Degradation [%]	0
total elimination from waste water [%]	3.3

These values calculated with SimpleTreat are only of theoretical interest as no nitrobenzene is supposed to enter municipal waste water treatment plants.

Considering the high elimination rates of the industrial WWTPs (over 90%) the regional and continental concentrations were calculated with an average elimination rate of the industrial WWTPs (see also Section 3.1.8).

3.1.3.3 Accumulation and metabolism

Bioaccumulation

In the MITI-list (CITI 1992) the bioaccumulation of nitrobenzene in the fresh water species *Cyprinus carpio* was ascertained. The used guideline corresponds to the guideline OECD

305 C "Bioaccumulation: Test for the degree of bioconcentration in fish". The test concentrations were 0.125 and 0.0125 mg/l, respectively, at 25 ± 2°C and the lipid content of the test organisms varied between 2 and 6%. At a nitrobenzene concentration of 0.125 mg/l a BCF in the range of 3.1-4.8 was determined during an exposure period of 42 days. At the concentration of 0.0125 mg/l the BCF varied between 1.7 and 7.7.

The bioaccumulation of nitrobenzene in fish, algae and activated sludge was also examined (Freitag et al. 1982). Experimental protocols were described in detail in Korte et al., 1978. For the fish test the golden orfe *Leuciscus idus melanotus* was chosen as test organism. Five fish weighing about 1.5 g each were exposed to 50 µg/l of ^{14}C-labelled nitrobenzene for three days in a closed system. The fish were not fed during this time and no aeration took place. After three days the radioactivity in the whole fish was determined and referred to the average constant concentration of nitrobenzene in the water. A BCF of < 10 (related to wet weight) was calculated. For the algae test the green alga *Chlorella fusca* was used. Algae (20 mg d.w./200ml) were exposed to 50 µg/l ^{14}C-labelled nitrobenzene for 24 hours. After this time algal cells were separated by centrifugation and the radioactivity was measured in the algae and in the supernatant. A BCF of 24 (related to wet weight) could be determined. In the third test activated sludge from a municipal sewage treatment plant (1 g dw/l) was exposed to 50 µg/l ^{14}C-labelled nitrobenzene in a nutrient solution for five days. Then an aliquot was taken and filtered. From measurement of the radioactivity in the filtrate and in the residue the distribution of nitrobenzene between activated sludge and water was obtained. An enrichment factor of 40 (related to dry weight) could be calculated.

In another study (Geyer et al., 1984) bioaccumulation of nitrobenzene in the alga *Chlorella fusca var. vacuolata* was examined. Algae were exposed to a nitrobenzene concentration of 50 µg/l in nutrient solution at room temperature (20–25°C). The experimentally determined bioconcentration factor is 24.

Also experiments with female guppies (*Poecilia reticulata,* 5 to 8 months old) were performed (Deneer et al., 1987). The mean fat content was 8 ± 2%. The test concentration was 1/5 of the LC_{50} (100 µmol/l=12.3 mg/l). Nitrobenzene solutions were renewed daily. After 3 days the nitrobenzene content of the individual fish was determined. The BCF_{fish} on the basis of fat weight varied from 22.4 to 38.9. The authors state that the relatively low BCF for nitrobenzene might be due to experimental difficulties in the determination of nitrobenzene in fish, due to the relatively high volatility of this compound.

According to the relationship developed by Veith et al. (1979) and proposed in the Technical Guidance Documents, a BCF of 7.6 $l \cdot kg^{-1}_{wet\ fish}$ can be estimated from log BCF = 0.85 · log Kow. This value is in good accordance with the measured values.

On a worst case basis, the experimentally derived mean BCF of 30.6 (Deneer et al., 1987, see above) is used for all further calculations.

Summary of bioaccumulation

The different experiments show that nitrobenzene seems to have a low bioaccumulation potential. In all available tests conducted with fish BCF values were clearly below 100.

Geoaccumulation

Both the calculated and measured solid-specific partition coefficients do not indicate a significant potential for geoaccumulation. If nitrobenzene is released or deposited to soil, most of the substance is expected to leach through soil into the groundwater and partly volatilise to the atmosphere.

3.1.4 Aquatic compartment (incl. sediment)

3.1.4.1 Calculation of predicted environmental concentrations (PEC_{local})

In the Technical Guidance Document a generic (i.e. non site-specific) exposure scenario for the release of intermediates to surface water during production and processing is proposed. This scenario is described in the Emission Scenario Document (ESD) IC -3- "chemicals used in synthesis; intermediates" and reflects a realistic worst case situation. For this generic local exposure estimation an average production volume of 300,000 tonnes/annum, which is processed on site, is used, as the production volume of the three greatest producers is between 200,000 and about 380,000 tonnes/annum.

3.1.4.1.1 Calculation of PEC_{local} for production and processing

a) Estimation of C_{local} for production and processing / Generic approach

The generic exposure scenario for production and processing of 300,000 tonnes nitrobenzene/year leads to a $C_{localwater}$ = 1.790 mg/l.

Default emission factors of 0.3% for production and 0.7% for processing and 300 days of emission per year were used for the calculation. According to the TGD $C_{localwater}$ was calculated with a default effluent discharge rate of an industrial STP of 10,000 m^3/day and a default dilution factor of 40.

The WWTP elimination rate used for calculation was 92.8%. It is the mean value of the six known elimination rates of the companies industrial waste water treatment plants (data from companies B, D, E, F, G and H).

b) Estimation of C_{local} for production and processing/Site-specific approach

The discharges of nitrobenzene during production and processing are assessed as point source emissions because the individual production/processing sites are identifiable. For the site-specific scenarios all nitrobenzene producers as well as all known nitrobenzene processing sites are considered. The emission factors are calculated from site-specific yearly releases into the respective waste water treatment plants or, at the site(s) without WWTP, to surface water and the production/processing amount. For the sites where production and processing takes place these factors are in the range of 0.006 to 0.04 kg/tonne and hence are considerably lower than the TGD default values. Two of the mere processing sites have the highest emission factors. These are higher than the TGD defaults. However, there results no concern for the environment out of this relatively high emission factors as the corresponding industrial WWTPs have high elimination rates.

For the Ceffluent, which is the basis for the assessment of treatment plants, the 90 percentile value or, if the compound was not detected, the detection limit is used.

For releases into rivers, the C_{local} is calculated with the $C_{effluent}$ and a dilution factor resulting from waste water and river low flow (10 percentile or 1/3 of the mean flow). According to new TGD the maximum dilution factor is 1,000.

The PEC_{local} includes the $PEC_{regional}$ of 0.01 µg/l (see Section 3.1.8).

There are 5 sites where production and processing takes place. At 3 sites only processing occurs. The following table lists the calculated PECs and the respective data used in the calculations (for calculation see confidential files). The detailed information provided and the calculations themselves are not included in this report. They can be made available to Member States Competent Authorities, as a confidential annex, on request.

The PEC for microorganisms in the STP (PEC_{stp}) equals the concentration in the effluent of a STP. The concentrations in the specific STPs vary from < 1 µg/l to 140 µg/l. However, at site E, a much higher PEC_{stp} of 1,000 µg/l occurs.

The total discharge during nitrobenzene production and processing for all known production and processing sites are summarised to be 6.6 tonnes/annum released directly to surface water and about 14 tonnes/annum directed to industrial waste water treatment plants.

In the TGD a calculation method for the estimation of PEC_{local} in sediment is proposed. As nitrobenzene is not expected to adsorb to organic matter a $PEC_{sediment}$ is only calculated for site C because it shows the highest PEC_{local} for water. Using the corresponding $PEClocal_{water}$ of 8.35 µg/l and the calculated partition coefficient between suspended matter and water (ksusp-water = 3.849 $m^3 \cdot m^{-3}$) the following $PEC_{sediment}$ was calculated (see **Appendix B**)

$$PEC_{sediment} = 0.03 \text{ mg/kg ww}$$

Table 3.7 Data used in local aquatic exposure assessment

Site		Site specific information	Release Factor [kg/t] *)	Clocal $_{water}$ [µg/l]	PEClocal $_{water}$ [µg/l]
A	Production Processing	Effluent concentration, river flow rate	$3.5 \cdot 10^{-4}$	0.86	0.87
B	Production Processing	Effluent concentration and effluent discharge rate, river flow rate	0.03	0.07	0.08
C	Production Processing	No WWTP	0.017	8.33	8.35
D	Production Processing	Effluent concentration and effluent discharge rate, river flow rate, emission days	0.007	0.02	0.03
E	Production Processing	Effluent concentration and effluent discharge rate, river flow rate	0.01	2.77	2.78
F	Processing	Effluent discharge rate, river flow rate	0.05	$1 \cdot 10^{-3}$	0.01
G	Processing	generic	3.5	$6 \cdot 10^{-3}$	0.02
H	Processing	Effluent concentration, river flow rate	26.1	0.003	0.02

*) For sites where both production and processing takes place release factors have not been calculated separately for production and processing, respectively,.

Site B $Clocal_{water}$ was calculated on the basis of the 90 percentile value of the WWTP effluent. There were only 16 random sampling measured over a period of 18 months. Hence the value for $clocal_{water}$ might be an underestimation of the real situation, also due to the fact that there are inexplicable fluctuations in the biodegradation behaviour of nitrobenzene. However, all measured values are under the $PNEC_{surfacewater.}$

Site E At this site, not a conventional WWTP is used but a set of four reed beds (constructed wetland). The effluent of this constructed wetland is emitted into a channel, for which only an average flow is available.

Site F $clocal_{water}$ was calculated on the basis of the annual discharge rate.

3.1.4.1.2 Calculation of PEC_{local} for formulation

As no formulation takes place a calculation for a separate PEC_{local} is not necessary.

3.1.4.1.3 Calculation of PEC_{local} for the use in consumer products

As no information is available on the use of nitrobenzene in consumer products no such scenario was calculated.

3.1.4.2 Measured levels

The large amount of nitrobenzene monitoring data provides a basis for comparing the calculated exposure data with measured ones. However, the available monitoring data are partly relatively old and cannot be assigned to the individual emission sources. They only provide an indication of the orders of magnitude which are to be expected.

Most of these monitoring data refer to the German river Rhine, but data on other rivers, as Elbe, Main, Ruhr etc. also exist. **Tables C1** and **C6** in **Appendix C** present summaries of published data for surface water (**Table C1**) and ground water (**Table C6**). Additional monitoring data for the hydrosphere from other countries (Japan, USA and the Czech Republic) are also compiled in these tables.

Most of the 90-percentile values in surface water are below 1 µg/l. There are a few measured maximum values that exceed 1 µg/l in the river Rhine which are in the range between 1.2 µg/l and 22.5 µg/l. The highest value was measured in the river Rhine at Mainz. The monitoring data for the river Elbe show values of about 0.5 µg/l at Zollenspieker (the city Hamburg is situated there) and Semannshöft (also close to Hamburg), respectively. Only in the Czech Republic higher concentrations for the river Elbe of maximum 5.2 µg/l were measured.

Nitrobenzene was detected in groundwater near a former ammunition plant in Leverkusen (Germany) at a concentration of 1 µg/l.

Sediment

Sediment monitoring data are scarcely found in the literature (see **Appendix C**, **Table C2**) because nitrobenzene is not likely to adsorb to organic matter. The low water/soil and water/sediment partition coefficients of 3.7-3.8 m^3/m^3 (**Table 3.4**) confirm this.

Sediment concentrations in samples of the river Rhine in Germany at different locations are found to be less than 10 µg/ kg dry substance with two exceptions of 18 and 26 µg/kg dry substance (LWA NRW, 1989).

3.1.4.3 Comparison between predicted and measured levels

The available monitoring data cannot be assigned to the individual emission sources. They only provide an indication of the orders of magnitude which are to be expected. However, the comparison of monitored and predicted water concentrations in fresh water rivers show good accordance. Both the measured and the predicted concentrations are mostly below 1 µg/l.

The default TGD calculation on production/processing shows a nitrobenzene concentration in the aquatic compartment that cannot be confirmed by monitoring data.

Monitoring data show regional differences in pollution levels. The river Rhine is the only river in Germany with monitoring data of nitrobenzene exceeding 1 µg/l.

The calculated $PECregional_{surfacewater}$ of 0.01 µg/l is confirmed by these monitoring investigations.

3.1.5 Terrestrial compartment

The release of nitrobenzene to soil occurs through atmospheric deposition after local releases to the atmosphere at the production and processing sites. The input through sludge application on agricultural soil is considered negligible. Nitrobenzene does not partition to a significant extent to sewage sludge in the WWTP (according to Simple Treat only 0.8% of the nitrobenzene in a WWTP enters the sludge). The log Pow of 1.86 (Koc = 118 l/kg) also indicates a low potential for adsorption to organic matter. In addition all nitrobenzene enters industrial WWTPs which sludges are not applied to agricultural soil.

3.1.5.1 Calculation of PEC_{local}

3.1.5.1.1 Calculation of PEC_{local} for production and processing

With the worst case deposition rate of $DEPtotal_{ann}$ of 0.84 $\mu g \cdot m^2 \cdot d^{-1}$ calculated for site C in Section 3.1.6.1.1 the maximum equilibrium soil concentration in the vicinity of a production/processing plant can be calculated according to the procedure proposed in the TGD. The calculations are presented in **Appendix H**, the resulting concentrations in natural soil and in agricultural soil are equal.

bulk soil concentration: $PEClocal_{soil} = 2.3 \cdot 10^{-3}$ mg/kg ww
porewater concentration: $PEClocal_{soil\text{-}porew} = 1.1$ µg/l

3.1.5.1.2 Calculation of PEC_{local} for formulation

No PEC_{local} for formulation has to be calculated because no formulation takes place.

3.1.5.1.3 Calculation of PEC_{local} for the use in consumer products

As no nitrobenzene is used in consumer products no PEC_{local} was calculated for this scenario.

3.1.5.2 Measured levels

Measured nitrobenzene values in soil are only available for 3 sites in Ontario and Quebec (Canada). There 100-150 µg/kg dry soil were found in agricultural soil (Webber and Wang, 1995).

These values are considerably higher than the calculated values in this report. But there is no information available whether possible entries of nitrobenzene via sludge in these soils took place. Of the 10 sites examined in different provinces of Canada nitrobenzene was only found in these 3 samples. In the other seven soil samples no nitrobenzene could be detected.

3.1.6 Atmosphere

Direct releases of nitrobenzene into the atmosphere occur during production and processing . Releases from industrial waste water treatment plants can be expected. With a Henry constant of 1.3 $Pa \cdot m^3 \cdot mol^{-1}$(calculated) the substance can be regarded as moderate volatile from aqueous solution. Using the SIMPLETREAT model releases from WWTPs are estimated to be 2.4% of the total quantity entering the waste water treatment plant.

3.1.6.1 Calculation of PEC_{local}

3.1.6.1.1 Calculation of PEC_{local} for production

For all production/processing sites specific air emission data are available. All data refer to the year 2000, with the exception of site H, for which data refer to 1996.

As for sites A and G no current figures were available the emission data from former years, which refer to other production/processing figures, were used and with the production/processing figures of the year 2000 converted to the respective emission data.

The emission factors (kg/tonne) are calculated from site-specific yearly release into air and the production/processing amount. For the sites where production and processing take place these factors are in the range between $3 \cdot 10^{-6}$ and $2 \cdot 10^{-3}$ kg/tonne and hence are considerably lower than the TGD default values. The calculations are presented in confidential files.

The results of the calculations are summarised in the following table.

