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Environmental risk assessment of the polycyclic musks AHTN and HHCB according to the EU-TGD

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PREFACE

This report has been prepared by the National Institute of Public Health and the Environment and BKH Consulting Engineers.

Results have been discussed in a task-force consisting of F. Balk (BKH Consulting Engineers), T.J. v. Bergen (NEA), R.A. Ford (RIFM), H-D. Gaisser (NEA), J.D. Middleton (NEA), E.J. v.d. Plassche (National Institute of Public Health and the Environment) and P.T.J. v.d. Zandt (National Institute of Public Health and the Environment).

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SUMMARY

An environmental risk assessment has been carried out for the polycyclic musks AHTN and HHCB according to the EU Technical Guidance Document for Environmental Risk Assessment for New and Existing Substances. AHTN and HHCB are used in fragrances for cosmetics and detergents. Both substances are high volume chemicals with a use volume for Europe of 585 and 1482 tonnes in 1995, respectively.

The environmental risk assessment is based on information and results of studies provided by the fragrance industry as represented in the Netherlands by its association NEA, by the Research Institute for Fragrance Materials (RIFM) and international open literature. Endpoints in the assessment were aquatic organisms, sediment dwelling organisms, soil organisms, fish-eating predators and worm-eating predators. Predicted Environmental Concentrations (PECs) were calculated with the European Union System for the Evaluation of Substances (EUSES). Since monitoring data were available for several media, measured concentrations could be compared with predicted ones. Subsequently, one of the two was selected as the exposure concentration used for the risk characterization. Risk Characterization Ratios (RCRs) are presented in the tables below.

AHTN	exposure concentrations	PNEC	RCR
aquatic organisms (μg/l)	0.2 (m)	3.5	0.057
sediment organisms (mg/kg dw)	0.48 (m) * 10[1]	11	0.44
soil organisms (mg/kg dw)	0.26 (p)	0.32	0.81
fish-eating predators (mg/kg)	0.146 (m)	10	0.015
worm-eating predators (mg/kg)	0.78 (p)	10	0.078

HHCB	exposure concentrations	PNEC	RCR
aquatic organisms (μg/l)	0.5 (m)	6.8	0.074
sediment organisms (mg/kg dw)	0.16 (m) * 10[1]	25	0.064
soil organisms (mg/kg dw)	0.38 (p)	0.32	1.2
fish-eating predators (mg/kg)	0.125 (m)	100	0.0013
worm-eating predators (mg/kg)	1.7 (p)	100	0.017

(m): measured concentration
(p): predicted concentration
[1]: measured concentration multiplied by 10 for AHTN and HHCB as log Kow is above 5 (TGD)

The environmental risk assessment can be further refined by carrying out more studies on the effects or exposure side. The latter is considered more relevant, especially for the soil compartment where no biodegradation is assumed although there are indications that biodegradation in soil by fungi is possible. A monitoring study is carried out at the moment in the Netherlands, in which concentrations in fish, sewage sludge, surface water, influent and effluent are measured.

SAMENVATTING

Een risico-evaluatie van de polycyclische musken AHTN en HHCB in het milieu is uitgevoerd volgens het “EU Technical Guidance Document for Environmental Risk Assessment for New and Existing Substances”. AHTN en HHCB worden gebruikt in geurstoffen die toegepast worden in cosmetica en wasmiddelen. Het zijn stoffen met een hoog volume waarvoor in 1995 voor Europa hoeveelheden van 585 ton voor AHTN en 1482 ton voor HHCB zijn gerapporteerd.

De informatie die in deze evaluatie is gebruikt, is afkomstig van studies die aangeleverd zijn door de geurstoffen industrie, die in Nederland vertegenwoordigd wordt door de Vereniging van Geur- en Smaakstoffenfabrikanten (NEA) en het Research Institute for Fragrance Materials (RIFM). Daarnaast is gebruik gemaakt van gegevens uit de openbare literatuur.

Het risico is bepaald voor waterorganismen, sedimentorganismen, bodemorganismen en vis-etende en worm-etende predatoren. De ‘Predicted Environmental Concentrations’ (PEC; voorspelde concentraties in het milieu) zijn berekend met het “European Union System for the Evaluation of Substances” (EUSES). Omdat monitoringgegevens beschikbaar waren voor diverse milieucompartimenten, zijn de voorspelde concentraties vergeleken met de gemeten concentraties. Vervolgens is één van deze concentraties gekozen voor de risicokarakterisering. Risicokarakterisering Ratio’s (RKR’s) zijn weergegeven in onderstaande tabellen.

AHTN	blootstellingconcentratie	PNEC	RKR
water organismen (μg/l)	0.2 (g)	3.5	0.057
sediment organismen (mg/kg dw)	0.48 (g) * 10[1]	11	0.44
bodem organismen (mg/kg dw)	0.26 (v)	0.32	0.81
vis-etende predatoren (mg/kg)	0.146 (g)	10	0.015
worm-etende predatoren (mg/kg)	0.78 (v)	10	0.078

HHCB	blootstellingconcentratie	PNEC	RKR
water organismen (μg/l)	0.5 (g)	6.8	0.074
sediment organismen (mg/kg dw)	0.16 (g) * 10[1]	25	0.064
bodem organisms (mg/kg dw)	0.38 (v)	0.32	1.2
vis-etende predatoren (mg/kg)	0.125 (g)	100	0.0013
worm-etende predatoren (mg/kg)	1.7 (v)	100	0.017

(g): gemeten concentratie
(v): voorspelde concentratie
[1]: omdat de log Kow van AHTN en HHCB groter is dan 5 zijn de gemeten concentraties vermenigvuldigd met een factor 10 (TGD)

Verfijning van de risico-evaluatie is mogelijk door het uitvoeren van aanvullende studies op het gebied van effecten of blootstelling. Studies gericht op het verkrijgen van meer inzicht in de blootstelling worden het meest relevant geacht, met name voor het compartiment bodem omdat aangenomen is dat AHTN en HHCB niet afbreken in de bodem, hoewel er aanwijzingen zijn dat biodegradatie in bodems door schimmels mogelijk is. Op dit moment wordt een monitoring studie uitgevoerd in Nederland, waarin concentraties in vis, zuiveringsslib, oppervlaktewater, influent en effluent gemeten worden.

1. INTRODUCTION

The polycyclic musk ingredients AHTN and HHCB are used in fragrances for cosmetics and detergents, fabric softeners, household cleaning products, air fresheners etc. AHTN and HHCB represent about 95% of the market in the European Union (EU) for all polycyclic musks (letter from RIFM, 09-09-1997). Both AHTN and HHCB have been found in the environment, e.g. in river water and fish (Eschke et al., 1994; 1995a) and in samples of human fat and milk (Eschke et al., 1995b; Müller et al., 1995).

In 1996 the Dutch Consumer Association informed the minstry of VROM regarding their concerns about the use of these fragrance ingredients and their detection in the environment. In a letter d.d. 13-06-1996 to the Dutch Consumers Association the ministry of VROM stated that an environmental risk assessment was being prepared for the polycyclic musks at that moment on behalf of the Dutch Association of Fragrance and Flavour Producers (NEA) and the Research Institute for Fragrance Materials (RIFM) (letter of Minister de Boer, 13-06-1996). The ministry of VROM asked the National Institute of Public Health and the Environment (RIVM) to evaluate this environmental risk assessment. The present report contains the results of the environmental risk assessment for AHTN and HHCB as evaluated by RIVM.