Table 3.8 Data used in local atmospheric exposure assessment

Site		Site specific release information	Release Factor [kg/t]	$clocal_{air\_ann}$ [mg/m³]	$PEClocal_{air\_ann}$ [mg/m³]	$DEPtotal_{ann}$ [mg/(m² · d)]
A	Production Processing	x	$2.3 \cdot 10^{-5}$	$2.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	$3.4 \cdot 10^{-4}$
B	Production Processing	x	$1.5 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$
C	Production Processing	x	$1.6 \cdot 10^{-3}$	$4.6 \cdot 10^{-4}$	$4.6 \cdot 10^{-4}$	$8.4 \cdot 10^{-4}$
D	Production Processing	x	$4.6 \cdot 10^{-4}$	$5.6 \cdot 10^{-5}$	$5.7 \cdot 10^{-5}$	$1.1 \cdot 10^{-4}$
E*)	Production Processing	x	$3.0 \cdot 10^{-6}$	$3.0 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$	$4.4 \cdot 10^{-5}$

Table 3.8 continued overleaf

Table 3.8 continued Data used in local atmospheric exposure assessment

Site		Site specific release information	Release Factor [kg/t]	clocal$_{air_ann}$ [mg/m^3]	PEClocal$_{air_ann}$ [mg/m^3]	DEPtotal$_{ann}$ [mg/(m^2 · d)]
F	Processing	x	$6.0 \cdot 10^{-7}$	$4.4 \cdot 10^{-5}$	$4.4 \cdot 10^{-5}$	$6.3 \cdot 10^{-5}$
G	Processing	TGD, B-table	0.001	$2.1 \cdot 10^{-5}$	$2.1 \cdot 10^{-5}$	$3.5 \cdot 10^{-5}$
H	Processing	x	0.82	$6.2 \cdot 10^{-5}$	$6.3 \cdot 10^{-5}$	$1.6 \cdot 10^{-4}$

*) At this site a set of four reed beds (constructed wetland) is used as a WWTP, covering a total area of 10,000 m^2. It can be assumed that considerably higher air emissions occur at this site than at the other sites with conventional WWTPs. But these air emissions are not quantifiable and hence all figures were calculated with the fraction of emission directed to air (2.5 %) which was obtained by Simple Treat calculation.

3.1.6.1.2 Calculation of PEC_{local} for formulation

No PEC_{local} for formulation has to be calculated because no formulation takes place.

3.1.6.1.3 Calculation of PEC_{local} for the use in consumer products

As nitrobenzene is not used in consumer products no PEC_{local} was calculated for this scenario.

3.1.6.2 Measured levels

For Europe no measured air concentrations are available.

For the US some data for exist. In an industrial area in New Jersey (US) values in the same order of magnitude as the predicted values were measured; the average value was 0.4 µg/m^3 and the maximum value was 3.5 µg/m^3 (Bozzelli and Kebbukus, 1982). In urban areas of New Jersey nitrobenzene in a concentration range of 0.36-0.51 µg/m^3 was measured in summer (average values). In winter the average values were less than the detection limit of 0.26 µg/m^3. (Harkov et. al, 1984). Measured data from a smog episode over Los Angeles, California, gave 0.05 µg/m^3 as the highest value (Fraser et. al, 1998).

3.1.6.3 Comparison between predicted and measured levels

The predicted air concentrations are in the range of 0.02-0.5 µg/m^3. These values refer to all industrial sites and not to residential areas. These data are in good accordance with the measured values from the US.

3.1.7 Secondary poisoning

Nitrobenzene has some potential for persistence. But there are no indications for bioaccumulation potential of nitrobenzene. Neither has nitrobenzene a log Kow ≥ 3 nor is it highly adsorptive or belongs to a class of substances known to have a potential to accumulate in living organisms. The TGD indicates that substances which have a potential to cause toxic

effects if accumulated in higher organisms should be considered in the effects assessment for secondary poisoning only if there is an indication of their bioaccumulation potential.

As nitrobenzene has only a low bioaccumulation potential it is not necessary to carry out a risk characterization for secondary poisoning.

3.1.8 Calculation of $PEC_{regional}$ and $PEC_{continental}$

All releases from point sources are considered in the determination of a regional background concentration. The calculations for the regional PECs are performed with Simple Box 2.0 (see **Appendix E**).

Sources for the release into the aquatic compartment and the atmosphere

The local emissions from the production and/or processing of nitrobenzene (8 sites within the EU) are summarised and distributed to the regional and continental area in a ratio of 10% to 90%.

Table 3.9 shows releases of nitrobenzene to the aquatic compartment and atmosphere.

As it is described in Section 3.1.3.1.4 "Summary of environmental degradation" nitrobenzene is considered to be not inherently biodegradable and the rate constant for the degradation of nitrobenzene in WWTPs is therefore 0 d^{-1}.

Nevertheless, industry data show clearly that nitrobenzene is efficiently eliminated in industrial WWTPs. Because of the high elimination rates in the industrial WWTPs the calculations of the regional PECs were conducted with the mean value (92.8%) of the six known elimination rates of the companies industrial waste water treatment plants (data from companies B, D, E, F, G and H).

Table 3.9 Releases to aquatic compartment and atmosphere

Site/scenario	Total release into the hydrosphere [t/a]		Total release into the atmosphere [t/a]
	Directly to surface water	via WWTP	
regional	0.66	1.44	0.08
continental	5.93	12.95	0.74
total	6.59	14.39	0.82

Point releases to soil:

No direct point releases to soil were identified.

In **Appendix E** the input and output figures of the Simple Box 2.0 calculation adapted to the TGD and EUSES 1.00 are presented. (The results of this calculation are consistent with EUSES) The resulting regional concentrations are:

$PECregional_{surface\ water} = 0.01\ \mu g/l$
$PECregional_{air} = 0.05\ ng/m^3$
$PECregional_{agr\ soil} = 5.4\ ng/kg_{ww}$
$PECregional_{agr\ soil\ porewater} = 2.5\ ng/l$
$PECregional_{sediment} = 0.04\ \mu g/kg_{ww}$

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

3.2.1 Aquatic compartment (incl. sediment)

Many investigations are available concerning the toxicity of nitrobenzene to aquatic organisms from different systematic classes including also several non-standard tests. Tests were regarded as valid if they were performed according to national or international test guidelines or if they are sufficiently documented and scientifically acceptable.

3.2.1.1 Toxicity test results

3.2.1.1.1 Fish

Acute toxicity

The following table gives an overview of the sensitivity of different fish species to nitrobenzene in short-term tests. It covers the full range of species tested. For each species the lowest available valid test was selected, respectively.

Table 3.10 Acute toxicity data to fish

Species	Endpoint	Effect concentrations [mg/l]	Test system	Reference
Brachydanio rerio	96-hour LC_{50}	112.5 (nc)	Static (no standard method)	(Wellens H, 1982)
Brachydanio rerio	96-hour LC_{50}	92 (mc)	Flow-through (OECD Guideline)	(Roederer, 1990)
Brachydanio rerio	14-day NOEC	5 (mc)	Flow-through (OECD Guideline)	(Roederer, 1990)
Leuciscus idus	48-hour LC_0 48-hour LC_{100}	50 (nc) 100 (nc)	Static (no standard method)	(Wellens H, 1982)
Leuciscus idus	48-hour LC_{50}	60 (nc)	Static (no standard method)	(Juhnke and Luedemann, 1978)
Oryzias latipes	48-hour LC_{50}	20 (nc)	static (Japanese Industrial Standards Committee)	(Tonogai et al., 1982)
Oryzias latipes	48-hour LC_{50}	70 (nc)	Semi-static(OECD Guideline)	(Yoshioka and Ose, 1993)
Oryzias latipes	48-hour LC_{50}	125 (nc)	Semi-static	(CITI, 1992)
*Oryzias latipes**	48-hour LC_{50}	1.8 (no information)	No information	(Yoshioka et al., 1986b)

Table 3.10 continued overleaf

* Only very few information are given on the test design and test conditions. The results are presented only in tabular form and can therefore not be validated.

Table 3.10 continued Acute toxicity data to fish

Species	Endpoint	Effect concentrations [mg/l]	Test system	Reference
Pimephales promelas	96-hour LC_{50}	117 (mc)	Flow-through (method: US-EPA)	(Holcombe et al., 1984)
Pimephales promelas	96-hour LC_{50}	119 (mc)	Flow-through (no standard method)	(Geiger et al., 1985)
Pimephales promelas	96-hour LC_{50} 7-day LC_{50} 7-day NOEC (growth)	44 (nc) 39 (nc) < 10.2 (nc)	Flow-through larval test (method: US-EPA) Effect: growth, survival	(Marchini et al., 1992)
Lepomis macrochirus	48-hour LC_{50}	43 (nc)	Static (method: US-EPA)	(Buccafusco et al., 1981)
Cyprinodon variegatus (saltwater)	96-hour LC_{50}	59 (nc)	Static (method: US-EPA)	(Heitmuller et al., 1981)
Poecilia reticolata	14-day LC_{50}	61.7 (mc)	Semi-static (no standard method)	(Deneer et al., 1987)

In acute toxicity tests to fresh (and one salt) water species values in the range from 20 mg/l (*Oryzias latipes*) to 125 mg/l (*Oryzias latipes*) were obtained.

The most sensitive fish species in fresh water seems to be *Oryzias latipes*. A 48-hour LC_{50} of 20 mg/l based on nominal concentrations was calculated (Tonogai et al., 1982). The test was conducted according to the procedure of Japan Industrial Standards (Japanese Industrial Standards Committee, 1971). Fish of the same age were chosen and acclimated for 10 days in tap water before the start of the test. The nitrobenzene test solution was prepared without the use of solvents.

Prolonged toxicity tests with *Pimephales promelas*, exposition at larval stage, showed a 7-day NOEC less than 10.2 mg/l for the endpoint growth and a NOEC (survival) of 38.3 mg/l (Marchini et al., 1992).

In a 14-day prolonged toxicity test, conducted according to OECD Guideline 204, *Brachydanio rerio* showed a NOEC of 5 mg/l (Roederer, 1990).

The experimental values are in reasonable agreement with the QSAR estimation according to the TGD (1996) which results in a fish (96-hour) LC_{50} of 37 mg/l for polar narcotic acting substances.

Long-term toxicity

Only one long-term toxicity test with *Oncorhynchus mykiss* exists (Black et al., 1982).

Log probit analysis was used by the authors to determine the LC_{50} at hatching and 4 days after hatching. Values of 0.002 mg/l for both points of time were obtained.

Table 3.11 Embryo-larval test with *Oncorhynchus mykiss* (Black et al., 1982).

Nitroenzene conc. [mg/l]	Percent hatchability	Percent survival normal organisms	Percent survival normal organisms
		at hatching	4 days posthatching
0.001	64	62	62
0.010	24	21	21
0.12	5	3	3
0.36	0	0	0
0.91	0	0	0
11.9	0	0	0

The effect values found by Black et al. (1982) for several substances other than nitrobenzene (e.g. benzene, toluene) are usually very low compared to effect values found by other authors. No explanation for these large discrepancies could be found. A careful examination of the entire information provided by Black et al. gave no plausible reason for the inconsistency of the data. However, as it was not possible to reproduce the effect values found by Black and his co-workers, it was decided by the EU member states not to use these data for a derivation of a PNECaqua if other valid fish early life stage tests are available. Concerning nitrobenzene no other fish early life stage tests exists. Nevertheless, the effect values found by Black et al. for *Oncorhynchus mykiss* are not employed in the further effects assessment because for other substances it was not possible to confirm the low effect values and it can be assumed that the value for nitrobenzene is also not representative.

3.2.1.1.2 Aquatic invertebrates

Acute toxicity

Table 3.12 shows the available test results for nitrobenzene obtained in short-term tests with aquatic invertebrates.

Table 3.12 Acute toxicity data to aquatic invertebrates

Species	Endpoint	Effect concentrations [mg/l]	Test system	Reference
Daphnia magna	24-hour EC_{50}	50 (nc)	Static (German DIN method) Endpoint: immobilisation	(Bringmann and Kühn, 1982)
Daphnia magna	48-hour EC_{50}	35 (nc)	Semistatic (OECD proposal 1979) Endpoint: behaviour	(Canton et al., 1985)
Daphnia magna	48-hour LC_{50}	27 (nc)	Static (method: US-EPA) Endpoint: mortality	(LeBlanc, 1980)

Table 3.12 continued overleaf

Table 3.12 continued Acute toxicity data to aquatic invertebrates

Species	Endpoint	Effect concentrations [mg/l]	Test system	Reference
Daphnia magna	24-hour EC_{50}	11.2 (mc)	Static (OECD Guideline 202) Endpoint: immobilisation	(Tosato et al., 1991)
Ceriodaphnia dubia	24-hour LC_{50}	54 (mc)	Static (method: US-EPA) Endpoint: mortality	(Marchini et al., 1993)
Mysidopsis bahia[*1]	96-hour EC_{50}	6.68		(LeBlanc, 1984)
Dugesia japonica[*2]	7-day EC_{50} 7-day LC_{50}	1.5 2.0	Endpoint: head regeneration	(Yoshioka et al. 1986b)

Short-term effect values for fresh-water invertebrates between 11 mg/l and 54 mg/l were reported. The most sensitive species seems to be Daphnia magna with a 24-hour EC_{50} of 11 mg/l. The test was conducted according OECD-Guideline 202 in a static test system with analytical monitoring. The concentration of the test solution was determined at the beginning and the end of the test. Test solutions were prepared without solubilising agents. For the further risk assessment the 24-hour EC_{50} of 11 mg/l is used as effect value for short-term toxicity of nitrobenzene to invertebrates.

The experimental EC_{50} values (48-hour) for *Daphnia* are in reasonable agreement with QSAR estimations according to the TGD (1996) which result in a Daphnia (48-hour) EC_{50} of 18 mg/l for polar narcotic acting substances

Long-term toxicity

There are three valid tests on chronic toxicity to Daphnia magna available. A LC50 of 24 mg/l and a LOEC of 18 mg/l were determined in a 21-day reproduction rate test (Maas-Diepeveen and van Leeuwen, 1986). In a semi-static chronic test to daphnia magna a 21-day NOEC of 12.5 mg/l based on nominal concentrations was found. Based on the measured concentration at day 3 after renewal of the test solution the NOEC is 2.6 mg/l (Kühn et al., 1988).

The lowest long-term effect value for *Daphnia magna* is a 21-day NOEC of 1.9 mg/l (measured) with the endpoint reproduction rate (Canton et al., 1985). No information about test conditions is given in this article, but for the performance of the standard tests the authors refer to their former publications (Canton and Slooff, 1982) and Slooff and Canton, 1983. According to this all daphnids (one day old) had been obtained from standardised laboratory cultures, whereas the tests were carried out in analogy to the rules of the Dutch Standardisation Organisation (NEN 6501, 6502, 6504 and 6506 DSO 1980). 25 organisms per group were used and the test volume per group was 1 litre. Daphnids were fed with Chlorella and the test solution was renewed three times a week. In addition to the test description of the Dutch Standardisation Organisation, where only nominal concentrations were reported, the actual concentrations of the test substance were measured in the present test.

[*1] This value is only a numeric value in a table in the cited study. It refers to an unpublished US-EPA study (68-01-4646, 1978). No further information concerning test design and test conditions is given in the EPA-study, hence the value can not be validated.

[*2] Relevant information are missing which allow to assess the validity and reliability of the results of the study. The results are presented only as graphs and in tabular form and can therefore not be validated.

3.2.1.1.3 Algae

In the following table the toxicity data to algae are listed.

Table 3.13 Toxicity data to algae

Species	Endpoint	Effect concentrations [mg/l]	Test system	Reference
Chlorella pyrenoidosa	96-hour EC_{50}	18 (no data whether nc or mc)	Static (OCED-Guideline 201) Endpoint: growth inhibition	(Maas-Diepeveen and van Leeuwen, 1986)
Chlorella pyrenoidosa	72-hour EC_{10} 72-hour NOEC	8.5 (mc) 9.2 (mc)	Static (no standard method) Endpoint: growth inhibition	(Ramos et al., 1999)
Microcystis aeruginosa *Scenedesmus quadricauda*	8-day EC_3 8-day EC_3	1.9 (nc) 33 (nc)	Static (no standard method) Endpoint: growth inhibition	(Bringmann and KühnKühn, 1978)
Scenedesmus obliquus	48-hour EC_{50}	67.7 (nc)	Static (OCED-Guideline 201) Endpoint: growth inhibition	(Liu and Lang, 1995)
Selenastrum capricornutum	96-hour EC_{50}	23.8 (no data whether nc or mc)	Static (US-standard test) Endpoint: growth inhibition	(Bollmann et al., 1989)
Skeletonema costatum	96-hour EC_{50}	10.3*)	Endpoint: photosynthesis effects	(LeBlanc, 1984)

*) This value is only a numeric value in a table in the cited study. It refers to an unpublished US-EPA study (68-01-4646, 1978). No further information concerning test design and test conditions is given in the EPA-study, hence the value can not be validated.