The polycyclic musks are important fragrance ingredients, because of their musky scent and their substantive properties. These substantive properties relate to their poor water solubility and high octanol-water partition coefficient. These properties are shared with another group of fragrance ingredients, the nitromusks, which otherwise differ completely in chemical structure and biological properties. As a consequence of publications by the Dutch Consumer Association RIVM, at the request of the ministry of VROM, recently completed an environmental risk assessment on musk xylene and musk ketone, the most important and highest volume nitromusks (Tas and Van de Plassche, 1996). This environmental risk assessment was based on information provided by NEA and RIFM. The Ministry of VROM subsequently concluded that there was no immediate cause for direct risk management decisions (letter of Minister de Boer, 13-06-1996). However, as a consequence of the results for the compartments sediment and soil, a further refinement of the assessment was considered necessary. In the mean time new test results for these compartments have become available (Tas et al., 1997). Both substances will be evaluated again within the EU program of existing substances. The Netherlands is rapporteur for musk ketone as well as musk xylene.

The environmental risk assessment for AHTN and HHCB is based on results available within RIFM and on data obtained from the international scientific literature. For the risk assessment to humans from their use as fragrance ingredients in cosmetics, reference is made to the current review in the EU Scientific Committee for Cosmetology (SCC).

All original test reports and information provided by RIFM have been screened according to the QA-procedures applied within the Centre for Substances and Risk Assessment of RIVM (RIVM/CSR). The risk assessment uses the method as described in the Technical Guidance Documents for New and Existing Substances, part II: Environmental Risk Assessment (EC, 1996), applying the European Union System for Evaluation of Substances (EC, 1997; Vermeire et al., 1997)[1]. This method is available for risk assessment throughout the EU.

In an environmental risk assessment the Predicted Environmental Concentration (PEC) and/or measured concentrations are compared to the Predicted No Effect Concentration (PNEC). Risk is expressed as the Risk Characterization Ratio (RCR): the PEC/PNEC ratio or as the ratio of actually measured concentrations over PNEC. In general, if the ratio exceeds 1, this is considered as a trigger for further refinements of the risk assessment or for risk management. Depending on the extent of the use of measured exposure and toxicity data in the derivation of the PEC/PNEC ratio, this involves a stepwise development of additional exposure and toxicity data.

Some refinement has already taken place as studies have been conducted beyond the so-called 'base-set' on the exposure as well as the effects side. This allows e.g. to predict the environmental distribution and fate processes more accurately, allowing a refinement of the PEC and the risk assessment where initial predicted ratios were above 1.

The following items are addressed in the report:

- calculation of PECs from information on use volume and applications;
- actual concentrations measured in the environment;
- comparison of PECs with those measured concentrations and subsequently a choice of which concentration (measured or predicted) will be used for the risk characterization;
- estimation of PNECs from (eco)toxicity studies for aquatic organisms, sediment-dwelling organisms, soil organisms and predators;
- calculation of the Risk Characterization Ratio (RCR) for aquatic organisms, sediment-dwelling organisms, soil organisms, fish-eating predators and worm-eating predators.

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[1] Throughout the present report referred to as TGD (EC, 1996) and EUSES (EC, 1997).

2 GENERAL INFORMATION

2.1 Function and use of AHTN and HHCB in perfumery

Both AHTN and HHCB are considered to be essential ingredients in fragrances for consumer products because of their typical musky scent and the effect they have on the quality of fragrances. They make a fragrance long lasting and have a positive effect on its balance. The balance is better because these materials bring the initial and residual smell in harmony. They form the foundation of modern fragrances, not least because of their ability to bind fragrances to fabrics. These properties are unique to the polycyclic musks. AHTN and HHCB are the two most important materials in this category and they are used in almost all fragrances and found in consumer products like extrait perfumes, cosmetics, soaps, shampoos, detergents, fabric conditioners and other household products. These two substances probably share over 95% of the market for polycyclic musks.

2.2 Physico-chemical properties

The chemical identity of AHTN and HHCB is described in Table 1. The acronym AHTN comes from the chemical name 7-Acetyl-1,1,3,4,4,6-Hexamethyl-1,2,3,4-TetrahydroNaphtalene. For technical reasons HHCB is commercially available only as an approximately 65% solution in a neutral solvent. The acronym HHCB comes from 1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-HexamethylCyclopenta-[gamma]-2-Benzopyran, the chemical description of the two diasteriomers, which are by far the main isomers of the product. Closely related structures such as the 6- and 8-ethyl substituted isomers of the same molecular formula ($C_{18}H_{26}O$) are minor product isomers. Identification and physico-chemical properties of the substances are presented in Table 1. Water solubility, melting point (AHTN only), vapour pressure, octanol-water partition coefficient and organic carbon partition coefficient were experimentally determined. The data for HHCB relate to the undiluted substance.

The vapour pressure was measured by the gas saturation method according to OECD Test Guideline 104 using ^{14}C-labelled AHTN and HHCB. A stream of nitrogen was equilibrated with the test substance. The test substance was adsorbed from the gas stream by a sorbent, XAD-2. The mass of the adsorbed test substance was determined by LSC. Vapour pressures at 25°C were $6.82*10^{-2}$ Pa (s.d. $1.23*10^{-2}$ Pa) for AHTN and $7.27*10^{-2}$ Pa (s.d. $1.20*10^{-2}$ Pa) for HHCB (MacGillivray, 1996a,b).

The water solubility was measured using ^{14}C-labelled AHTN and HHCB in three buffer solutions (pH 5, 7 and 9) at 25°C. The procedure is based on the "flask method" in accordance with OECD Test Guideline 105. Tubes were filled with a solution of the test substance in ethanol. Ethanol was removed by evaporation, leaving the test material as tiny droplets on the bottom of the tubes and the buffer solutions were added. The system was agitated and samples were taken after centrifugation (2,655 g and 10,620 g). The concentrations of AHTN and HHCB were determined by LSC at days 1, 2 ,5 and 7. After 7 days of equilibrium the average water solubility of AHTN was 1.31 mg/l at pH 5 and 1.22 mg/l at pH 7 and pH 9 (Edwards, 1996a). Water solubility of HHCB was 1.99 mg/l at pH 5, 1.65 mg/l at pH 7 and 1.60 mg/l at pH 9 (Edwards, 1996b). The water solubility may also be calculated using QSARs based on log Kow and molecular weight as applied in USES (Uniform System for the Evaluation of Substances;

RIVM, VROM, WVC, 1994). The results are lower than the experimentally determined values but well within the range of reliablity of this type of QSARs (Table 1).

Henry's law constant is calculated using molecular weight, vapour pressure and measured solubility in water (TGD).

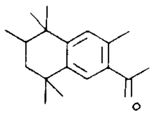
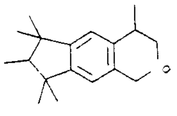
The octanol-water partition coefficient log Kow was determined with the reversed-phase HPLC method according to OECD Test Guideline 117. HPLC was performed with acetonitrile/water 65:35 (v/v) as the mobile phase; column: 250 x 4 mm, packed with Nucleosil 120-5 C_{18}, 5µ. The detection wavelength was 260 nm for AHTN and 210 nm for HHCB, temperature of the determination was 24 °C. Reference substances were thiourea, aniline, acetophenone, benzophenone, naphthalene, 1,2,4-trichlorobenzene, n-butylbenzene and triphenylamine, spanning a range of log Kow between 0.9 and 5.7. Log Kow was 5.7 for AHTN. For HHCB log Kow was determined for two isomers in a mixture. Log Kow was 5.8 for the main isomer and 6.0 for the other isomer. The average log Kow for HHCB was 5.9 (Rudio, 1993a,b). Log Kow may also be calculated from Hydrophobic Fragmental Constants. For the calculations the Syracuse program (SRC) is used. These values are 0.75 and 0.36 log unit higher than the experimental results for AHTN and HHCB, respectively (Table 1).

The sorption to activated sludge was determined from a sorption isotherm experiment producing the Freundlich isotherm constants for the test substances. LSC analysis (liquid scintillation counting) was used as a non-specific analytical technique. The activated sludge samples were freeze-dried, heated (~103°C) and washed to remove excessive TOC. The test was carried out with 2.5 g SS/l (19% OC) and 10, 50, 150 and 300 µg test substance/l. The system was equilibrated for 16 hours. Oxidation of sludge solids followed by LSC produced the best mass balance but direct measurement of sludge scintillation activity (without combustion) was carried out as well. The total recovery for the treatment including combustion was 81 to 91% for AHTN and 89 to 105% for HHCB. The sorption isotherm was linear. The sorption coefficient Kd (determined after sludge combustion) was 10,040 l/kg for AHTN and 12,780 l/kg for HHCB, the sorption coefficient related to organic carbon was 55,176 l/kg (log Koc = 4.74) for AHTN and 70,221 l/kg (log Koc = 4.85) for HHCB. In another way of calculating Koc, the activity on solids was measured indirectly by taking the total ^{14}C dose applied minus the residual amount of ^{14}C activity in the supernatant at the end of the sorption study. Sorption coefficients were only marginally higher: Kd was 11,586 l/kg for AHTN and 13,600 for HHCB, the sorption coefficient related to organic carbon was 63,658 l/kg (log Koc = 4.80) for AHTN and 72,473 l/kg (log Koc = 4.86) for HHCB (MacGillivray, 1996c,d). The higher values were used in the calculations with EUSES.

In EUSES the Koc is estimated from the Kow if no experimental data are available. For non-polar organic chemicals the following QSAR is used: $Koc = 1.26\ Kow^{0.81}$ (Sabljic et al., 1995). Based on the experimental Kow values the resulting log Koc values are 4.71 and 4.88 for AHTN and HHCB, respectively. It can be conlcuded that the differences between the calculated values and the experimental ones is minor for AHTN and HHCB.

Summarizing, measured values are available for most physico-chemical properties of AHTN and HHCB. For Kow, water solubility, vapour pressure and log Koc these measured values are used in the calculations with EUSES.

Table 1. Identification and properties of AHTN and HHCB

	AHTN	**HHCB**
Identification		
CAS - No	1506-02-1; 21145-77-7	1222-05-5
Molecular formula	$C_{18}H_{26}O$	$C_{18}H_{26}O$
Chemical name	7-acetyl-1,1,3,4,4,6-hexamethyl-1,2,3,4-tetrahydronaphtalene	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-cyclopenta[gamma]2-benzopyran
Structural formula		
Molecular weight	258.4	258.4
Properties		
Physical state	solid	viscous liquid
Odour	musky	musky
Boiling point [°C]	n.a.	n.a.
Melting point (measured) [°C]	54.5	not applicable
Vapour pressure (measured) [Pa]	0.0608*	0.0727*
Solubility in water [mg/l]		
measured	1.25*	1.75*
calculated (USES)	0.36	0.19
Henry's law constant [Pa.m^3/mol]	12.5*	11.3*
Octanol/water partition coefficient		
(log Kow) [-]: measured	5.7*	5.9*
calculated (SRC, version 1.35a)	6.35	6.26
Partition coefficient organic carbon-water (log Koc) [l/kg]: measured	4.80*	4.86*
calculated (Sabljic et al.; EUSES)	4.71	4.88

	AHTN	HHCB
Degradation		
Hydrolysis	no data	no data
Photolysis t½ [h], (predicted, SRC version 1.5)	8	3.22
Biodegradation	assumed not mineralized during areobic sewage treatment	assumed not mineralzied during aerobic sewage treatment
Rate constant	assumed biodegradation rate constant = 0 [hr^{-1}]*	assumed biodegradation rate constant = 0 [hr^{-1}]*

* used for the calculations with EUSES

2.3 Biodegradability

Mineralization

AHTN

The inherent biodegradability of AHTN has been assessed in various tests. The probability of adaptation was increased in several ways:

- by inoculation of "adapted" activated sludge from an industrial wastewater treatment plant at an AHTN production facility (Rudio, 1993c);
- by inoculation of "adapted" bacteria from effluent of SCAS units after 8 weeks of adaptation to the test substance (King, 1994a);
- by using extended test periods up to 7 weeks and repetitive addition of test substance (Boersma and Hagens, 1991).

The bioavailability of the poorly water soluble substance was promoted by the following different dispersion techniques:

- fine grinding combined with ultrasonic dispersion (Rudio, 1993c);
- melting at 60 °C in combination with ultrasonic dispersion (Rudio, 1993c);
- using methylene chloride as a solvent followed by evaporation of the solvent to create a thin film on the glass wall of the test vessel (Rudio, 1993c);
- emulsification with Tween 80 (King, 1994a).

The following test methods have been used: (a) modified MITI II for oxygen uptake over 28 days (OECD Test Guideline 302 C, Rudio, 1993c), (b) sealed vessel headspace test with TIC (total inorganic carbon) analysis for CO_2 evolution according to Birch and Fletcher (1991). The inoculum was the filtered effluent from a SCAS system that had been dosed with AHTN for 8 weeks (King, 1994a), (c) two-phase closed bottle BOD method for oxygen uptake after repetitive additions (RDA = Repetitive-die-away test, NEN 6515, Boersma and Hagens, 1991) and (d) modified Sturm test for CO_2-evolution (OECD Test Guideline 301 B, EEC Procedure C.5, Jenkins, 1991a). Test conditions and results are summarized in Table 2. All test results show that the level of mineralisation is insignificant or incomplete. The results in the RDA test indicate a minor oxidation between 10 and 20% of the Theoretical Oxygen Demand (ThOD).