EC_{50}-values for different algal species are in the range from 18 mg/l to 68 mg/l. The lowest effect value from a test with a standardized exposure time of 96 hours was found by Maas-Diepeveen with *Chlorella pyrenoidosa* with a 96-hour EC_{50} of 18 mg/l.

For *Microcystis aeruginosa* Bringmann and Kühn found an 8-day EC_3 of 1.9 mg/l. However, after 8 days the algae may no longer be in the exponential growth phase and this can have a negative influence on the test result. Therefore this low effect value should be used with care.

There are additional toxicity data to algae in the USEPA report "Nitrobenzene Ambient Water Quality Criteria. EPA 440/5-80-061". A 96-hour EC_{50} for the freshwater alga *Selenastrum capricornutum* of 44.1 and 42.8 mg/l based on chlorophyll-A and cell numbers respectively, and a 96-hour EC_{50} for the salt-water alga *Skeletonema costatum* of 10.3 and 9.7 mg/l based on chlorophyll-A and cell numbers are mentioned. These algal data are only figures in a table and have apparently not been published (US EPA 1978, Contract No. 68-01-4646). No test protocol or test description is available and hence the data can not be validated.

3.2.1.1.4 Microorganisms

The following table shows the effect values available for microorganisms. The effect concentrations for bacteria range from 24-hour IC_{50}=0.92 mg/l (*Nitrosomonas*) to 49-hour IC_{50}=370 mg/l (aerobic heterotrophs).

For protozoa the effect data show a range from 1.9 mg/l (72-hour TGK *Entosiphon sulcatum*) up to 98 mg/l (24-hour EC_{50} *Tetrahymena pyriformis*).

Table 3.14 Toxicity to microorganisms

Species	Duration	Effect concentrations [mg/l]	Effect	Reference
Aerobic heterotrophs	49 hours	IC_{50} = 370 (nc)	Inhibition of oxygen uptake	(Blum and Speece, 1991)
Activated sludge	3 hours	EC_{50} = 100 (nc)	Inhibition of oxygen uptake	(Yoshioka et al., 1986a)
Vibrio harveyi	5 hours	EC_{50} = 17.5 (nc)	growth inhibition	(Thomulka et al., 1992)
Methanogens	13 days	NOEC = 10 (mc)	Inhibition of gas production	(Bhattacharya et al., 1996)
Methanogens	96 hours	IC_{50}= 13 (nc)	Inhibition of gas production	(Blum and Speece, 1991)
Nitrosomonas	24 hours	IC_{50} = 0.92 (nc)	Inhibition of ammonia consumption	(Blum and Speece, 1991)
Chilomonas paramaecium (cryptomonad)	48 hours	TGK = 17 (nc) 1)	Inhibition of cell multiplication	(Bringmann et al., 1980)
Entosiphon sulcatum (euglenoid)	72 hours	TGK = 1.9 (nc) 1)	Inhibition of cell multiplication	(Bringmann and Kühn, 1980a)
Tetrahymena pyriformis (ciliate)	24 hours	EC_{50} = 98 (nc)	growth inhibition	(Yoshioka et al., 1985)
Uronema parduczi (ciliate)	20 hours	TGK = 15 (nc) 1)	Inhibition of cell multiplication	(Bringmann and Kühn, 1980b)

1) TGK= toxic threshold concentration, defined as 5% effect compared to the control

There is one study with activated sludge of one of the production sites (BASF AG, 1979). Industrial activated sludge was incubated with nitrobenzene in the presence of nutrient salts, but the exposure period was not reported. An EC_{20} of 1,000 mg/l was found.

The most sensitive microorgamism species is *Nitrosomonas*. The test was conducted in a closed system. Sealed serum bottles were prepared with ammonia feed and 20 ml of surcharged oxygen. Ammonia was measured at the end of the assay period using an ammonia selective electrode. Nitrite was checked to ensure that only toxicity to *Nitrosomonas* and not toxicity to *Nitrobacter* was controlling the rate of metabolic activity. Therefore, the effect value from this test will be used for the risk assessment of sewage treatment plants.

However, according to expert judgement the process of nitrification is not the main mechanism in a constructed wetland like the one used as a WWTP at site E. The activated sludge respiration inhibition test is considered more relevant for the reed bed system and therefore this test will be used for assessing the risk at this specific site.

3.2.1.1.5 Amphibians

There are two studies on amphibians available.

An acute test to *xenopus laevis* (African clawed frog) resulted in a 96-hour LC_{50} of 121 mg/l and in a 96-hour EC_{50} of 54 mg/l (Canton et al., 1985). The description of the method was given by another publication (Canton and Slooff, 1982). Ten animals per group (3-4 weeks old) were exposed to nitrobenzene test solutions over a period of 96 hours in a semi-static test system (renewal of the test substance once a day). Besides the endpoint mortality the effect "behaviour" was not further explained.

In another test to *rana pipiens* (northern leopard frog) a 9-day LC_{50} of 0.640 mg/l was obtained (Black et al., 1982). These effect values found by Black et al. for *rana pipiens* are not employed in the further effects assessment (for explanation please see Section 3.2.1.1.1 Fish – long-term toxicity).

3.2.1.2 Calculation of Predicted No Effect Concentration (PNEC)

Calculation of $PNEC_{aqua}$

For vertebrates, invertebrates and algae no significant differences in sensitivity between marine and freshwater species are recorded.

Results from acute toxicity tests with species from 3 trophic levels are available. The most sensitive organisms from standard tests (EC_{50}) are *Oryzias latipes, Daphnia magna* and *Chlorella pyrenoidosa.*

Reliable long-term NOECs are available for invertebrates (*Daphnia magna*) and several algae species. For fish and other vertebrates only prolonged tests results are available which are not regarded as long-term tests.

Thus, according to the EU Technical Guidance Document the assessment factor is set at 50 for the aquatic compartment as data from valid long-term tests on 2 trophic levels are available. The most sensitive value has been determined for *Daphnia magna* with a 21-day NOEC of 1.9 mg/l.

The PNECaqua is calculated as follows:

$$PNECaqua = 1.9 \text{ mg/l} / 50 = 0.038 \text{ mg/l} = 38 \text{ µg/l}$$

Calculation of the $PNEC_{WWTP}$

For the determination of the $PNEC_{WWTP}$ different tests with microorganisms, bacteria and protozoa, are available.

The lowest effect concentration found was for *Nitrosomonas* with a 24-hour IC_{50} of 0.92 mg/l. Applying an assessment factor of 10 leads to a $PNEC_{WWTP}$ = 92 µg/l. This PNEC is used for the risk characterisation of WWTP at all sites except site E.

For the assessment of the reed bed system at site E the activated sludge respiration inhibition test was considered. It leads to a 3-hour EC_{50} of 100 mg/l. Applying an assessment factor of 100 results in a $PNEC_{WWTP}$ of 1 mg/l for the assessment of this specific site.

3.2.1.3 Toxicity test results for sediment organisms

No sediment tests with nitrobenzene and sediment-dwelling organisms are available.

Nitrobenzene reaches waste water by production and processing industries. From Henry's law constant and the log Pow it can be concluded that nitrobenzene will remain mostly in water and only a small part of it will adsorb to the sediment.

3.2.1.4 Calculation of Predicted No Effect Concentration (PNEC) for sediment organisms

As there is a lack of tests on sediment-dwelling organisms the equilibrium partitioning method can be used as surrogate to calculate the $PNEC_{sediment}$.

$PNEC_{sediment} = K_{susp\text{-}water} / RHO_{susp} \cdot PNEC_{water} \cdot 1{,}000$

where $K_{susp\text{-}water} = 3.85\ m^3/m^3$
$RHO_{susp} = 1{,}150\ kg/m^3$
$PNEC_{water} = 0.038\ mg/l$

The $PNEC_{sed.}$ is 0.127 mg/kg wet weight obtained by this calculation. Using the default water content of sediment from the Technical Guidance Document of 80% by volume or 61.54% by weight this value can be converted to a $PNEC_{sed.}$ = 0.331 mg/kg dry weight.

3.2.2 Terrestrial compartment

3.2.2.1 Toxicity test results

There are toxicity test results both on plants and on terrestrial invertebrates (earthworms) available.

3.2.2.1.1 Plants

In a 72 hours phytotoxicity test eight species of plants were exposed to nitrobenzene in exposure chambers (McFarlane et al., 1990). All plant species examined in this study were provided with nutrient medium containing nitrobenzene. Phytotoxicity to nitrobenzene varies considerably between species. When roots were dosed at 8 mg/l the photosynthesis and transpiration responses vary from no effect to complete suppression.

No visible symptoms or changes in the transpiration or photosynthetic rates occurred with soybeans (*glycine maximus*), barley (*hordeum vulgare*), honeysuckle (*lonicera tatarica*) and poplar (*populus robusta*). For these species the 72-hour NOEC ≥ 8 mg/l. Green ash (*fraxinus pennsylvanica*) and lettuce (*lactuca sativa*) showed no visible symptoms but suffered an initial decrease in both transpiration and photosynthesis rate. The ash plants started recovery after about 10 hours. Lettuce plants recovered much more slowly, the photosynthetic rate started to increase after about 60 hours. Two *Elaeagnus* species seem to be the most sensitive to nitrobenzene. Autumn olive (*Elaeagnus umbellata*) did not survive the dosing of 8 mg/l (LC_{100} = 8 mg/l). Shortly after dosing the transpiration and photosynthetic rate decreased rapidly and did not recover, leaves dropped spontaneously and by the end of the study all remaining leaves dropped when the plants were touched. Russian olive plants (*Elaeagnus angustifolia*) were similar to the autumn olive in that some of the leaves on some of the plants dropped. However, the newest leaves and all leaves on one plant remained intact and continued to function (photosynthesis and transpiration), although at reduced rates. Recovery started after about 10 hours and was complete at the end of the experiment.

Inhibition of root growth of soybean plants (*glycine maximus*) without an accompanied impairment of transpiration and photosynthesis rate was also observed (Fletcher J et al., 1990). The plants were exposed to nitrobenzene concentrations of 0.02 to 100 mg/l via roots and

harvested after 72 hours. The lower concentration of nitrobenzene did not appear to cause plant damage or alter shoot growth. But a visual examination of roots before and after nitrobenzene exposure indicated that the highest concentration inhibited root growth.

3.2.2.1.2 Earthworm

The following table shows the results of the toxicity tests to four earthworm species (Neuhauser et al., 1986). All of the reported concentrations are nominal concentrations.

Table 3.15 Toxicity towards earthworm

Species	Duration	Effect concentrations [mg/l]	Effect
Allolobophora tuberculata	48 hours	LC_{50} = 11.6 µg/cm² filter paper	Mortality
	14 days	LC_{50} = 362 mg/kg soil dw	Mortality
Eisenia fetida	48 hours	LC_{50} = 16 µg/cm² filter paper	Mortality
	14 days	LC_{50} = 319 mg/kg soil dw	Mortality
Eudrilus eugeniae	48 hours	LC_{50} = 5.5 µg/cm² filter paper	Mortality
	14 days	LC_{50} = 226 mg/kg soil dw	Mortality
Perionyx excavatus	48 hours	LC_{50} = 10.4 µg/cm² filter paper	Mortality
	14 days	LC_{50} = 343 mg/kg soil dw	Mortality

In the 48-hour test filter paper soaked with 1 ml nitrobenzene solution was put into a glass vial and one animal per glass vial was added. After 48 hours at 20°C in the dark mortality was determined

For the 14 day tests 10 worms per assay were exposed to soil containing various concentrations of nitrobenzene. The artificial soil consisted of 10% peat, 20% kaolinite clay, 69% fine sand and 1% calcium carbonate. An aqueous nitrobenzene solution was then added (water content = 35% of dry weight).

3.2.2.2 Calculation of Predicted No Effect Concentration (PNEC)

From the tests to plants no EC_{50} or NOEC can be derived. Hence for the calculation of the $PNEC_{soil}$ there is only one terrestrial test result available (earthworm). It is calculated with the most sensitive of the earthworm species *Eudrilus eugeniae* with a 14-day LC_{50} of 226 mg/kg soil dw and an assessment factor of 1,000, as results from long-term tests are not available.

$$PNEC_{soil} = 0.226 \text{ mg/kg dw}$$

As there is only one terrestrial test result available the TGD instructs that the risk assessment should be performed both on this test result and on the basis of the outcome of the aquatic toxicity data in this case. A PNECsoil can be derived by using the equilibrium partitioning method.

$$PNEC_{soil} = K_{soil\text{-}water} / RHO_{soil} \cdot PNEC_{water} \cdot 1{,}000$$

With:

$K_{soil\text{-}water} = 3.74 m^3/m^3$
$RHO_{soil} = 1{,}700 \text{ kg/m}^3$
$PNEC_{water} = 0.038 \text{ mg/l}$

A $PNEC_{soil}$ of 0.084 mg/kg ww is obtained by this method. Using the default water content of soil from the Technical Guidance Document of 20% by volume or 11.8% by weight this value can be converted to $PNEC_{soil}$ = 0.10 mg/kg dry weight.

The use of the equilibrium partitioning method based on the $PNEC_{water}$ results in a lower $PNEC_{soil}$. Thus, the $PNEC_{soil}$ derived from the equilibrium partitioning is used for risk assessment.

3.2.3 Atmosphere

There is one short-term test with wheat plants (*Tritium aestivum*) reported (Christ, 1996).

Ten days old plants were kept under greenhouse conditions using a flow-through system with a flow of air containing various concentrations of nitrobenzene (2 m^3/hour) in an exposure chamber of 260 litres. The test lasted over three hours. The maximum light intensity was about 50% compared to outdoor conditions. The endpoint photosynthetic rate was measured as the differences in the CO_2-content between incoming and outgoing air compared to a control without nitrobenzene. Apparently no analytical measurement took place. The following LOEC was found:

Triticum aestivum endpoint: photosynthetic rate 3-hour LOEC = 150 mg/m^3

The author classifies nitrobenzene as a substance which is dangerous to plants at low concentrations.

3.2.4 Secondary poisoning

Nitrobenzene has some potential for persistence. However, there are no indications for bioaccumulation potential of nitrobenzene. Neither has nitrobenzene a log Kow ≥ 3 nor is it highly adsorptive or belongs to a class of substances known to have a potential to accumulate in living organisms. The TGD indicates that substances which have a potential to cause toxic effects if accumulated in higher organisms should be considered in the effects assessment for secondary poisoning only if there is an indication of their bioaccumulation potential. Nitrobenzene does not present an indication of a bioaccumulation potential. An effect assessment for secondary poisoning is therefore not considered necessary.

3.3 RISK CHARACTERISATION

3.3.1 Aquatic compartment (incl. sediment)

Surface water

The PEC/PNEC ratios are below 1 for all production and/or processing sites. The currently available data do not indicate any risk to the aquatic biocenosis. Regarding the $PNEC_{aqua}$ of 38 µg/l the following PEC/PNEC ratios can be calculated:

Table 3.16 PEC/PNEC ratios for the aquatic compartment

Scenario	Site specific PEC_{aqua} [µg/l]	PEC/PNEC
Production/processing sites:		
A	0.87	0.02
B	0.08	< 0.01
C	8.35	0.22
D	0.03	< 0.01
E	2.78	0.07
F	0.01	< 0.01
G	0.02	< 0.01
H	0.02	< 0.01

Sediment

The highest PEC/PNEC ratio for sediment is the same as for water at site C as both the PEC and the PNEC are calculated from the respective water values. Hence no risk for sediment dwelling organisms can be detected.

Conclusion (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.

Conclusion (ii) applies to surface water and sediment regarded for the production and/or processing of nitrobenzene. All PEC/PNEC ratios are below 1.

Waste-water treatment plants

A possible risk to microorganisms is only evaluated for industrial waste water treatment plants as no nitrobenzene is expected to enter municipal waste water treatment plants.

Effluent concentrations (=PEC_{stp}) between < 1 µg/l and 140 µg/l were given for the industrial WWTPs at the production/processing sites except for site E where a PEC_{WWTP} of 1,000 µg/l is reported. All data are based on measurements at the respective sites.