HHCB

HHCB was tested in (a) the sealed vessel headspace test with TIC analysis for CO_2 evolution and an adapted inoculum (King, 1994b) and (b) the modified Sturm test for CO_2-evolution (OECD Test Guideline 301 B, EEC Procedure C.5, Jenkins, 1991b). In (a) HHCB was tested as one of the commercially available qualities containing isopropyl myristate, which, as a dispersant, should promote the bioavailability of the poorly water soluble HHCB. The CO_2 evolution in the test was attributed to the biodegradation of isopropyl myristate. Both tests show the absence of mineralisation.

Primary degradation

All test methods mentioned above aim to measure complete mineralisation and therefore primary biodegradation of the parent substances cannot be excluded by these results. Two studies were carried out that show biotransformation of both AHTN and HHCB.

HHCB

Uniformly radio-labeled HHCB was added to different fungal species growing in mats on growth medium in closed vials at 30 °C at pH 4.5. Fungi were pure cultures of *Phanerochaete chrysosporium* (two strains) and species isolated from spontaneously air-infected cultures. Nominal concentrations of HHCB were 50 - 100 mg/l.

After 6 weeks of incubation no radio-labeled volatile organics or carbon dioxide were produced. For the various strains, however, significant amounts of radio-activity (5-30-50-77%) was associated with metabolites. The mass balance for the radio-activity was complete (recovery in extract 98 - 105%, from TLC 90 - 103%).

Metabolites were extracted in ethyl acetate and separated on TLC with hexane:ethanol 80:20 solvent mixture. According to the Rf-values, metabolites were more polar than HHCB (Rf 0.89): e.g., HHCB-lactone (Rf 0.67), and polarity further increased during 6 weeks (from Rf 0.57 to Rf 0.38). In a second test the most active strain (from air-infected culture) was incubated with nutrients and spiked with HHCB. HHCB was transformed 95 % in 4 weeks. HHCB-lactone accounted for 20% of the radio-activity and 75% consisted of other, more polar products (Envirogen, 1997a).

This work shows that several pure cultures of fungi have the capability for primary biodegradation (loss of parent structure) of HHCB, without mineralisation. The most active fungus culture was identified as *Cladosporium cladospoiodes* (Envirogen, 1997a), a common fungus that is found in several environmental compartments including leaf litter and soils (Kuthubutheen and Pugh, 1979, Wookey et al., 1991). Similar effects in activated sludge cannot be excluded. The tests with activated sludge bacteria carried out so far (King, 1994; Jenkins 1991) were not designed for the detection of metabolites other than carbon dioxide. Recent sludge studies carried out in the Netherlands also indicate a significant loss of parent material during the wastewater treatment and sludge digestion process (see § 3.6).

In another experiment in the Envirogen study, after 4 weeks of incubation the fungal medium was adjusted to pH 7 and amended with additional nutrients and an inoculum from mixed soil and sludge samples. After 140 days mineralisation was shown as about 18% of the radio-activity was trapped in the form of $^{14}CO_2$ (Envirogen, 1997).

AHTN and HHCB

A variety of 64 soil samples from different soil types and localities in The Netherlands were screened for the presence of micro-organisms able to transform these polycyclic musks into metabolites with a more polar behaviour indicated by the lower Rf-value on TLC plates. About 1/3 to 1/2 of the samples showed a positive degrading potential towards one or both polycyclic musks.

Several pure cultures of fungi *Aureobasidium pullulans* and *P. chrysosporium* were incubated with AHTN, AHTN-alcohol, and HHCB. In cultures of *A. pollulans* about 80% of AHTN disappeared in 3 weeks. GC-MS analysis of the ethylacetate extracts indicated reduction of the acetyl-group.

In cultures of *P. chrysosporium* HHCB and AHTN disappeared within 3 and 6 days, respectively. GC-MS analysis of the metabolites of AHTN in ethylacetate extracts showed the temporary presence of small amounts of AHTN + O and AHTN + 2 O. It is suggested that later stages of degradation were too polar to be extracted by ethyl acetate (PFW, 1996).

These results show that polycyclic musks in soil are likely to be transformed to polar intermediates by soil-born fungi. Some published data on biodegradation of polycyclic aromatic hydrocarbons (PAH) with white rot fungus indicate the presence of extra-cellular enzymes able to attack macromolecules with similar structures (e.g., lignin, humic compounds) to the polycyclic musks (Field et al., 1992; Bumpus, 1989). These results need further quantification before they can actually be used in the risk assessment.

Overall conclusion

Mineralization of AHTN and HHCB appears to be insignificant in several standard test systems. However, it has been shown that primary degradation of AHTN and HHCB does occur by soil-born fungi. These results need further quantification in the sense of a rate constant, before they can be used in the calculations with EUSES. Therefore, the biodegradation rate constant is set at 0 hr^{-1} in the Sewage Treatment Plant (STP), and in the sediment and soil compartment in the calculations with EUSES.

Table 2. Summary of biodegradation tests

AHTN	
Test method	**OECD 302C: modified MITI II**, respirometric method
Inoculum	Adapted Industrial Sludge 100 mg/l
Test substance	AHTN, nominal 30 mg/l
Dispersion	1) grinding + ultrasonic 2) melting + ultrasonic 3) solvent + evaporation
Test duration	28 days
Controls	Reference substance aniline No toxicity control
Results	% oxidation: zero, no additional BOD in comparison with blank.
Reference	Rudio, 1993c
Test method	**Modification of OECD 301B**, Sealed vessel TIC test acc. to Birch and Fletcher, 1991
Inoculum	Effluent from SCAS after 8 weeks adaptation
Test substance	AHTN, 1.34 mg C/l; carbon 83.72% w/w
Dispersion	In Tween 80
Test duration	28 days
Controls	Reference substance benzyl alcohol No toxicity control
Results	% CO_2 release: zero
Reference	King, 1994a
Test method	**Two-phase closed bottle test, NEN 6515, 1989** Oxygen uptake
Inoculum	Activated sludge from communal STP, 30 mg/l
Test substance	AHTN, nominal 22 mg C/l, repetitive additions after 4 and 5 weeks
Dispersion	no
Test duration	7 weeks
Controls	Reference substances Sodium acetate and diethylene glycol; Toxicity control
Results	21% oxidation after 3 weeks 12% oxidation after 7 weeks
Reference	Boersma and Hagens, 1991
Test method	**Modified Sturm test OECD 301B**, CO_2-evolution
Inoculum	sewage effluent, 1 drop/l
Test substance	AHTN, nominal 10 and 20 mg/l
Dispersion	no
Test duration	28 days
Controls	Reference substance sodium benzoate; Toxicity control
Results	% CO_2 release: zero
Reference	Jenkins, 1991a

HHCB	
Test method	**Modification of OECD 301B**, Sealed vessel TIC test acc. to Birch and Fletcher, 1991
Inoculum	Effluent from SCAS after 8 weeks adaptation
Test substance	HHCB in isopropyl myristate, 10.97 mg C/l; 32.2% IPM, two identified HHCB isomers totalled 51.8% (26.4% and 25.4%), carbon 80.56% w/w
Dispersion	Injection in isopropyl myristate
Test duration	28 days
Controls	Reference substance benzyl alcohol No toxicity control
Results	% CO_2 release: zero (corrected for isopropyl myristate)
Reference	King, 1994b
Test method	**Modified Sturm test OECD 301B**, CO_2-evolution
Inoculum	sewage effluent, 1 drop/l
Test substance	HHCB, nominal 10 and 20 mg/l
Dispersion	no
Test duration	28 days
Controls	Reference substance Sodium benzoate; Toxicity control
Results	% CO_2 release: zero
Reference	Jenkins, 1991b