Applying the $PNEC_{microorganisms}$ of 92 µg/l for the industrial WWTPs at all sites except for site E and the $PNEC_{microorganisms}$ of 1,000 µg/l for the constructed wetland at site E all ratios of $PEC/PNEC_{microorganisms}$ are ≤ 1.

The maximum effluent concentration at one site is above the PNEC (140 µg/l). At this site daily measurements of the effluent concentrations of the industrial WWTP took place in the year 2000. Only 5 out of 352 values were above the detection limit (12 µg/l) and thereof only two were in the range of the $PNEC_{WWTP}$. Hence, it can be assumed that there is no risk to the WWTP microorganisms at this site.

Conclusion (i) There is a need for further information and/or testing.

No **conclusion (i)** was drawn

Conclusion (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.

Conclusion (ii) applies to all of the industrial WWTPs at sites A, B, D, E, F, G and H.

3.3.2 Terrestrial compartment

The comparison of $PEClocal_{soil}$ at site C of $2.3 \cdot 10^{-3}$ mg/kg ww with the $PNEC_{soil}$ of 0.084 mg/kg ww indicates no risk for the terrestrial compartment.

Conclusions to the risk assessment for the terrestrial compartment:

Conclusion (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.

3.3.3 Atmosphere

There are no representative fumigation tests for nitrobenzene available. An quantitative effect assessment for this compartment therefore can not be performed.

The only result is a 3-hour LOEC of 150 mg/m^3. Comparing this result with the highest $PEClocal_{air\_annual}$ of $4.6 \cdot 10^{-4}$ mg/m^3 at site C no risk to terrestrial plants via air emissions of nitrobenzene can be found as the ratio of $PEClocal_{air\_annual}$ /LOEC is very small ($3 \cdot 10^{-6}$).

Nitrobenzene may be dangerous for the atmospheric environment at low concentrations as it is classified as R48 (”Danger of serious damage to health by prolonged exposure”). There are no long-term or chronic data available that could help decide whether further plant fumigation toxicity data were needed. However, the comparison of the PEC with the LOEC, which leads to a very small risk quotient, indicates in a first approach that nitrobenzene might pose no risk to plants.

The potential of a contribution of nitrobenzene to the formation of harmful ground-level ozone is an aspect which can not be excluded. Nitrobenzene has a relative long half life in the atmosphere ($t_{1/2}$ = 66 days) but, on the other hand, releases to the atmosphere take only place from point sources and no additional entry into the atmosphere, e.g. from traffic emissions, occur. There are no data available on the ozone formation potential of nitrobenzene and no measured air concentrations exist for Europe.

Conclusions to the risk assessment for the atmosphere:

Conclusion (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.

3.3.4 Secondary poisoning

Nitrobenzene has some potential for persistence. But there are no indications for bioaccumulation potential of nitrobenzene. Neither has nitrobenzene a log Kow ≥ 3 nor is it highly adsorptive or belongs to a class of substances known to have a potential to accumulate in living organisms. The TGD indicates that substances which have a potential to cause toxic effects if accumulated in higher organisms should be considered in the effects assessment for secondary poisoning only if there is an indication of their bioaccumulation potential.

As nitrobenzene has only a low bioaccumulation potential no risk characterization for secondary poisoning has to be conducted.

3.3.5 PBT-assessment

The following table shows the PBT/vPvB criteria as defined in the TGD and the values relevant for nitrobenzene. The description of the relevant tests can be found in Section 3.1.3.1 (B), 3.1.3.3 (P) and in Section 3.2.1.1 (T).

Table 3.17 Data for nitrobenzene and PBT/vPvB criteria according to TGD

Criterion	PBT-criteria	vPvB-criteria	Nitrobenzene
P	Half-life > 60 days in marine water or > 40 days in freshwater or half-life > 180 days in marine sediment or > 120 days in freshwater sediment	Half-life > 60 days in marine- or freshwater or half-life > 180 days in marine or freshwater sediment	non biodegradable (surface water) no degradation rate constant for the sediment could be derived.
B	BCF > 2,000	BCF > 5,000	BCF (fish) = 30.6
T	Chronic NOEC < 0.01 mg/l or CMR or endocrine disrupting effects	Not applicable	72-hour NOEC (algae): 9.2 mg/l 21-day NOEC (*Daphnie Magna*) = 1.9 mg/l Carcinogenic Cat. 3 Toxic for Reproduction Cat. 3

Nitrobenzene has to be considered as non biodegradable in surface water. No degradation rate constants for degradation of nitrobenzene in sediment or soil could be derived.

The highest measured BCF in fish is 30.6.

The lowest long-term effect value of 1.9 mg/l was found for *Daphnia magna*.

Nitrobenzene is classified as Carcinogenic (Cat. 3) and Toxic for Reproduction (Cat. 3). There is evidence of serious damage to health by prolonged exposure through inhalation and contact with skin (T, R48/23/24).

It can be concluded that nitrobenzene could possibly fulfil the P/vP-criteria. The B- and T-criteria are not fulfilled. Overall nitrobenzene does not meet the PBT criteria.

4 HUMAN HEALTH

4.1 HUMAN HEALTH (TOXICITY)

4.1.1 Exposure assessment

4.1.1.1 General discussion

4.1.1.2 Occupational exposure

4.1.1.3 Consumer exposure

4.1.1.4 Humans exposed via the environment

Indirect exposure via the environment is calculated using data for oral intake via food, drinking water and air (for calculation see **Appendix A**). One local scenario, site C with the highest PEClocal for surface water, was considered. Following the data for the regional scenario the total daily dose is smaller. The resultant daily doses for the uptake of nitrobenzene are:

DOSEtot = 0.42 µg / kg bodyweight and day (local scenario site C)

DOSEtot = 0.57 ng/kg bodyweight and day (regional background concentrations)

Table 4.1 Results of calculation of the indirect exposure

Intake route	% of total intake	
	Local site C	Regional
Drinking water	47.0	64.9
Air	23.7	1.95
Stem	6.31	0.56
Root	2.44	4.23
Meat	< 0.01	< 0.01
Milk	< 0.01	< 0.01
Fish	20.6	28.4

5 RESULTS

5.1 INTRODUCTION

5.2 ENVIRONMENT

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

No **conclusion (iii)** was drawn.

Conclusion (i) There is a need for further information and/or testing.

No **conclusion (i)** was drawn

Conclusion (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.

Conclusion (ii) applies to surface water, sediment, the atmosphere and the terrestrial compartment regarded for the production and/or processing of nitrobenzene. All PEC/PNEC ratios are below 1. This conclusion also applies to the industrial WWTPs of all sites.

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Abbreviations

ADI	Acceptable Daily Intake
AF	Assessment Factor
ASTM	American Society for Testing and Materials
ATP	Adaptation to Technical Progress
AUC	Area Under The Curve
B	Bioaccumulation
BBA	Biologische Bundesanstalt für Land- und Forstwirtschaft
BCF	Bioconcentration Factor
BMC	Benchmark Concentration
BMD	Benchmark Dose
BMF	Biomagnification Factor
BOD	Biochemical Oxygen Demand
bw	body weight / *Bw*, *bw*
C	Corrosive (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)
CA	Chromosome Aberration
CA	Competent Authority
CAS	Chemical Abstract Services
CEC	Commission of the European Communities
CEN	European Standards Organisation / European Committee for Normalisation
CEPE	European Committee for Paints and Inks
CMR	Carcinogenic, Mutagenic and toxic to Reproduction
CNS	Central Nervous System
COD	Chemical Oxygen Demand
CSTEE	Scientific Committee for Toxicity, Ecotoxicity and the Environment (DG SANCO)
CT_{50}	Clearance Time, elimination or depuration expressed as half-life
d.wt	dry weight / dw
dfi	daily food intake
DG	Directorate General
DIN	Deutsche Industrie Norm (German norm)
DNA	DeoxyriboNucleic Acid
DOC	Dissolved Organic Carbon
DT50	Degradation half-life or period required for 50 percent dissipation / degradation
DT90	Period required for 90 percent dissipation / degradation
E	Explosive (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)
EASE	Estimation and Assessment of Substance Exposure Physico-chemical properties [Model]

EbC50	Effect Concentration measured as 50% reduction in biomass growth in algae tests
EC	European Communities
EC10	Effect Concentration measured as 10% effect
EC50	median Effect Concentration
ECB	European Chemicals Bureau
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECVAM	European Centre for the Validation of Alternative Methods
EDC	Endocrine Disrupting Chemical
EEC	European Economic Communities
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of New Chemical Substances
EN	European Norm
EPA	Environmental Protection Agency (USA)
ErC50	Effect Concentration measured as 50% reduction in growth rate in algae tests
ESD	Emission Scenario Document
EU	European Union
EUSES	European Union System for the Evaluation of Substances [software tool in support of the Technical Guidance Document on risk assessment]
F(+)	(Highly) flammable (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)
FAO	Food and Agriculture Organisation of the United Nations
FELS	Fish Early Life Stage
foc	Organic carbon factor (compartment depending)
GLP	Good Laboratory Practice
HEDSET	EC/OECD Harmonised Electronic Data Set (for data collection of existing substances)
HELCOM	Helsinki Commission -Baltic Marine Environment Protection Commission
HPLC	High Pressure Liquid Chromatography
HPVC	High Production Volume Chemical (> 1000 tonnes/annum)
IARC	International Agency for Research on Cancer
IC	Industrial Category
IC50	median Immobilisation Concentration or median Inhibitory Concentration
ILO	International Labour Organisation
IPCS	International Programme on Chemical Safety
ISO	International Organisation for Standardisation
IUCLID	International Uniform Chemical Information Database (existing substances)
IUPAC	International Union for Pure and Applied Chemistry
JEFCA	Joint FAO/WHO Expert Committee on Food Additives
JMPR	Joint FAO/WHO Meeting on Pesticide Residues

Koc	organic carbon normalised distribution coefficient
Kow	octanol/water partition coefficient
Kp	solids-water partition coefficient
L(E)C50	median Lethal (Effect) Concentration
LAEL	Lowest Adverse Effect Level
LC50	median Lethal Concentration
LD50	median Lethal Dose
LEV	Local Exhaust Ventilation
LLNA	Local Lymph Node Assay
LOAEL	Lowest Observed Adverse Effect Level
LOEC	Lowest Observed Effect Concentration
LOED	Lowest Observed Effect Dose
LOEL	Lowest Observed Effect Level
MAC	Maximum Allowable Concentration
MATC	Maximum Acceptable Toxic Concentration
MC	Main Category
MITI	Ministry of International Trade and Industry, Japan
MOE	Margin of Exposure
MOS	Margin of Safety
MW	Molecular Weight
N	Dangerous for the environment (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC
NAEL	No Adverse Effect Level
NOAEL	No Observed Adverse Effect Level
NOEL	No Observed Effect Level
NOEC	No Observed Effect Concentration
NTP	National Toxicology Program (USA)
O	Oxidising (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)
OC	Organic Carbon content
OECD	Organisation for Economic Cooperation and Development
OEL	Occupational Exposure Limit
OJ	Official Journal
OSPAR	Oslo and Paris Convention for the protection of the marine environment of the Northeast Atlantic
P	Persistent
PBT	Persistent, Bioaccumulative and Toxic
PBPK	Physiologically Based PharmacoKinetic modelling

PBTK	Physiologically Based ToxicoKinetic modelling
PEC	Predicted Environmental Concentration
pH	logarithm (to the base 10) (of the hydrogen ion concentration $\{H^+\}$
pKa	logarithm (to the base 10) of the acid dissociation constant
pKb	logarithm (to the base 10) of the base dissociation constant
PNEC	Predicted No Effect Concentration
POP	Persistent Organic Pollutant
PPE	Personal Protective Equipment
QSAR	(Quantitative) Structure-Activity Relationship
R phrases	Risk phrases according to Annex III of Directive 67/548/EEC
RAR	Risk Assessment Report
RC	Risk Characterisation
RfC	Reference Concentration
RfD	Reference Dose
RNA	RiboNucleic Acid
RPE	Respiratory Protective Equipment
RWC	Reasonable Worst-Case
S phrases	Safety phrases according to Annex IV of Directive 67/548/EEC
SAR	Structure-Activity Relationships
SBR	Standardised birth ratio
SCE	Sister Chromatic Exchange
SCHER	Scientific Committee on Health and Environmental Risks
SDS	Safety Data Sheet
SETAC	Society of Environmental Toxicology And Chemistry
SNIF	Summary Notification Interchange Format (new substances)
SSD	Species Sensitivity Distribution
STP	Sewage Treatment Plant
T(+)	(Very) Toxic (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)
TDI	Tolerable Daily Intake
TG	Test Guideline
TGD	Technical Guidance Document
TNsG	Technical Notes for Guidance (for Biocides)
TNO	The Netherlands Organisation for Applied Scientific Research
ThOD	Theoritical Oxygen Demand
UC	Use Category
UDS	Unscheduled DNA Synthesis
UN	United Nations

UNEP	United Nations Environment Programme
US EPA	Environmental Protection Agency, USA
UV	Ultraviolet Region of Spectrum
UVCB	Unknown or Variable composition, Complex reaction products of Biological material
vB	very Bioaccumulative
VOC	Volatile Organic Compound
vP	very Persistent
vPvB	very Persistent and very Bioaccumulative
v/v	volume per volume ratio
w/w	weight per weight ratio
WHO	World Health Organisation
WWTP	Waste Water Treatment Plant
Xn	Harmful (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)
Xi	Irritant (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)

Appendix A Indirect exposure via the environment

INDIRECT EXPOSURE VIA THE ENVIRONMENT

(TGD On New and Existing Chemicals, chapter 2)

Parameter [Unit]	*Symbol*
Definitions (for the use in this document)	
definition of the unit 'kg$_{bw}$' for body weight	$kg_{bw} := 1 \cdot kg$
definition of the unit 'd' for day	$d := 1 \cdot Tag$
	$scenario := 1 .. 2$
	$local := 1$ $regional := 2$
Constants	
gas - constant R	$R := 8.314 \cdot J \cdot K^{-1} \cdot mol^{-1}$
Defaults	
volumefraction air in plant tissue [-]	$Fair_{plant} := 0.3$
volumefraction water in plant tissue [-]	$Fwater_{plant} := 0.65$
volumefraction lipids in plant tissue [-]	$Flipid_{plant} := 0.01$
bulk density of plant tissue [kg$_{wet\ plant}$ *m$_{plant}$ $^{-3}$]	$RHO_{plant} := 700 \cdot kg \cdot m^{-3}$
leaf surface area [m^2]	$AREA_{plant} := 5 \cdot m^2$
conductance (0.001 m*s^{-1}) [m*d^{-1}]	$g_{plant} := 0.001 \cdot m \cdot s^{-1}$
shoot volume [m^3]	$V_{leaf} := 0.002 \cdot m^3$
transpiration stream [m^3*d^{-1}]	$Q_{transp} := 1 \cdot 10^{-3} \cdot m^3 \cdot d^{-1}$
correction exponent for differences between plant lipids and octanol [-]	$b := 0.95$
growth rate constant for dilution by growth [d^{-1}]	$kgrowth_{plant} := 0.035 \cdot d^{-1}$
pseudo-first order rate constant for metabolism in plants [d^{-1}]	$kmetab_{plant} := 0 \cdot d^{-1}$
pseudo-first order rate constant for photolysis in plants [d^{-1}]	$kphoto_{plant} := 0 \cdot d^{-1}$

concentration in meat and milk

daily intake of grass
[$kg_{wetgrass}*d^{-1}$]

$IC_{grass} := 67.6 \cdot kg \cdot d^{-1}$

daily intake of soil
[$kg_{wet\ soil}*d^{-1}$]

$IC_{soil} := 0.46 \cdot kg \cdot d^{-1}$

daily intake of air
[$m_{air}{}^{3}*d^{-1}$]

$IC_{air} := 122 \cdot m^3 \cdot d^{-1}$

daily intake of drinkingwater
[$l*d^{-1}$]

$IC_{drw} := 55 \cdot l \cdot d^{-1}$

daily intake for human

daily intake for the several pathways
[$kg_{chem}*d^{-1}$] or [$m^{3}*d^{-1}$]