3 EXPOSURE ASSESSMENT

3.1 Release estimation

The estimation of the release of substances like AHTN and HHCB starts with their use pattern. Although both substances are produced in the EU, the present report focusses only on the release due to private use as this is considered the main route by which AHTN and HHCB enter the environment. The TGD distinguishes three types of categories: (1) main category, describing the exposure relevance of the use of a substance, (2) industrial category and (3) function or use category. For AHTN and HHCB the predicted environmental concentration (PEC) is calculated using industrial category 5: Personal Domestic Use, use category 9: Cleaning/washing agents and additives, and assuming that emission takes place only via the life cycle stage private use. Although not all material is used in the category Cleaning/washing agents and additives, this scenario is used as the use category: Cosmetics will give the same results. In both use categories it is assumed that the entire use volume is disposed of down the drain and is treated by a sewage treatment plant (STP). It is assumed that no AHTN and HHCB remains on fabric, skin or surfaces, or volatilises to air during use.

The quantities of AHTN and HHCB released from point sources are assessed for a generic local environment (TGD). This is not an actual site but a hypothetical one with predefined, agreed environmental characteristics, the so-called 'standard environment'. PEClocal represents the concentration expected at a certain distance from the source (e.g. a STP). PEC is also calculated for a standardised regional environment taking into account the further distribution and fate of a substance upon release from point and diffuse sources over a wider area (PECregional). The standard regional environment is a densely populated area with $20 * 10^6$ inhabitants in a region of $200 * 200\ km^2$. The PECregional is used also as background concentration for the local scale (TGD).

The amount of AHTN and HHCB used in Europe is based on a survey by the Research Institute of Fragrance Materials (RIFM, 1997). RIFM carried out two surveys, one in 1993 and one in 1996, relating to volumes of use in compounding fragrances for 1992 and 1995, respectively. Results are presented in Table 3.

Table 3. Use volumes of AHTN and HHCB in Europe (RIFM, 1997)

	AHTN [tonnes]	HHCB[1] [tonnes]
1992	885	2400
1995	585	1482

[1] refers to undiluted HHCB (due to the high viscosity of pure HHCB commercial HHCB is a c. 65% solution in a neutral solvent)

In 1993 100% of the large companies responded to the survey and enough smaller companies to cover 90% of their use. In 1996 32 companies supplied data. These companies included the major producers of fragrance compounds in Europe. According to RIFM the volumes for 1995 account for approximately 88% with a range of 81 to 95% of the total use volume (RIFM, 1997). The figures for 1992 as well as 1995 have not been corrected for export of fragrance compounds containing AHTN and HHCB outside Europe. RIFM reports that industry has estimated that 20-30% of AHTN and HHCB is exported (RIFM, 1997). This estimation does not include export of consumer products containing AHTN or HHCB; it only refers to export by fragrance suppliers. Currently a new survey is being undertaken to obtain 1996 figures. According to RIFM it cannot be concluded whether the decrease in use volumes for both substances represents a downward trend in use or is caused by market fluctuations in use from year to year.

In the standard scenario in the TGD it is assumed that 10% of the total volume in the EU is used on a regional scale unless specific information on use or emission is available. Deviating from this scenario it may be assumed for HHCB and AHTN (which are used in consumer products only) that the use per capita is the same all over the EU and that all compounded material is marketed and used in the EU (as the volume exported outside the EU is unknown and only an estimation is available).

In order to justify this alternative scenario two aspects are investigated:

1. variability in use of consumer products containing ATHN or HHCB within the EU countries;
2. verification of the use volume based on use per capita with data on use of consumer products containing AHTN and HHCB and data on the content of AHTN and HHCB in consumer products.

ad 1) AHTN and HHCB are used in cosmetics and detergents. Statistics on the use of detergents has been published by the Association Internationale de la Savonnerie, de la Détergence et des produits d'Entretien (AISE, 1996) for consumer soap, detergent and cleaning products. In Figure 1 the use of these products in the EU in 1995 is presented for those products having a total use volume of more than 5% of the total use volume for all consumer soap, detergent and cleaning products, being the categories: fabric washing powders, fabric washing liquids, fabric rinsing products, machine dish cleaning and surface cleaning - general purpose and others. Raw data are given in Appendix 2 together with the mean use per capita per country for each product category and the ratio between the maximum and mean value and between the mean and minimum value as an indication for the variation among countries.

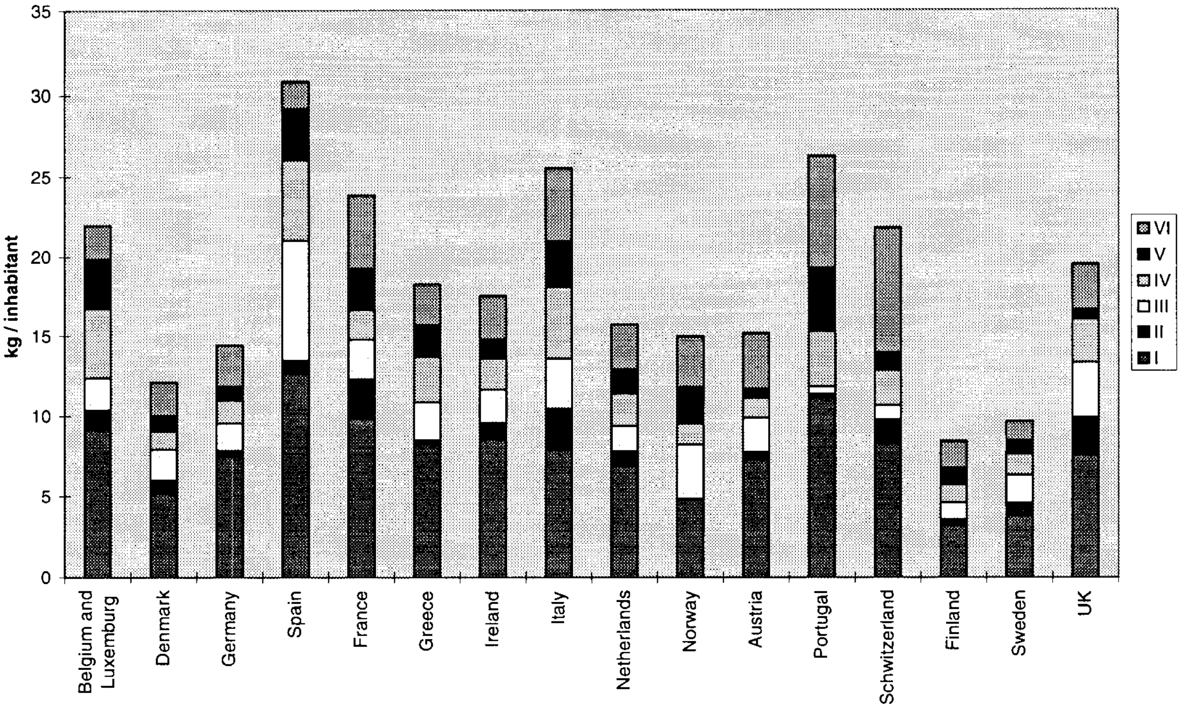


Figure 1. Use of consumer soap, detergent and cleaning products in kg/inhabitant within the EU for 1995 (I: fabric washing powders, II: fabric washing liquids, III: fabric rinsing products, IV: machine dish cleaning, V: surface cleaning - general purpose and VI: others). Weighted mean is 18.5 kg/inhabitant.