$IH_{drw} := 2 \cdot l \cdot d^{-1}$

$IH_{fish} := 0.115 \cdot kg \cdot d^{-1}$

$IH_{stem} := 1.2 \cdot kg \cdot d^{-1}$

$IH_{root} := 0.384 \cdot kg \cdot d^{-1}$

$IH_{meat} := 0.301 \cdot kg \cdot d^{-1}$

$IH_{milk} := 0.561 \cdot kg \cdot d^{-1}$

$IH_{air} := 20 \cdot m^3 \cdot d^{-1}$

bioavailability through route of intake
[-]

$BIO_{inh} := 0.75$

$BIO_{oral} := 1.0$

average body weight of human
[kg]

$BW := 70 \cdot kg_{bw}$

Name: **Nitrobenzene** CAS - No.: 98 – 95 – 3

Input

chemical properties

octanol-water partitioning coefficient [-]	$\log K_{OW} := 1.86$ $K_{OW} := 10^{\log K_{OW}}$
Henry - partitioning coefficient [Pa*m^3*mol^{-1}]	$HENRY := 1.296 \cdot Pa \cdot m^3 \cdot mol^{-1}$
air-water partitioning coefficient [-]	$K_{air\_water} := 5.32 \cdot 10^{-4}$
fraction of the chemical associated with aerosol particles [-]	$F_{ass\_aer} := 5 \cdot 10^{-6}$
half-life for biodegration in surface water [d]	$DT_{50\_bio\_water} := 1000000\,d$

environmental concentrations

annual average local PEC in surface water (dissolved) [mg$_{chem}$ * l$_{water}^{-1}$] , (from open use)	$PEClocal_{water\_ann} := 6.85 \cdot 10^{-3} \cdot mg \cdot l^{-1}$
annual average local PEC in air (total) [mg$_{chem}$ * m$_{air}^{-3}$] (from open use)	$PEClocal_{air\_ann} := 4.6 \cdot 10^{-4} \cdot mg \cdot m^{-3}$
local PEC in grassland (total), averaged over 180 days [mg$_{chem}$ * kg$_{soil}^{-1}$]	$PEClocal_{grassland} := 2.36 \cdot 10^{-3} \cdot mg \cdot kg^{-1}$
local PEC in porewater of agriculture soil [mg$_{chem}$ * l$_{porewater}^{-1}$]	$PEClocal_{agr\_soil\_porew} := 1.05 \cdot 10^{-3} \cdot mg \cdot l^{-1}$
local PEC in porewater of grassland [mg$_{chem}$ * l$_{porewater}^{-1}$]	$PEClocal_{grassland\_porew} := 1.07 \cdot 10^{-3} \cdot mg \cdot l^{-1}$
local PEC in groundwater under agriculture soil [mg$_{chem}$ * l$_{water}^{-1}$]	$PEClocal_{grw} := 1.05 \cdot 10^{-3} \cdot mg \cdot l^{-1}$
regional PEC in surface water (dissolved) [mg$_{chem}$ * l$_{water}^{-1}$]	$PECregional_{water} := 1.3 \cdot 10^{-5} \cdot mg \cdot l^{-1}$
regional PEC in air (total) [mg$_{chem}$ * m$_{air}^{-3}$]	$PECregional_{air} := 5.2 \cdot 10^{-8} \cdot mg \cdot m^{-3}$
regional PEC in agriculture soil (total) [mg$_{chem}$*kg$_{soil}^{-1}$	$PECregional_{agr\_soil} := 5.4 \cdot 10^{-6} \cdot mg \cdot kg^{-1}$
regional PEC in porewater of agriculture soils [mg$_{chem}$*l$_{water}^{-1}$	$PECregional_{agr\_soil\_porew} := 2.5 \cdot 10^{-6} \cdot mg \cdot l^{-1}$

Definition of the concentrations used for indirect exposure

$C_{water_{local}} := PEClocal_{water\_ann}$ $C_{water_{regional}} := PECregional_{water}$

$C_{air_{local}} := PEClocal_{air\_ann}$ $C_{air_{regional}} := PECregional_{air}$

$C_{grassland_{local}} := PEClocal_{grassland}$ $C_{grassland_{regional}} := PECregional_{agr\_soil}$

$C_{agr\_porew_{local}} := PEClocal_{agr\_soil\_porew}$ $C_{agr\_porew_{regional}} := PECregional_{agr\_soil\_porew}$

$C_{grass\_porew_{local}} := PEClocal_{grassland\_porew}$ $C_{grass\_porew_{regional}} := PECregional_{agr\_soil\_porew}$

$C_{grw_{local}} := PEClocal_{grw}$ $C_{grw_{regional}} := PECregional_{agr\_soil\_porew}$

bioconcentration in fish

bioconcentration factor for fish
[$m_{water}^3 * kg_{chem}^{-1}$]

$$BCF_{fish} := 10^{0.85 \cdot \log K_{OW} - 0.7} \cdot l \cdot kg^{-1}$$

modified equation for logKow > 6

$$BCF_{fish} := wenn\left[\log K_{OW} > 6, \left[-0.278 \cdot \left(\log K_{OW}\right)^2 + 3.38 \cdot \log K_{OW} - 5.94\right] \cdot l \cdot kg^{-1}, BCF_{fish}\right]$$

$$C_{fish_{scenario}} := BCF_{fish} \cdot C_{water_{scenario}}$$

bioconcentration in plants

$$K_{plant\_water} := Fwater_{plant} + Flipid_{plant} \cdot K_{OW}^{b}$$

$$Croot_{agr\_plant_{scenario}} := \frac{K_{plant\_water} \cdot C_{agr\_porew_{scenario}}}{RHO_{plant}}$$

$$TSCF := 0.784 \cdot e^{\frac{-\left(\log K_{OW} - 1.78\right)^2}{2.44}}$$

remark: for $\log K_{OW}$ out of the range from -0.5 to 4.5
the TSCF is limited by the values for $\log K_{OW}$ = -0.5 resp. 4.5

$$TSCF := wenn\left(\log K_{OW} < -0.5, 0.903, TSCF\right)$$

$$TSCF := wenn\left(\log K_{OW} > 4.5, 0.832, TSCF\right)$$

$$K_{leaf\_air} := Fair_{plant} + \frac{K_{plant\_water}}{K_{air\_water}}$$

$$kelim_{plant} := kmetab_{plant} + kphoto_{plant}$$

$$\alpha := \frac{AREA_{plant} \cdot g_{plant}}{K_{leaf\_air} \cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant}$$

$$\beta_{agr\_plant_{scenario}} := C_{agr\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_crops_{scenario}} := \frac{\beta_{agr\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

$$\beta_{grass\_plant_{scenario}} := C_{grass\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_grass_{scenario}} := \frac{\beta_{grass\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

purification of drinking water

system may defined dependent from the aerobic biodegradation

$$system := wenn\left(DT_{50\_bio\_water} < 10 \cdot d, 0, 1\right)$$

select a column on dependence from log K_{OW}

$$FIndex := wenn\left(logK_{OW} < 4, 0, wenn\left(logK_{OW} > 5, 2, 1\right)\right)$$

$$Fpur_{logKow} := \begin{bmatrix} 1 & \frac{1}{4} & \frac{1}{16} \\ 1 & \frac{1}{2} & \frac{1}{4} \end{bmatrix}$$

$$Fpur := \frac{Fpur_{logKow_{system, FIndex}}}{wenn(HENRY > 100 \cdot Pa \cdot m^3 \cdot mol^{-1}, 2, 1)}$$

$$C_{drw_{scenario}} := wenn\left[C_{grw_{scenario}} > \left(C_{water_{scenario}} \cdot Fpur\right), C_{grw_{scenario}}, C_{water_{scenario}} \cdot Fpur\right]$$

Biotransfer to meat and milk

$$BTF_{meat} := 10^{-7.6 + logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for $logK_{OW}$ out of the range from 1.5 to 6.5
the BTF_{meat} is limited by the values for $logK_{OW}$ = 1.5 resp. 6.5

$$BTF_{meat} := wenn\left(logK_{OW} < 1.5, 7.943 \cdot 10^{-7} \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$BTF_{meat} := wenn\left(logK_{OW} > 6.5, 0.07943 \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$C_{meat_{scenario}} := BTF_{meat} \cdot \left(\begin{array}{l} C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \cdots \\ + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw} \end{array}\right)$$

$$BTF_{milk} := 10^{-8.1 + logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for $logK_{OW}$ out of the range from 3 to 6.5
the BTF_{milk} is limited by the values for $logK_{OW}$ = 1.5 resp. 6.5

$$BTF_{milk} := wenn\left(logK_{OW} < 3, 7.943 \cdot 10^{-6} \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$BTF_{milk} := wenn\left(logK_{OW} > 6.5, 0.02512\, kg^{-1} \cdot d, BTF_{milk}\right)$$

$$C_{milk_{scenario}} := BTF_{milk} \cdot \left(\begin{array}{l} C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \cdots \\ + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw} \end{array} \right)$$

total daily intake for human

daily dose through intake of several pathways

[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{drw_{scenario}} := \frac{C_{drw_{scenario}} \cdot IH_{drw}}{BW} \qquad DOSE_{air_{scenario}} := \frac{C_{air_{scenario}} \cdot IH_{air} \cdot BIO_{inh}}{BW \cdot BIO_{oral}}$$

$$DOSE_{stem_{scenario}} := \frac{C_{leaf\_crops_{scenario}} \cdot IH_{stem}}{BW} \qquad DOSE_{root_{scenario}} := \frac{Croot_{agr\_plant_{scenario}} \cdot IH_{root}}{BW}$$

$$DOSE_{meat_{scenario}} := \frac{C_{meat_{scenario}} \cdot IH_{meat}}{BW} \qquad DOSE_{milk_{scenario}} := \frac{C_{milk_{scenario}} \cdot IH_{milk}}{BW}$$

$$DOSE_{fish_{scenario}} := \frac{C_{fish_{scenario}} \cdot IH_{fish}}{BW}$$

total daily intake for human

total daily intake for human as sum of each pathway

[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{tot_{scenario}} := DOSE_{drw_{scenario}} + DOSE_{fish_{scenario}} + DOSE_{stem_{scenario}} + DOSE_{root_{scenario}} \ldots + DOSE_{meat_{scenario}} + DOSE_{milk_{scenario}} + DOSE_{air_{scenario}}$$

relative doses of specific different pathway (%)

$$RDOSE_{drw_{scenario}} := \frac{DOSE_{drw_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{air_{scenario}} := \frac{DOSE_{air_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{stem_{scenario}} := \frac{DOSE_{stem_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{root_{scenario}} := \frac{DOSE_{root_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{meat_{scenario}} := \frac{DOSE_{meat_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{milk_{scenario}} := \frac{DOSE_{milk_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{fish_{scenario}} := \frac{DOSE_{fish_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

Results of calculation

$DOSE_{tot_{local}} = 4.16297 \cdot 10^{-4} \circ \frac{mg}{kg_{bw} \cdot d}$

$DOSE_{tot_{regional}} = 5.72412 \cdot 10^{-7} \circ \frac{mg}{kg_{bw} \cdot d}$

$RDOSE_{drw_{local}} = 47.013124 \circ \%$

$RDOSE_{drw_{regional}} = 64.888324 \circ \%$

$RDOSE_{air_{local}} = 23.678143 \circ \%$

$RDOSE_{air_{regional}} = 1.94665 \circ \%$

$RDOSE_{stem_{local}} = 6.305251 \circ \%$

$RDOSE_{stem_{regional}} = 0.561165 \circ \%$

$RDOSE_{root_{local}} = 2.440699 \circ \%$

$RDOSE_{root_{regional}} = 4.226292 \circ \%$

$RDOSE_{meat_{local}} = 1.010229 \cdot 10^{-3} \circ \%$

$RDOSE_{meat_{regional}} = 1.006768 \cdot 10^{-3} \circ \%$

$RDOSE_{milk_{local}} = 8.218654 \cdot 10^{-3} \circ \%$

$RDOSE_{milk_{regional}} = 8.190497 \cdot 10^{-3} \circ \%$

$RDOSE_{fish_{local}} = 20.553555 \circ \%$

$RDOSE_{fish_{regional}} = 28.368371 \circ \%$

Appendix B Calculation of PEC_{local} for sediment

Calculation of PEC_{local} for Sediment

Chemical: Nitrobenzene - Prod.

concentration in surface water during emission period $PEClocal_{water} := 0.00835 mg \cdot l^{-1}$

partition coefficient suspended matter-water: $K_{susp\_water} := 3.849 \cdot m^3 \cdot m^{-3}$

bulk density of (wet) suspended matter $RHO_{susp} := 1150 \cdot kg \cdot m^{-3}$

$$PEClocal_{sed} := \frac{K_{susp\_water}}{RHO_{susp}} \cdot PEClocal_{water}$$

$$PEClocal_{sed} = 2.79 \cdot 10^{-2} \ mg \cdot kg^{-1}$$

Appendix C Monitoring data of surface water (Table C1), sediment (Table 2), wastewater treatment plants (Table C3), sewage of agricultural soils (Table C4), air (Table C5) and soild and groundwater (Table C6)

Table C1 Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany Rhine at Götterswickerhamm	1.0	1985	detection limit: 0.1 µg/l	LWA NRW 1986
Germany Rhine at mouth from the Emscher	0.3	1985	detection limit: 0.1 µg/l	LWA NRW 1986
Germany river Rhine at Leverkusen	max.: 0.7	1984	detection limit: 0.1 µg/l extraction with Hexan GC with ECD	LWA NRW 1985
Germany river Rhine tributarie: Lippe	0.1	1984	dto.	LWA NRW 1985
Germany river Rhine at Bad Honnef	percentil-50: < 0.1 percentil-90: 0.3	1984	dto.	LWA NRW 1985
Germany river Rhine at Düsseldorf-Flehe	 0.15 0.32 0.08 0.11 0.28 0.33 0.18 0.19 0.10 0.47 0.07	1986 Feb. March April May June July Aug. Sept. Oct. Nov. Dec.		ARW 1986
Germany river Rhine at Wiesbaden	 < 0.02 0.20 < 0.02 < 0.02 0.10 0.66 0.55	1986 Feb. March April May June Aug. Dec.		ARW 1986

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Rhine at Wesel	 0.17 0.04 0.05 0.10 0.03 0.12 0.26 0.15 0.05 0.06 0.02	1986 Feb. March April May June July Aug. Sept. Oct. Nov. Dec.		ARW 1986
Germany river Rhine at Köln	 0.12 0.36 0.07 0.10 0.06 0.12 0.21 0.25 0.16 0.05 0.65 0.15	1986 Jan. Feb. March April May June July Aug. Sept. Oct. Nov. Dec.		ARW 1986 ARW 1986
Germany river Rhine at Wiesbaden	0.05-1.6	1987	concentration fluctuations max.-min.concen-tration	IAWR 1986/87
Germany river Rhine at Köln	0.07-0.80	1987	dto.	LAWR 1986/87
Germany river Rhine at Düsseldorf	0.07-0.81	1987	dto.	LAWR 1986/87
Germany river Rhine at Lobith	< 0.1-3.6	1987	dto.	LAWR 1986/87
Germany river Rhine at Lobith road.km 862	max.: 8.4	08./09.02. 1987	Detected pollution by cases of damage and illegal introduction origin. a cause unknown	LAWR 1986/87
Germany river Rhine at Lobith	middle: 0.2 north: 0.2	1986	detection limit: 0.1 µg/L extraction with Hexan GC with ECD	LWA NRW1987
Germany river Rhine at Lobith	average: 0.2 max.: 3.6	1987	detection limit at the year: 0.1µg/L number of samples: 47	RIWA 1987/88
Germany river Rhine at Lobith	average: 0.3 max.: 1.3	1988	detection limit at the year: 0.1 µg/L number of samples: 51	RIWA 1987/88

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Rhine at Bad Honnef road km 640	1.2	03.03.1988	deceted pollution by cases of damage and illegal introduction origin. a cause unknown	RIWA 1987/88
Germany river Rhine at Bad Honnef. Düsseldorf	max.: 3	12.02.1989	case of damage origin. a cause unknown extraction with Hexan GC with ECD	LWA NRW 1990
Germany river Rhine at Bad Honnef. Düsseldorf	max.: 3 µg/L at Bad Honnef max.: 6 µg/L at Düsseldorf	1.08.1989	the BASF announced the introduction of 400 kg Nitrobenzene methods of analysis: extraction with Hexan. GC with ECD	LWA NRW 1990
Germany river Rhine at Bad Honnef. Düsseldorf	a freight of 1.2 t at Bad Honnef max.: 19 µg/L at Düsseldorf	04.11.1989	the BASF announced the introduction of 650 kg method of analysis: dto.	LWA NRW 1990
Germany river Rhine coordinated application of the measuring chips of Iffezheim to Bimmen	km 641.5: 0.059 km 733.2:0.055 km 745.6:0.047 km 777.8: 0.056 km 800: 0.055 km 869.4: 0.067	1992	the limit determination varies depending upon substance (24 single materials) between 0.01 and 0.1 µg/L	Deutsche Kommission zur Reinhaltung des Rheins 1994
Germany river Rhine (north) tributaries: Sieg, Wupper, Erft, Ruhr, Emscher and Lippe	Rhine north: 1.0 Tributaries < 0.5	1990	detection limit: 0.5 µg/L	LWA NRW 1991
Germany river Rhine (south. middle. north) tributaries: Sieg. Wupper. Erft. Ruhr (east and west) Emscher and Lippe	not detected	1992	detection limit: 0.5 µg/L	LWA NRW 1993
Gemany river Rhine (south. middle. north) tributaries: Sieg. Wupper. Erft. Ruhr (east and west). Emscher and Lippe	not detected	1993	detection limit: 0.5 µg/L	LUA NRW 1997
Germany river Rhine Rhine-km 163.9 pipe-water- with drawal-place IWB	< 0.02 < 0.02 < 0.02 < 0.02 < 0.02	01.03.1994 03.05.1994 30.08.1994 29.11.1994 average	liquidchromatographie with DAD- and fluorescence detection after solid phase-extraction of the sample	Gewässer-schutzamt Basel-Stadt 1994
Germany river Rhine Rhine-km 163.9 pipe-water-withdrawal-place IWB	< 0.02 < 0.02 < 0.02 < 0.02 < 0.02	07.03.1995 06.06.1995 03.10.1995 05.12.1995 average		AWBR 1995

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Rhine at Öhningen	average: < 0.05 percentil-90: < 0.05 max.: 0.06	1989	number of samples: 24	Umweltbundes-amt Berlin (UBA)1996
Germany river Rhine at Öhningen	average: < 0.05 percentil-90: < 0.05 max.: < 0.05	1990	number of samples: 26	UBA 1996
Germany river Rhine at Öhningen	average: < 0.05 percentil-90: < 0.05 max: < 0.05	1991	number of samples: 26	UBA 1996
Germany river Rhine at Öhningen	average: < 0.05 percentil-90: < 0.05 max.: < 0.05	1992	number of samples: 13	UBA 1996
Germany river Rhine at Öhningen	average: < 0.05 max.: < 0.05	1993	number of samples: 3	UBA 1996
Germany river Rhine at Dogern	average: < 0.05 percent.-90: <0.05 max: < 0.05	1993	number of samples: 13	UBA 1996
Germany river Rhine at Village-Neuf	average: < 0.05 percentil-90: 0.07 max.: 0.07	1989	number of samples: 14	UBA 1996
Germany river Rhine at Village-Neuf	average: < 0.05 percentil-90: 0.06 max.: 0.10	1990	Number of samples: 25	UBA 1996
Germany river Rhine at Village-Neuf	average: < 0.05 percentil-90: 0.07 max.: 0.08	1991	Number of samples: 22	UBA 1996
Germany river Rhine at Seltz	average: < 0.05 percentil-90: 0.10 max.: 0.13	1989	Number of samples: 21	UBA 1996
Germany river Rhine at Seltz	average: < 0.05 percentil-90: 0.09 max.: 0.15	1990	Number of samples: 25	UBA 1996
Germany river Rhine at Seltz	average: < 0.05 percentil-90: 0.07 max.: 0.07	1991	Number of samples: 15	UBA 1996
Germany river Rhine at Karlsruhe	average:< 0.05 percentil-90: 0.05 max.: 0.05	1993	Number of samples: 14	UBA 1996
Germany river Rhine at Maxau	average: < 0.05 percentil-90: 0.07 max.: 0.12	1989	Number of samples: 26	UBA 1996
Germany river Rhine at Maxau	average: < 0.05 percentil-90:0.08 max.: 0.21	1990	Number of samples: 24	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Rhine at Maxau	average: < 0.05 percentil-90: 0.07 max.: 0.09	1991	number of samples: 25	UBA 1996
Germany river Rhine at Mannheim	average: < 0.05 percentil-90:< 0.05 max.: < 0.05	1990	number of samples: 21	UBA 1996
Germany river Rhine at Mannheim	average: < 0.02 percentil-90: 0.03 max.: 0.08	1991	number of samples: 24	UBA 1996
Germany river Rhine at Mannheim	average: < 0.05 percentil-90:< 0.05 max.: < 0.05	1992	number of samples: 13	UBA 1996
Germany river Rhine at Mainz	average: 0.23 percentil-90: 0.37 max.: 2.70	1989	number of samples: 25	UBA 1996
Germany river Rhine at Mainz	average: < 2 percentil-90:< 2 max.: 22.50	1989	number of samples: 151	UBA 1996
Germany river Rhine at Mainz	average: 0.09 percentil-90: 0.17 max.: 0.20	1990	number of samples: 26	UBA 1996
Germany river Rhine at Mainz	average: 0.07 percentil-90: 0.10 max.: 0.21	1991	number of samples: 25	UBA 1996
Germany river Rhine at Mainz	average: < 0.05 percentil-90: 0.06 max.: 0.11	1992	number of samples: 26	UBA
Germany river Rhine at Mainz	average: < 2 percentil-90: < 2 max.: < 2	1993	number of samples: 25	UBA 1996
Germany river Rhine at Mannheim	average: 0.80 percentil-90: 0.86 max.: 12.80	1989	number of samples: 25	UBA 1996
Germany river Rhine at Mannheim	average: 0.25 percentil-90: 0.79 max.: 1.01	1990	number of samples: 26	UBA 1996
Germany river Rhine at Mannheim	average : 0.14 percentil-90: 0.26 max.: 0.59	1991	number of samples: 26	UBA 1996
Germany river Rhine at Koblenz	average: < 0.05 max.:< 0.05	1993	number of samples: 10	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Rhine at Koblenz	average: 0.14 percentil-90: 0.45 max.: 0.72	1989	number of samples: 26	UBA 1996
Germany river Rhine at Koblenz	average: 0.08 percentil-90: 0.11 max.: 0.60	1990	number of samples: 26	UBA 1996
Germany river Rhine at Koblenz	average: 0.08 percentil-90: 0.12 max.: 0.40	1991	number of samples:26	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.1 percentil-90: 0.30 max.:0.30	1984	number of samples: 13	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.1 percentil-90: 0.44 max: 0.70	1985	number of samples: 13	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.1 percentil-90: < 0.1 max.:< 0.1	1986	number of samples: 13	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.1 max.: 0.10	1987	number of samples: 7	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.1 max.: < 0.1 < 0.1	1988	number of samples: 5	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.1 percentil-90: < 0.1 max: < 0.1	1989	number of samples: 13	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1990	number of samples: 13	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1991	number of samples: 35	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1992	number of samples: 13	UBA 1996
Germany river Rhine at Bad Honnef	average: < 0.5 percentil-90: < 0.5 max.:< 0.5	1993	number of samples: 13	UBA 1996
Germany river Rhine at Düsseldorf	average: 0.28 percentil-90: 1.25 max.: 1.60	1989	number of samples: 25	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Rhine at Düsseldorf	average: 0.06 percentil-90: 0.09 max.: 0.11	1990	number of samples: 25	UBA 1996
Germany river Rhine at Düsseldorf	average: 0.07 percentil-90: 0.13 max.: 0.18	1991	number of samples: 24	UBA 1996
Germany river Rhine at Lobith	average: 0.19 percentil-90: 0.42 max.: 1.20	1989	number of samples: 26	UBA 1996
Germany river Rhine at Lobith	average: 0.06 percentil-90: 0.10 max.: 0.11	1990	number of samples: 26	UBA 1996
Germany river Rhine at Lobith	average: 0.06 percentil-90: 0.12 max.: 0.15	1991	number of samples: 26	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: < 0.1 percentil-90: 0.22 max.: 0.30	1984	number of samples: 13	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: 0.12 percentil-90: 0.56 max: 0.80	1985	number of samples: 12	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: < 0.1 percentil-90: 0.20 max.: 0.20	1986	number of samples: 12	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: 0.14 percentil-90: 0.68 max.: 1.00	1987	number of samples: 13	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: < 0.1 max.: < 0.1	1988	number of samples: 8	UBA 1996
Germany river Rhine at Kleve-Bimmen	average:< 0.1 percentil-90: < 0.1 max.: 0.10	1989	number of samples: 13	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: <0.5 percentil-90: < 0.5 max.: < 0.5	1990	number of samples: 13	UBA 1996
Germany river Rhine at Kleve-Bimmen	average:< 0.5 percentil-90:< 0.5 max.:< 0.5	1991	number of samples: 51	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1992	number of samples: 13	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Rhine at Kleve-Bimmen	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1993	number of samples: 13	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: 0.13 percentil-90: 0.29 max.: 0.76	1989	number of samples: 25	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: 0.06 percentil-90: 0.13 max.: 0.17	1990	number of samples: 25	UBA 1996
Germany river Rhine at Kleve-Bimmen	average: 0.06 percentil-90: 0.09 max.: 0.13	1991	number of samples: 26	UBA 1996
Czech Republic river Elbe at Valy	average: 1.8 max.: 5.2 min.: 0.3:	Jan. to Oct. 1994	9 of 11 samples were positive	Medek et al. 1995
Germany river Elbe at Dresden	1.6 µg/L (90-Per-zentil) the total of Nitrobenzene and the three of Nitrotoluenes	1994	freezingdried sample extraction with Toluol/ Aceton or Toluol. GC/MS	HlfU 1997
Germany river Elbe at Zollenspieker river Elbe at Seemannshöft	median: 0.25 percentil-90: 0.53 max.: 0.60 median: 0.196 max.: 0.568	1992/93	unfiltered samples	Freie und Hansestadt Hamburg. Umweltbe-hörde 1995
Germany river Elbe at Zollenspieker	average: 0.35 percentil-90: 0.55 max.: 0.60	1992	number of samples: 12	UBA 1996
Germany river Elbe at Zollenspieker	average: 0.19 max.: 0.53	1993	number of samples: 8	UBA 1996
Germany river Elbe at Seemannshöft	average: 0.28 percentil-90: 0.48 max.: 0.57	1992	number of samples: 12	UBA 1996
Germany river Elbe at Seemannshöft	average: 0.19 max.: 0.50	1993	number of samples: 8	UBA 1996
Germany river Donau at Ulm	average: < 0.05 percentil-90: < 0.05 max.: < 0.05	1990	number of samples: 12	Umwelt-bundesamt Berlin 1996
Germany river Donau at Ulm	average: < 0.02 percentil-90: < 0.02 max.: < 0.02	1991	number of samples: 13	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Donau at Ulm	average: < 0.05 percentil-90: < 0.05 max.: < 0.05	1992	number of samples: 12	UBA 1996
Germany river Donau at Ulm	average: < 0.05 percentil-90: < 0.05 max.: < 0.05	1993	number of samples: 15	UBA 1996
Germany river Main at Bischofsheim	Percentil-90: 0.05	1995. weekly sampling	Freeze-dried sample extraction with Toluol/ Aceton or Toluol (GC/MS)	HLfU 1997
Germany river Main at Bischofsheim	average: 0.13 percentil-90: 0.26 max.: 0.64	1989	number of samples: 25	UBA 1996
Germany river Main at Bischofsheim	average: 0.14 percentil-90: 0.31 max.: 0.50	1990	number of samples: 26	UBA 1996
Germany river Main at Bischofsheim	average: 0.15 percentil-90: 0.20 max.: 0.62	1991	number of samples: 26	UBA 1996
Germany river Main at Bischofsheim	max.: 0.04	1991	number of samples: 1	UBA 1996
Germany river Main at Bischofsheim	max.: 0.06	1992	number of samples: 1	UBA 1996
Germany river Main at Bischofsheim	average: 0.10 percentil-90: 0.22 max.: 0.36	1992	number of samples: 16	UBA 1996
Germany river Main at Bischofsheim	average: 0.08 percentil-90: 0.12 max.: 0.37	1993	number of samples: 53	UBA 1996
Germany river Mosel at Palzem	average: < 2 percentil-90: < 2 max.: < 2	1992	number of samples: 13	UBA 1996
Germany river Mosel at Palzem	average: < 0.4 percentil-90: < 0.4 max.: < 0.4	1993	number of samples: 13	UBA 1996
Germany river Neckar at Poppenweiler	average: < 0.05 percentil-90:< 0.05 max.: < 0.05	1990	Number of samples: 13	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Neckar at Mannheim/Neckar	average: < 0.05 percentil-90:< 0.05 max.: < 0.05	1990	number of samples:23	UBA 1996
Germany river Neckar at Mannheim/Neckar	average: < 0.02 percentil-90: < 0.02 max.: < 0.02	1991	number of samples: 22	UBA 1996
Germany river Neckar at Mannheim/Neckar	average: < 0.05 percentil-90: < 0.05 max.: < 0.05	1992	number of samples: 16	UBA 1996
Germany river Neckar at Mannheim/Neckar	average: < 0.05 percentil-90: < 0.05 max.: < 0.05	1993	number of samples: 13	UBA 1996
Germany river Erft at Neuss	average: < 0.1 max.: < 0.1	1985	number of samples: 5	UBA 1996
Germany river Erft at Neuss	average: < 0.1 max.: < 0.1	1986	number of samples: 7	UBA 1996
Germany river Erft at Neuss	average: < 0.1 max.: < 0.1	1987	number of samples: 7	UBA 1996
Germany river Erft at Neuss	average: < 0.1 max.: < 0.1	1988	number of samples: 7	UBA 1996
Germany river Erft at Neuss	average: < 0.1 percentil-90: < 0.1 max.:< 0.1	1989	number of samples: 13	UBA 1996
Germany river Erft at Neuss	average: < .05 percentil-90: < 0.5 max.: < 0.5	1990	Number of samples: 12	UBA 1996
Germany river Erft at Neuss	average: < 0.5 max.: < 0.5	1991	Number of samples: 8	UBA 1996
Germany river Erft at Neuss	average: < 0.5 max.: < 0.5	1992	number of samples: 3	UBA 1996
Germany river Erft at Neuss	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1993	Number of samples: 13	UBA 1996
Germany river Fulda at Wahnhausen	max.: < 0.02	1991	Number of samples: 1	UBA 1996
Germany river Fulda at Wahnhausen	max.: < 0.05	1992	Number of samples: 1	UBA 1996
Germany river Lahn at Limburg-Staffel	max.: 0.02	1991	Number of samples: 1	UBA 1996
Germany river Lahn at Limburg-Staffel	max.: < 0.05	1992	Number of samples: 1	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Lippe at Wesel	average.: < 0.1 max.: 0.10	1984	Number of samples: 7	UBA 1996
Germany river Lippe at Wesel	average: < 0.1 max.: < 0.1	1985	Number of samples: 5	UBA 1996
Germany river Lippe at Wesel	average: < 0.1 max.: < 0.1	1986	Number of samples: 7	UBA 1996
Germany river Lippe at Wesel	average: < 0.1 max.: < 0.1	1987	Number of samples: 7	UBA 1996
Germany river Lippe at Wesel	average: < 0.1 max.: < 0.1	1988	Number of samples: 6	UBA 1996
Germany river Lippe at Wesel	average: 0.11 percentil-90: 0.39 max.: 0.43	1989	Number of samples: 13	UBA 1996
Germany river Lippe at Wesel	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1990	Number of samples: 12	UBA 1996
Germany river Lippe at Wesel	average: < 0.5 percentil-90: < 0.5 max: < 0.5	1991	number of samples: 45	UBA 1996
Germany river Lippe at Wesel	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1992	number of samples: 13	UBA 1996
Germany river Lippe at Wesel	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1993	number of samples: 13	UBA 1996
Germany river Nidda at Frankfurt-Nied	max.: 0.02	1991	number of samples: 1	UBA 1996
Germany river Pleiße at Gößnitz	average: < 0.1 max.: < 0.1	1993	number of samples: 4	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.1 max.: < 0.1	1984	number of samples: 7	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.1 max.:< 0.1	1985	number of samples: 6	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.1 max.: < 0.1	1986	number of samples: 7	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.1 max.: < 0.1	1987	number of samples: 7	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.1 max.: < 0.1	1988	number of samples: 6	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.1 max.: < 0.1	1989	number of samples: 10	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1990	number of samples: 13	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.5 max: 0.66	1991	number of samples: 8	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.5 max.: < 0.5	1992	number of samples: 3	UBA 1996
Germany river Ruhr at Duisburg-Ruhrort	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1993	number of samples: 13	UBA 1996
Germany river Saale at Camburg-Stöben	average: < 0.1 max.: < 0.1	1993	number of samples: 4	UBA 1996
Germany river Saar at Kanzem	average: < 2 percentil-90: < 2 max.: < 2	1992	number of samples: 13	UBA 1996
Germany river Saar at Kanzem	average: < 0.4 percentil-90: < 0.4 max.: < 0.4	1993	number of samples: 13	UBA 1996
Germany river Sieg at Bergheim	average: < 0.1 max.: < 0.1	1984	number of samples: 7	UBA 1996
Germany river Sieg at Bergheim	average: < 0.1 max.: < 0.1	1985	number of samples: 6	UBA 1996
Germany river Sieg at Bergheim	average: < 0.1 max.: < 0.1	1986	number of samples: 7	UBA 1996
Germany river Sieg at Bergheim	average: < 0.1 max.: < 0.1	1987	number of samples: 7	UBA 1996
Germany river Sieg at Bergheim	average: < 0.1 max.: < 0.1	1988	number of samples: 6	UBA 1996
Germany river Sieg at Bergheim	average: < 0.1 percentil-90: < 0.1 max.: < 0.1	1989	number of samples: 13	UBA 1996
Germany river Sieg at Bergheim	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1990	number of samples: 13	UBA 1996
Germany river Sieg at Bergheim	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1991	number of samples: 13	UBA 1996
Germany river Sieg at Bergheim	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1992	number of samples: 13	UBA 1996