From this figure it can be seen that the variability in use volumes for the different product categories is not that high: the maximum is a factor 1.7-5.2 higher than the mean for the individual product categories, while the mean is a factor 2.4-6.7 higher than the minimum (see Appendix 2). The lowest variability is found for fabric washing powders constituting about 40% of the total use volume.

For cosmetics no data are available on use volumes per country. However, the European Cosmetic Toiletry and Perfumery Association Colipa has presented market volume data at retail sales prices for 1995 (Colipa, 1996). In Figure 2 the national market volumes in ECU/inhabitant are presented for all product categories: perfumes and fragrances, decorative cosmetics, skin care products, hair care products and toiletries. Raw data are given in Appendix 2 together with the mean per capita per country for each product category and the ratio between the maximum and mean value and between the mean and minimum value.

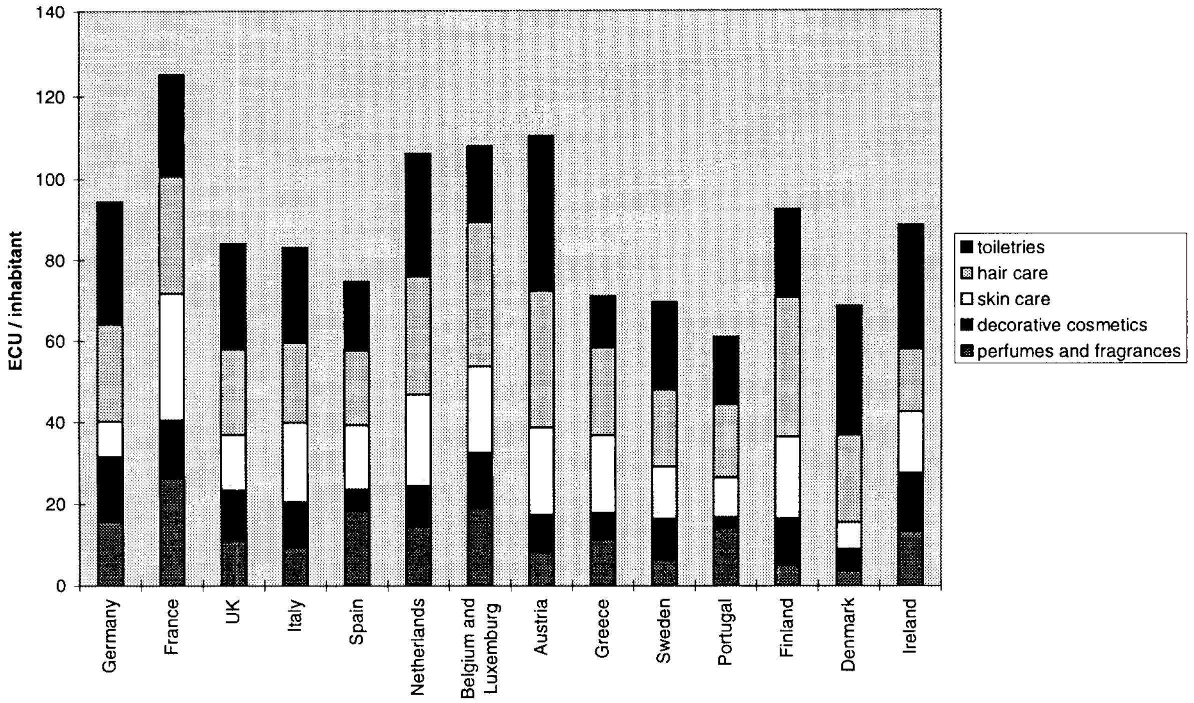


Figure 2. National market volumes at retail sales prices (ECU/inhabitant) for 1995 in the EU for the product categories perfumes and fragrances, decorative cosmetics, skin care products, hair care products and toiletries. Weighted mean is 88.4 ECU/inhabitant.

From this figure it can be seen that the variability for cosmetics, toiletry and perfumery products is smaller compared to consumer soap, detergent and cleaning products: the maximum is a factor 1.5-2.1 higher than the mean while the mean is a factor 1.6-3.3 higher than the minimum (see Appendix 2). Although the real use is unknown there is certainly a relation between the market volumes at retail sales prices and the use expressed in kg per inhabitant.

ad 2) Based on an EU population of 3.65 * 10^8 inhabitants (European Commission, 1995) the use per capita in 1995 is:

* for AHTN: 585 / 3.65 * 10^8 = 1.6 g/year or 4.4 mg/day;

* for HHCB: 1482 / 3.65 * 10^8 = 4.1 g/year or 11.1 mg/day.

These calculations can be verified using information on the use of consumer soap, detergent and cleaning products and cosmetics, toiletry and perfumery products and the content of AHTN and HHCB in these products. Taking the Netherlands as an example the use per inhabitant is 23.4 and 58.6 tonnes in 1995 assuming a population of 14.3 * 10^6 inhabitants (European Commission, 1995). Assuming 25% export and that these figures represent 88% of the 'real' volume, the total use volume for the Netherlands of AHTN and HHCB is estimated to be 71 tonnes.

In Table 4 the use of polycyclic musks is calculated assuming an average of 5% total polycyclic musks in a fragrance in consumer soap, detergent and cleaning products (NEA, 1997). The figure of 5% is a best estimate for the average content in perfumes which may vary between 4 and 6% (NEA, 1997).

Table 4. Estimation of use volumes of polycyclic musks in consumer soap, detergent and cleaning products in the Netherlands in 1995.

product	tonnage (kton)	fragrance concentration (%)	fragrance tonnage (ton)	tonnage polycyclic musks (ton)
toilet soap	12.3	1	123	6.15
fabric washing powder	106.5	0.4	426	21.3
hard soap	0.6	0.5	3	0.15
fabric rinsing	24.3	0.3	72.9	3.6
fabric washing liquids	14.0	0.3	42	2.1
fabric washing auxilliary	1.4	0.3	4.2	0.21
hand dish cleaning	30.7	0.3	92.1	4.6
machine dish cleaning	9.6	0.3	28.8	1.4
surface cleaning	43.3	0.2	86.6	4.3
total	242.7		874.4	43.9

To the tonnage of 43.9 the quantity used in cosmetics, toiletry and perfumery must be added. However, accurate figures on use of these products within the EU are unknown and the statistics in monetary values from Colipa cannot be readily converted. According to Somogyi et al. (1995) the use of fragrance oils per product category in Europe is as follows (Table 5):

Table 5. Use of fragrance oils per product category in the EU (Somogyi et al., 1995)

detergents (fabric & dishwashers)	24.3%
fabric softeners	14.2%
soaps (fabric, skin, surface bar & surface liquid)	9.1%
personal care (cosmetics, creams/milks, deo's)	13.2%
fine fragrances (perfumes, eau de perfume, eau de toilette, colognes)	5.1%
hair care (shampoo, conditioner, styling, colour)	10.2%
bath & shower (gels, oils, pearls, powder)	10.2%
industrial and household cleaners (surface, al purpose, scourers, lavatory)	7.6%
other (room airfreshener; candles, potpourri, masking, paper)	6.1%

Of these product categories soaps, fabric softeners, detergents and cleaners account for 55% of the total use, i.e. the 43.9 tonnes from Table 4. Adding the remainder of 45% gives a total use of 43.9 + 35.9 = 79.8 tonnes in 1995. This figure corresponds well to the volume of 71 tonnes given above for AHTN and HHCB based on equal use per inhabitant in the EU.