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Germany river Sieg at Bergheim	average: < 0.5 percentil-90: < 0.5 max.: < 0.5	1993	number of samples: 13	UBA 1996
Germany river Schwarzbach at Trebur-Astheim	max.: < 0.02	1991	number of samples: 1	UBA 1996
Germany River Unstrut	average: < 0.1 max.: < 0.1	1993	number of samples: 4	UBA 1996
Germany River Weisse Elster	average: < 0.1 max.: < 0.1	1993	number of samples: 4	UBA 1996
Germany River Werra at Gerstungen	average: < 0.1 max.: < 0.1	1993	number of samples: 4	UBA 1996
Germany River Werra at "Letzter Heller"	< 0.02 < 0.05	1991 1992	number of samples: 1 number of samples: 1	UBA 1996
Germany River Wipper at Hachelbich	average: < 0.1 max.: < 0.1	1993	number of samples: 4	UBA 1996
Germany River Pleisse at Gößnitz	average: < 0.1 max.: < 0.1	1993	number of samples: 4	UBA 1996
Germany river Ilm at Niedertrebra	average: < 0.1 max.: < 0.1	1993	Number of samples: 4	UBA 1996
Belgium River Scheldt (estuarine water) between Antwerp and the North See	0.13	1986	number of samples: 1	UBA 1996
Japan not given	0.0001-0.0014 ppm	1976	detection limit: 0.00003-0.0004 ppm	Environment Agency Japan 1985
Japan not given	0.00013-0.0038 ppm	1977	detection limit: 0.0001-0.03 ppm	Environment Agency Japan 1985
Japan southwest and middle Japan Sendai Bay rivers in Hanamaki City, lake Hachiro Tomakomai port mouth of Ishikari	0.1-1.4 ppb	1976	detection limit: 0.003-0.4 ppb	JETOC 1993
Japan dto.	0.13-3.8 ppb	1977	detection limit: 0.1-30 ppb	JETOC 1993
Japan dto.	0.17 ppb	1991	detection limit: 0.15 ppb	JETOC 1993
Japanese river water and seawater	0.16-0.99 ppb		but not quantified in seawater in the Kitakyushi area of Japan	Spectrum Laboratories 08.01.01

Table C1 continued overleaf

Table C1 continued Surface Water

Location	Concentration [µg/l]	Period	Remark	Reference
Netherlands river Waal river Maas river Rhine	[ppb] average: 1.7 max.: 13.8 average: < 0.1 max.: 0.3 0.5			Spectrum Laboratories 08.01.01
USA Buffalo river Cuyahoga river St. Joseph river lake Erie Bansin lake Michigan Bansin	not detected			Spectrum Laboratories 08.01.01

Table C2 Sediment

Location	Concentration	Period	Remark	Reference
Germany river Rhine right bank Rhine-km:	[µg/kg dry substance]		rub the sediment with water-free Natrium-sulfat Soxhlet-extraction with Hexan clean up with TBA-reagent Florisil-säulenchro-matografie	LWA NRW 1990
659.8	< 10	04/1989	with I-Octanol/Toluol (95/5)	
659.8	< 10	09/1989	and Hexan/Diethylether (1/1)	
687.3	< 10	09/1989		
706.9	< 10	07/1989		
706.9	26	09/1989		
743.1	18	09/1989		
814.6	< 10	04/1989		
814.6	< 10	09/1989		
830.0	< 10	04/1989		
830.0	< 10	09/1989		
Germany river Rhine left bank Rhine-km:	[µg/kg dry substance]		dto.	LWA NRW 1990
639.1	< 10	04/1989		
639.1	< 10	09/1989		
773.6	< 10	04/1989		
807.2	< 10	04/1989		
829.5	< 10	04/1989		
829.5	< 10	09/1989		
863.8	< 10	04/1989		
863.8	< 10	09/1989		

Table C3 Waste Water Treatment Plants: Influents and Effluents

Location	Concentration	Period	Remark	Reference
Czech Republic river Elbe at Synthesia a.s.	[µg/l] outflow A average: 84 max.: 210 min.: 13 outflow R average : 1150 max.: 4000 min.: 85	Jan. to Oct. 1994	16 of 18 samples were positive 16 of 16 sample were positive	Medek et al. 1995
Norway 28 samples of industrial effluents polluted fjords	not detected			Spectrum Laboratories 08.01.01
USA mutagenic secondary effluents from industrial plants and publicly-owned treatment works Lockport - petroleum refinery Sauget – heavy chemical plant. although manufactures of alloys and metal tubin	found. however no exact specification available		GC-MS	Ellis et al. 1982
USA following industrial category: leather tanning petroleum refining nonferrous metals organics and plastics inorganic chemicals pulp and paper auto and other laundries pesticides manufactures explosives organic chemical	effluents frequency of ocurrence/median [ppb] 1; 3.7 1; 7.7 1; 47.7 13; 3876.7 3; 1995.3 1; 124.3 1; 40.4 1;16.3 8; 51.7 36; 43.7 100.245 highest effluent conc. in the organics and plastics industry		of the 1245 stations reporting nitrobenzene in industrial effluents in EPA STORET database. 1.8% contanined detectable levels of the chemical	Spectrum Laborates 08.01.01
USA Los Angeles municipal wastewater treatment plants	final effluent 20 ppb < 10 ppb			Spectrum Laboratories 08.01.01

Table C4 Sewage sludge of agricultural Soils

Location	Concentration	Period	Remark	Reference
Canada	[µg/kg dry soil] Ontario maize field: 100 Ontario apple plantation: 150 Quebec corn field: 100		In 3 out of 10 agricultural samples values > detection limit (60 µg/kg dry soil) were found	Webber MD and Wang C 1995

Table C5 Air

Location	Concentration	Period	Remark	Reference
USA New Jersey	[µg/m³] 2 residential areas: average: 0.06 max. 1.6 industrial areas: average: 0.40 max: 3.5	1978	6-20 l per sample, 20 min. sample period. 6 samples/day. 3 days/week 4-9 weeks	Bozelli JW, Kebbukus BB 1982
USA Southern California Long Beach Central LA Azusa Claremont	[ng/m³] Long Beach: 4.45 Central LA: 8.99 Azusa: 16.98 Claremont: 20.74 12-4a.m: 5.41 6-10a.m.: 10.6 12-4p.m.: 18.0 6-10p.m.: 17.0	08.- 09. Sept. 1993	samples at all times aggregated by sampling site samples at all urban sites aggregated by time of day	Fraser et al. 1998

Table C6 Soil and Groundwater

Location	Concentration [µg/l]	Period	Remark	Reference
Germany Leverkusen former ammunition production site	groundwater 17 samples > DL max. 1.0	May 1990	Detection limit (GC-MC) not given	IWS 1994

Appendix D Calculation of Kpsewage and the factor for the adsorption on suspended matter

Calculation of Kp_{sewage} and the factor for the adsorption on suspended matter

Chemical: Nitrobenzene

$a := 0.63 \qquad b := 0.9$

$LOGP_{OW} := 1.86 \qquad P_{OW} := 10^{LOGP_{OW}} \qquad P_{OW} = 7.24436 \cdot 10^{1}$

$K_{OC} := 10^{a \cdot LOGP_{OW} + b} \cdot l \cdot kg^{-1} \qquad K_{OC} = 1.17978 \cdot 10^{2} \ l \cdot kg^{-1}$

$K_{p\_susp} := 0.1 \cdot K_{OC} \qquad c_{susp} := 15 \cdot mg \cdot l^{-1}$

$faktor := \left(1 + K_{p\_susp} \cdot c_{susp}\right)$

$faktor = 1.00018$

Sludge / Sewage

$K_{p\_raw\_sewage} := 0.3 \cdot K_{OC} \qquad K_{p\_activated\_sewage} := 0.37 \cdot K_{OC}$

$K_{p\_raw\_sewage} = 3.53933 \cdot 10^{1} \ l \cdot kg^{-1} \qquad K_{p\_activated\_sewage} = 4.36518 \cdot 10^{1} \ l \cdot kg^{-1}$

Calculation of the Henry coefficient

molecular weight: $MOLW := 0.12311 \cdot kg \cdot mol^{-1}$

vapour pressure: $VP := 2.0 \cdot 10^{1} \cdot Pa$

water solubility: $SOL := 1900 \cdot mg \cdot l^{-1}$

$$HENRY := \frac{VP \cdot MOLW}{SOL}$$

$HENRY = 1.29589 \ Pa \cdot m^{3} \cdot mol^{-1} \qquad \log\left(\frac{HENRY}{Pa \cdot m^{3} \cdot mol^{-1}}\right) = 1.1257 \cdot 10^{-1}$

Simple Treat 3.0 (debugged Version, 07.02.97) $k := 0$

Summary of distribution			
	to air	2.4	
	to water	96.7	
	via primary sludge	0.6	
	via surplus sludge	0.2	
	degraded	0.0	
	total	100.0	%

Appendix E Calculation of PECregional and PECcontinental

SimpleBox2.0a - Berechnung regionaler + kontinentaler PEC's

- Anpassung an TGD (1996) / EUSES 1.00: Michael Feibicke (06/98)

INPUT - Nitrobenzene			
Parameter names acc. SimpleBox20	Unit	Input	Parameter names according Euses
Physicochemical properties			
COMPOUND NAME	[-]	Nitrobenzene	Substance
MOL WEIGHT	[g.mol^{-1}]	123	Molecular weight
MELTING POINT	[° C]	5,26	Melting Point
VAPOR PRESSURE(25)	[Pa]	20	Vapour pressure at 25°C
log Kow	[log10]	1,86	Octanol-water partition coefficient
SOLUBILITY(25)	[mg.l^{-1}]	1900	Water solubility
Distribution - Partition coefficients			
- Solids water partitioning (derived from K_{oc})			
Kp(soil)	[l.kg$_d^{-1}$]	2,36	Solids-water partitioning in soil
Kp(sed)	[l.kg$_d^{-1}$]	5,9	Solids-water partitioning in sediment
Kp(susp)	[l.kg$_d^{-1}$]	11,8	Solids-water partitioning in sudpended matter
- Biota-water			
BCF(fish)	[l.kg$_w^{-1}$]	30,6	Biocentration factor for aquatic biota
Degradation and Transfromation rates			
- Characterisation and STP			
PASSreadytest	[y / n]	n	Characterization of biodegradability
- Environmental Total Degradation			
kdeg(air)	[d^{-1}]	1,06E-02	Rate constant for degradation in air
kdeg(water)	[d^{-1}]	6,93E-07	Rate constant for degradation in bulk surface water
kdeg(soil)	[d^{-1}]	6,93E-07	Rate constant for degradation in bulk soil
kdeg(sed)	[d^{-1}]	6,93E-07	Rate constant for degradation in bulk sediment
Sewage treatment (e.g. calculated by SimpleTreat)			
- Continental			
FR(volatstp) [C]	[-]	2,50E-02	Fraction of emission directed to air (STPcont)
FR(effstp) [C]	[-]	3,90E-02	Fraction of emission directed to water (STPcont)
FR(sludgestp) [C]	[-]	8,00E-03	Fraction of emission directed to sludge (STPcont)
- Regional			
FR(volatstp) [R]	[-]	2,50E-02	Fraction of emission directed to air (STPreg)
FR(effstp) [R]	[-]	3,90E-02	Fraction of emission directed to water (STPreg)
FR(sludgestp) [R]	[-]	8,00E-03	Fraction of emission directed to sludge (STPreg)
Release estimation			
- Continental			
Edirect(air) [C]	[t.y^{-1}]	0,739	Total continental emission to air
STPload [C]	[t.y^{-1}]	12,95	Total continental emission to wastewater
Edirect(water1) [C]	[t.y^{-1}]	5,933	Total continental emission to surface water
Edirect(soil3) [C]	[t.y^{-1}]	0	Total continental emission to industrial soil
Edirect(soil2) [C]	[t.y^{-1}]	0	Total continental emission to agricultural soil
- Regional			
Edirect(air) [R]	[t.y^{-1}]	0,0821	Total continental emission to air
STPload [R]	[t.y^{-1}]	1,44	Total continental emission to wastewater
Edirect(water1) [R]	[t.y^{-1}]	0,66	Total continental emission to surface water
Edirect(soil3) [R]	[t.y^{-1}]	0	Total continental emission to industrial soil
Edirect(soil2) [R]	[t.y^{-1}]	0	Total continental emission to agricultural soil

OUTPUT - Nitrobenzene

Zur **Neuberechnung der Daten**: ->Extras ->Optionen ->Berechnen -> Datei_berechnen -> F9 drücken, sonst keine komplette Neuberechnung aller Bezüge!!