Summarizing, the variation in use of cosmetics, toiletry and perfumery products within the EU is reasonably low: the maximum is less than a factor 2 higher than the mean value. The variation in use of consumer soap, detergent and cleaning products is somewhat higher, but still reasonably low for the most important product categories. Using information on the content of polycyclic musks in a fragrance, it can be concluded that estimating the use based on the ratio of the total volume used in the EU and the number of inhabitants, leads to a reasonable estimation of the 'real' use.

It is concluded that it is justified to deviate from the standard scenario in the TGD in which 10% of the total volume in the EU is used on a regional scale. The only 'hard' data on the use volumes of AHTN and HHCB available are the results from the RIFM survey. In the calculations with EUSES in the next paragraphs the use is therefore based on the total volume divided by the number of inhabitants, assuming that all compounded material is marketed within the EU.

3.2 Surface water

According to the emission scenario in the TGD, emission takes place only by private use and the total volume is discharged through a STP. In the STP the AHTN and HHCB partition between water and sludge; practically nothing goes to air for both substances. Part of the amount of AHTN and HHCB is released into the aquatic environment when the effluent is discharged and diluted in a river. Another part enters the terrestrial environment after adsorption to the sludge in the STP and applying sludge on agricultural land. The method described in the TGD will not be discussed extensively in the present report. For the description of the method reference is made to the TGD.

Table 6 presents the steps to derive the predicted environmental concentration in surface water for a generic local environment calculated with EUSES ($PEClocal_{water}$)[2]. Appendix 1 lists all input and output data of the EUSES calculations.

Table 6. Derivation of PECwater for the local environment

Step		AHTN	HHCB
1	Tonnage (EU) [tonnes/yr]	585	1482
2	Daily per capita release [mg/day]	4.4	11.1
3	Daily per capita release [mg/day] 'realistic worst case'	13.2	33.3
4	Total concentration influent STP [mg/l]	0.066	0.16
5	Total concentration effluent STP [mg/l]	0.011	0.025
6	Clocalwater, dissolved [mg/l]	0.00097	0.0023
7	PECregionalwater, dissolved [mg/l]	0.000054	0.00012
8	PEClocalwater, dissolved [mg/l]	0.0010	0.0024

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[2] In the present report several symbols are used for a concentration:
- PEC (Predicted Environmental Concentration): Predicted Environmental Concentration for the endpoints for the risk characterization: surface water, sediment, soil and predators;
- C (Concentration): other, not used for the risk characterization, predicted concentrations;
- *C* in italics (Concentration): measured concentration.

ad 1 and 2
Results from the 1995 survey (see § 3.1).

ad 3
It is assumed that 100% of the amount used is discharged through an STP. It is unlikely that the distribution of the consumption of AHTN and HHCB is even over the week or month. Therefore, the figures under 2 are multiplied with a factor 3 to reflect a 'realistic worst case' (Tas and Van de Plassche, 1996).

ad 4
The default sewage flow to the STP is 200 l/inhabitant equivalent (i.e.)/day. Subsequently, influent concentrations are for AHTN and HHCB 13.2 / 200 = 0.066 mg/l and 33.3 / 200 = 0.16 mg/l, respectively.

ad 5
In the STP the substances partition between water and sludge. The partitioning between sludge and water is determined by the default operation parameters of the STP (activated sludge reactor: sludge loading rate of 0.15 $kg_{BOD}.kg_{dwt}^{-1}.d^{-1}$; surface aeration) (EUSES; Chapter III). The Kow and H determine the fraction released to air, water and sludge. It is assumed that no biodegradation or hydrolysis takes place: the rate constants for abiotic as well as biotic degradation in an STP are therefore set at 0 hr^{-1} (TGD). Fractions to water and sludge are calculated assuming that AHTN and HHCB will partition between water and sludge determined by the partition coefficient water-sludge, calculated from the formula Kp = foc * Koc. Kp values are derived for raw sewage sludge, settled sewage sludge and activated sewage sludge (see Appendix 1). For AHTN and HHCB the fraction to air, water and sludge is 0.021, 0.17, 0.81 and 0.016, 0.16, 0.83, respectively. So, for both substances the total amount entering an STP will leave the STP mainly via effluent and sludge. The fraction to water includes a fraction of the chemical sorbed to suspended matter in the effluent.

ad 6
The standard dilution factor of effluent in surface water is 10. The factor 10 is applied to the total effluent concentration. The concentration in surface water is calculated taking also sorption to suspended matter into account applying the formula:

$$Clocal_{water} = Clocal_{eff} / [(1 + (Kp_{susp} * SUSP_{water}) * DILUTION] \qquad (1)$$

where:

DILUTION: dilution factor: 10;
$SUSP_{water}$: concentration suspended matter in river water: 15 mg/l for the local and regional scale;
Kp_{susp}: solids-water partition coefficient of suspended matter: 6310 and 7240 l/kg for AHTN and HHCB, respectively. For the local and regional scale 8.6% and 9.8% is sorbed to suspended matter for AHTN and HHCB, respectively.

ad 7

Regional background concentrations in water and the concentrations in water entering the region from other areas (continental scale) should be added to the local concentrations (TGD). According to the TGD 10% of the volume used in the EU is used as the regional tonnage while the EU volume minus the regional tonnage (i.e. 90% of the EU volume) is used as the continental tonnage. Here, for the calculations with EUSES the volume is based on use per capita as explained in § 3.1 for the local scenario. This leads to a regional tonnage of 23.4 and 58.6 tonnes for AHTN and HHCB, respectively. It is assumed that 70% of the discharged volume passes through a STP, whereas 30% bypasses sewage treatment and is discharged directly on surface water (TGD). The predicted concentrations are presented in Table 7.

Table 7. Derivation of PECwater for the regional and continental scale

	AHTN	HHCB
Tonnage Europe [tonnes/yr]	585	1482
Tonnage regional [tonnes/yr]	23.4	58.6
Tonnage continental [tonnes/yr]	562	1423
PECregional$_{water}$ [mg/l] dissolved	$5.4*10^{-5}$	$1.2*10^{-4}$
PECcontinental$_{water}$ [mg/l] dissolved	$1.6*10^{-5}$	$3.7*10^{-5}$

Background concentrations are low compared to the local concentrations. PECcontinental$_{water}$ is not considered further, while PECregional$_{water}$ is used for the estimation of PEC$_{oral, fish}$ (see § 3.5.2) and the PEClocal$_{water}$ (see below).

ad 8

The local concentration Clocal$_{water}$ and the background concentration (PECregional$_{water}$) are summed up to obtain PEClocal$_{water}$.