Parameter names acc. SimpleBox20	Unit	Output	Parameter names according Euses
Physicochemical properties			
COMPOUND NAME	[-]	Nitrobenzene	Substance
Output			
- Continental			
PECsurfacewater (total)	[mg.l^{-1}]	2,16E-06	Continental PEC in surface water (total)
PECsurfacewater (dissolved)	[mg.l^{-1}]	2,15E-06	Continental PEC in surface water (dissolved)
PECair	[mg.m^{-3}]	3,02E-08	Continental PEC in air (total)
PECagr.soil	[mg.kg$_{wwt}^{-1}$]	7,31E-07	Continental PEC in agricultural soil (total)
PECporewater agr.soil	[mg.l^{-1}]	3,32E-07	Continental PEC in pore water of agricultural soils
PECnat.soil	[mg.kg$_{wwt}^{-1}$]	2,14E-07	Continental PEC in natural soil (total)
PECind.soil	[mg.kg$_{wwt}^{-1}$]	2,14E-07	Continental PEC in industrial soil (total)
PECsediment	[mg.kg$_{wwt}^{-1}$]	6,80E-06	Continental PEC in sediment (total)
- Regional			
PECsurfacewater (total)	[mg.l^{-1}]	1,29E-05	Regional PEC in surface water (total)
PECsurfacewater (dissolved)	[mg.l^{-1}]	1,29E-05	Regional PEC in surface water (dissolved)
PECair	[mg.m^{-3}]	5,18E-08	Regional PEC in air (total)
PECagr.soil	[mg.kg$_{wwt}^{-1}$]	5,43E-06	Regional PEC in agricultural soil (total)
PECporewater agr.soil	[mg.l^{-1}]	2,47E-06	Regional PEC in pore water of agricultural soils
PECnat.soil	[mg.kg$_{wwt}^{-1}$]	3,66E-07	Regional PEC in natural soil (total)
PECind.soil	[mg.kg$_{wwt}^{-1}$]	3,66E-07	Regional PEC in industrial soil (total)
PECsediment	[mg.kg$_{wwt}^{-1}$]	3,95E-05	Regional PEC in sediment (total)

Appendix F Calculation of the Photolytical degradation in air

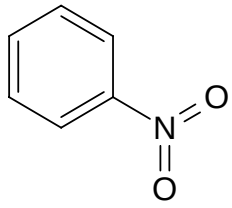
PropertEst :

Estimation of chemical´s properties with QSAR

Endpoint: Photolytical degradation in air

Substance :
Name: Nitrobenzene
Molekular weight : 123,11 g/mol
Sum forumula : C6 H5 N O2
SMILES-Code: c1(ccccc1)N(=O)=O

Strukture



Result:
k : 0.244E-12 cm³/molec/s (AOP v1.9)
$t_{(1/2)}$: 65.8 days

Description of the model:
Photolytical degradation of organic chemicals in the atomosphere is primarily due to their reaction with hydroxyl radicals.
With the programme AOP you can estimate the rate constant (k) for this reaction. Together with the concentration of the hydroxyl radicals (5E5 radicals/cm³ - 24-h mean value) in the atmosphere the half life of the organic chemical in the atmosphere can be calculated.

Source:
Atkinson, R.: "Estimation of Gas-Phase Hydroxyl Radical Rate Constants for organic Chemicals" Environ. Toxicol. Chem. 7, 435-442, 1988

Appendix G Distribution and fate

Distribution and Fate

Substance: Nitrobenzene

melting point:	$MP := 278.41 \cdot K$
vapour pressure:	$VP := 20 \cdot Pa$
water solubility:	$SOL := 1900 \cdot mg \cdot l^{-1}$
part. coefficient octanol/water:	$LOGP_{OW} := 1.86$
molecular weight:	$MOLW := 0.12311 \cdot kg \cdot mol^{-1}$
gas constant:	$R := 8.3143 \cdot J \cdot mol^{-1} \cdot K^{-1}$
temperature:	$T := 293 \cdot K$
conc. of suspended matter in the river:	$SUSP_{water} := 15 \cdot mg \cdot l^{-1}$
density of the solid phase:	$RHO_{solid} := 2500 \cdot kg \cdot m^{-3}$
volume fraction water in susp. matter:	$Fwater_{susp} := 0.9$
volume fraction solids in susp.matter:	$Fsolid_{susp} := 0.1$
volume fraction of water in sediment:	$Fwater_{sed} := 0.8$
volume fraction of solids in sediment:	$Fsolid_{sed} := 0.2$
volume fraction of air in soil:	$Fair_{soil} := 0.2$
volume fraction of water in soil:	$Fwater_{soil} := 0.2$
volume fraction of solids in soil:	$Fsolid_{soil} := 0.6$
aerobic fraction of the sediment comp.:	$Faer_{sed} := 0.1$
product of CONjunge and $SURF_{air}$:	$product := 10^{-4} \cdot Pa$

distribution air/water: Henry-constant

$$HENRY := \frac{VP \cdot MOLW}{SOL} \qquad HENRY = 1.296 \cdot Pa \cdot m^3 \cdot mol^{-1}$$

$$\log\left(\frac{HENRY}{Pa \cdot m^3 \cdot mol^{-1}}\right) = 0.113$$

$$K_{air\_water} := \frac{HENRY}{R \cdot T} \qquad K_{air\_water} = 5.32 \cdot 10^{-4}$$

solid/water-partition ceefficient Kp_{comp} and total compartment/water-partition coefficient K_{comp_water}

$a := 0.63$ (a,b from TGD, p. 539)

$b := 0.90$ $K_{OC} := 10^{a \cdot LOGP_{OW} + b} \cdot l \cdot kg^{-1}$ $K_{OC} = 117.978 \cdot l \cdot kg^{-1}$

Suspended matter

$Kp_{susp} := 0.1 \cdot K_{OC}$ $Kp_{susp} = 11.798 \cdot l \cdot kg^{-1}$

$K_{susp\_water} := Fwater_{susp} + Fsolid_{susp} \cdot Kp_{susp} \cdot RHO_{solid}$ $K_{susp\_water} = 3.849$

factor for the calculation of $Clocal_{water}$:

$faktor := 1 + Kp_{susp} \cdot SUSP_{water}$ $faktor = 1$

Sediment

$Kp_{sed} := 0.05 \cdot K_{OC}$ $Kp_{sed} = 5.899 \cdot l \cdot kg^{-1}$

$K_{sed\_water} := Fwater_{sed} + Fsolid_{sed} \cdot Kp_{sed} \cdot RHO_{solid}$ $K_{sed\_water} = 3.749$

Soil

$Kp_{soil} := 0.02 \cdot K_{OC}$ $Kp_{soil} = 2.36 \cdot l \cdot kg^{-1}$

$K_{soil\_water} := Fair_{soil} \cdot K_{air\_water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHO_{solid}$

$K_{soil\_water} = 3.739$

Sludge (activated sludge)

$K_{p\_sludge} := 0.37 \cdot K_{OC}$ $K_{p\_sludge} = 43.652 \cdot l \cdot kg^{-1}$

Raw sewage

$K_{p\_sewage} := 0.30 \cdot K_{OC}$ $K_{p\_sewage} = 35.393 \cdot l \cdot kg^{-1}$

Elimination in STPs

rate constant in STP: k = 0 d^{-1} elimination P = f (k, logpow, logH) =1.4

fraction directed to surface water $Fstp_{water}$ = 96.1

biodegradation in different compartments

surface water

$kbio_{water} := 0 \cdot d^{-1}$

soil

$DT50bio_{soil} := 1000000d$

$kbio_{soil} := \frac{\ln(2)}{DT50bio_{soil}}$ $kbio_{soil} = 6.931 \cdot 10^{-7} \ d^{-1}$

sediment

$kbio_{sed} := \frac{\ln(2)}{DT50bio_{soil}} \cdot Faer_{sed}$ $kbio_{sed} = 6.931 \cdot 10^{-8} \ d^{-1}$

degradation in surface waters

$khydr_{water} := 0 \cdot d^{-1}$

$kphoto_{water} := 5.2 \cdot 10^{-3} \cdot d^{-1}$ (Simmons and Zepp, 1986)

$kdeg_{water} := khydr_{water} + kphoto_{water} + kbio_{water}$

$kdeg_{water} = 5.2 \cdot 10^{-3} \ d^{-1}$

Atmosphere

calculation of CONjunge * SURFaer for the OPS-model

$VPL := \frac{VP}{\exp\left[6.79 \cdot \left(1 - \frac{MP}{285 \cdot K}\right)\right]}$ $VP := wenn(MP > 285 \cdot K, VPL, VP)$ $VP = 20 \ Pa$

$Fass_{aer} := \frac{product}{VP + product}$

$Fass_{aer} = 5 \cdot 10^{-6}$

degradation in the atmosphere

$kdeg_{air}$ = 4.4E-04 h^{-1} =1.06E-02 d^{-1} (see AOP-calculation)

Appendix H Exposure of soil

Exposure of Soil

chemical: Nitrobenzene

Defaults:

mixing depth of soil: $DEPTHsoil_i :=$

0.2·m
0.2·m
0.1·m

bulk density of soil: $RHO_{soil} := 1700 \cdot kg \cdot m^{-3}$

average time for exposure: $T_i :=$

30·d
180·d
180·d

partial mass transfer coefficient at air-side of the air-soil interface: $kasl_{air} := 120 \cdot m \cdot d^{-1}$

partial mass transfer coefficient at soilair-side of the air-soil interface: $kasl_{soilair} := 0.48 \cdot m \cdot d^{-1}$

partial mass transfer coefficient at soilwater-side of the air-soil interface: $kasl_{soilwater} := 4.8 \cdot 10^{-5} \cdot m \cdot d^{-1}$

fraction of rain water that infiltrates into soil: $Finf_{soil} := 0.25$

rate of wet precipitation: $RAINrate := 1.92 \cdot 10^{-3} \cdot m \cdot d^{-1}$

dry sludge application rate: $APPLsludge_i :=$

0.5·kg·m^{-2}·a^{-1}
0.5·kg·m^{-2}·a^{-1}
0.1·kg·m^{-2}·a^{-1}

Input:

annual average total deposition flux: $DEPtotal_{ann} := 8.4 \cdot 10^{-4} \cdot mg \cdot m^{-2} \cdot d^{-1}$

soil-water partitioning coefficient: $K_{soil\_water} := 3.739$

concentration in dry sewage sludge: $C_{sludge} := 0.0 \cdot \mu g \cdot kg^{-1}$

air-water partitioning coefficient: $K_{air\_water} := 5.32 \cdot 10^{-4}$

rate constant for for removal from top soil: $kbio_{soil} := 6.931 \cdot 10^{-7} \cdot d^{-1}$

PECregional: $PECregional_{natural\_soil} := 3.66 \cdot 10^{-7} \cdot mg \cdot kg^{-1}$

Calculation:

aerial deposition flux per kg of soil:

$$D_{air_i} := \frac{DEPtotal_{ann}}{DEPTHsoil_i \cdot RHO_{soil}}$$

rate constant for valatilisation from soil:

$$k_{volat_i} := \left[\left(\frac{1}{kasl_{air} \cdot K_{air\_water}} + \frac{1}{kasl_{soilair} \cdot K_{air\_water} + kasl_{soilwater}} \right) \cdot K_{soil\_water} \cdot DEPTHsoil_i \right]^{-1}$$

rate constant for leaching from soil layer:

$$k_{leach_i} := \frac{Finf_{soil} \cdot RAINrate}{K_{soil\_water} \cdot DEPTHsoil_i}$$

removal from top soil:

$$k_i := k_{volat_i} + k_{leach_i} + kbio_{soil}$$

concentration in soil

concentration in soil due to 10 years of continuous deposition:

$$Cdep_{soil\_10_i} := \frac{D_{air_i}}{k_i} \cdot \left(1 - \exp\left(-365 \cdot d \cdot 10 \cdot k_i\right)\right)$$

concentration just after the first year of sludge application:

$$Csludge_{soil\_1_i} := \frac{C_{sludge} \cdot APPLsludge_i \cdot a}{DEPTHsoil_i \cdot RHO_{soil}}$$

initial concentration in soil after 10 applications of sludge:

$$Csludge_{soil\_10_i} := Csludge_{soil\_1_i} \cdot \left(1 + \sum_{n=1}^{9} \exp\left(-365 \cdot d \cdot n \cdot k_i\right)\right)$$

sum of the concentrations due to both processes:

$$C_{soil\_10_i} := Cdep_{soil\_10_i} + Csludge_{soil\_10_i}$$

average concentration in soil over T days:

$$Clocal_{soil_i} := \frac{D_{air_i}}{k_i} + \frac{1}{k_i \cdot T_i} \cdot \left(C_{soil\_10_i} - \frac{D_{air_i}}{k_i} \right) \cdot \left(1 - \exp\left(-k_i \cdot T_i \right) \right)$$

$$PEClocal_{soil_i} := Clocal_{soil_i} + PECregional_{natural\_soil}$$

	$\frac{Clocal_{soil_i}}{ppt}$
$Clocal_{soil}$ =	$2.3102 \cdot 10^3$
$Clocal_{agr.soil}$ =	$2.314 \cdot 10^3$
$Clocal_{grassland}$ =	$2.361 \cdot 10^3$

	$\frac{PEClocal_{soil_i}}{ppt}$
$PEClocal_{soil}$ =	$2.3107 \cdot 10^3$
$PEClocal_{agr.soil}$ =	$2.3145 \cdot 10^3$
$PEClocal_{grassland}$ =	$2.3615 \cdot 10^3$

Indicating persistency of the substance in soil

initial concentration after 10 years:

$\frac{C_{soil\_10_i}}{ppt}$
$2.3094 \cdot 10^3$
$2.3094 \cdot 10^3$
$2.3608 \cdot 10^3$

initial concentration in steady-state situation:

$$C_{soil\_ss_i} := \frac{D_{air_i}}{k_i} + Csludge_{soil\_1_i} \cdot \left(\frac{1}{1 - \exp\left(-365 \cdot d \cdot k_i \right)} \right)$$

$\frac{C_{soil\_ss_i}}{ppt}$
$2.3612 \cdot 10^3$
$2.3612 \cdot 10^3$
$2.362 \cdot 10^3$

fraction of steady-state in soil achieved:

$$Fst\_st_i := \frac{C_{soil\_10_i}}{C_{soil\_ss_i}}$$

Fst_st_i
0.97805
0.97805
0.99952

calculated k-values

	$\frac{k_{volat_i}}{d^{-1}}$	$\frac{k_{leach_i}}{d^{-1}}$	$\frac{k_i}{d^{-1}}$
soil	$4.0375 \cdot 10^{-4}$	$6.4188 \cdot 10^{-4}$	$1.0463 \cdot 10^{-3}$
agriculture soil	$4.0375 \cdot 10^{-4}$	$6.4188 \cdot 10^{-4}$	$1.0463 \cdot 10^{-3}$
grassland	$8.075 \cdot 10^{-4}$	$1.2838 \cdot 10^{-3}$	$2.092 \cdot 10^{-3}$

concentration in pore water

$$Clocal_{soil\_porew_i} := \frac{Clocal_{soil_i} \cdot RHO_{soil}}{K_{soil\_water}}$$

	$Clocal_{soil\_porew_i}$ / ng·l^{-1}
$Clocal_{soil\_porew}$ =	$1.0504 \cdot 10^3$
$Clocal_{agr.soil\_porew}$ =	$1.0521 \cdot 10^3$
$Clocal_{grassland\_porew}$ =	$1.0735 \cdot 10^3$

$$PEClocal_{soil\_porew_i} := \frac{PEClocal_{soil_i} \cdot RHO_{soil}}{K_{soil\_water}}$$

	$PEClocal_{soil\_porew_i}$ / ng·l^{-1}
$PEClocal_{soil\_porew}$ =	$1.0506 \cdot 10^3$
$PEClocal_{agr.soil\_porew}$ =	$1.0523 \cdot 10^3$
$PEClocal_{grassland\_porew}$ =	$1.0737 \cdot 10^3$

concentration in ground water

$PEClocal_{grw} = PEClocal_{agr\_soil\_porew}$

European Commission

EUR 22480 EN **European Union Risk Assessment Report nitrobenzene, Volume 77**

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The report provides the comprehensive risk assessment of environment part of the substance nitrobenzene. It has been prepared by Germany in the frame of Council Regulation (EEC) No. 793/93 on the evaluation and control of the risks of existing substances, following the principles for assessment of the risks to humans and the environment, laid down in Commission Regulation (EC) No. 1488/94.

Part I – Environment

The evaluation considers the emissions and the resulting exposure to the environment in all life cycle steps. Following the exposure assessment, the environmental risk characterisation for each protection goal in the aquatic, terrestrial and atmospheric compartment has been determined.

The environmental risk assessment for nitrobenzene concludes that risks are not expected.

Part II – Human Health

This part of the evaluation will be published later.

The mission of the JRC is to provide customer-driven scientific and technical support for the conception, development, implementation and monitoring of EU policies. As a service of the European Commission, the JRC functions as a reference centre of science and technology for the Union. Close to the policy-making process, it serves the common interest of the Member States, while being independent of special interests, private or national.

European Commission – Joint Research Centre
Institute for Health and Consumer Protection
Toxicology and Chemical Substances (TCS)
European Chemicals Bureau (ECB)

European Union Risk Assessment Report

nitrobenzene

Part I - environment

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