3.3 Soil

A fraction of AHTN and HHCB in the STP partitions to the sludge. In the approach of the TGD digested surplus sludge is routinely applied to the soil. In the TGD, scenarios are available to determine the risk for the soil ecosystem, and for human health due to consumption of agricultural crops and meat and milk of cattle feeding on grass. In the Netherlands as well as in some other countries the application of sludge to agricultural soil is not common, as usually the sludge is burned or dumped in landfills. However, in other countries the use of sludge on agricultural land is common practice. Therefore, in the EU risk assessment this route of exposure is incorporated. Results with EUSES for the PEClocal$_{soil}$ used for assessing the risks for ecosystems are presented in Table 8. Appendix 1 lists all input and output data of the EUSES calculations.

Table 8. Derivation of PEClocalsoil for the local environment

Step		AHTN	HHCB
1	C_{sludge} [mg/kg dw]	132	336
2	Median measured concentration digested sludge: C_{sludge} [mg/kg dw]	16	23
3	$Clocal_{agricultural\ soil}$ [mg/kg ww]	0.23	0.33
4	$PECreg_{natural\ soil}$ [mg/kg ww]	$5.8 * 10^{-4}$	$2.3 * 10^{-3}$
5	$PEClocal_{soil}$ [mg/kg ww]	0.23	0.34
6	$PEClocal_{soil}$ [mg/kg dw]	0.26	0.38

ad 1

The default net rate of sewage sludge production is 71 g/d/i.e. The emission to sludge is divided by the amount of sewage sludge to obtain the predicted concentration in sludge (C_{sludge}).

ad 2

The scenario for the route to soil assumes that sludge is collected during some period of time, brought onto the land once per year and the $PEClocal_{soil}$ reflects the estimated situation after 10 consecutive applications. The measured concentrations in digested sludge deviate considerably from the model predictions: a factor 8.3 and 15 for the median of all measured concentrations for AHTN and HHCB, respectively (see § 3.7). Therefore, for further model calculations to predict the concentrations in soil, the measured concentrations in digested sludge were used. Fluctuations in sludge concentrations are smoothed and therefore the median concentration in digested sludge is relevant for the estimation of the concentration in soil. Maximum concentrations were a factor 1.4 higher than the median concentrations for both substances. For further details see § 3.7.

ad 3

Sludge is applied to soil once a year with a rate of 0.5 kg dw/m^2/y and ploughed to a depth of 0.20 m. The bulk density of the soil is taken to be 1700 kg/m^3. Potential loss processes in the soil are biodegradation, volatilisation and leaching. Although it was shown that primary degradation of AHTN and HHCB may occur in soil, this cannot yet be quantified and therefore loss through these processes is presumed to be negligible. $Clocal_{agricultural\ soil}$ used as the exposure concentration of the terrestrial ecosystem is the concentration 30 days after sludge application where sludge is assumed to be applied for 10 consecutive years (TGD).

ad 4

The concentration on the regional scale is used as a background concentration for the local one. The steady state concentration in natural soil is used, where input only occurs through atmospheric deposition. As both AHTN and HHCB are not very volatile substances, these regional concentrations are very low compared to the local concentrations.

ad 5
The local concentration $Clocal_{agricultural\ soil}$ and the background concentration ($PECreg_{natural\ soil}$) are summed to obtain $PEClocal_{soil}$.

ad 6
Concentrations in mg/kg ww are converted to mg/kg dw by multiplying the wet weight values with a factor 1.13 using the formula (EUSES):

$$CONV_{soil} = RHO_{soil} / (Fsolid_{soil} * RHOsolid) \qquad (2)$$

$CONV_{soil}$:	conversion factor for ww to dw;
RHO_{soil}:	wet bulk density of soil, being 1700 kg ww/m^3;
$Fsolid_{soil}$:	volume fraction of solids in soil, being 0.6 m^3/m^3;
RHOsolid:	density of solid phase, being 2500 kg/m^3.

3.4 Sediment

The discharged effluent is diluted in surface water and AHTN and HHCB partition between water and suspended solids in the surface water. In the TGD the concentration in freshly deposited sediment is assumed to equal the concentration in suspended solids in the water. Table 9 lists the steps included in the calculation of $PEClocal_{sed}$.

Table 9. Derivation of PEClocalsed

Step	Parameter	AHTN	HHCB
1	log Koc	4.71	4.88
2	Ksusp-water	1580	1810
3	$PEClocal_{sed}$ [mg/kg ww]	1.4	3.8
4	$PEClocal_{sed}$ [mg/kg dw]	3.6	9.8

ad 1
See § 2.2 and Table 1, Physico-chemical properties.

ad 2
The solids-water partition coefficient Kp is 6310 l/kg for AHTN and 7240 l/kg for HHCB. The partition coefficient Ksusp-water between suspended material and water is derived from Kp, involving correction for the fraction of water and solids (F) and for the density of water and solids (RHO) in suspended matter:

$$K_{susp-water} = Fwater_{susp} * RHOwater + Fsolid_{susp} * Kp * RHOsolid \qquad (3)$$

For AHTN: $K_{susp-water} = 0.9 * 1.0 + 0.1 * 6310 * 2.5 = 1580$.
For HHCB: $K_{susp-water} = 0.9 * 1.0 + 0.1 * 7240 * 2.5 = 1810$.

ad 3

$PEClocal_{sed}$ is derived from $PEClocal_{water}$ (see § 3.2) using $K_{susp\text{-}water}$ after correction for density differences between suspended matter and sediment:

$$PEClocal_{sed} = K_{susp\text{-}water} * PEClocal_{water} / RHO_{susp} \qquad (4)$$

For AHTN: $PEClocal_{sed}$ = 1580 * 0.0010 / 1.15 = 1.4 mg/kg ww.
For HHCB: $PEClocal_{sed}$ = 1810 * 0.0024 / 1.15 = 3.8 mg/kg ww.

ad 4

Concentrations in mg/kg ww are converted to mg/kg dw by multiplying the wet weight values with a factor 2.6 using the formula (EUSES):

$$CONV_{sed} = RHO_{sed} / (Fsolid_{sed} * RHOsolid)$$

$CONV_{sed}$: conversion factor for ww to dw;
RHO_{sed}: wet bulk density of sediment, being 1300 kg ww/m^3;
$Fsolid_{sed}$: volume fraction of solids in sediment, being 0.2 m^3/m^3;
RHOsolid: density of solid phase, being 2500 kg/m^3.

3.5 Predators

3.5.1 Bioconcentration in fish

Predators may take up these substances via their food. For the aquatic food chain fish-eating predators such as birds and mammals are considered. Fish can accumulate AHTN and HHCB from water. For the prediction of the concentration in fish from the predicted concentration in water the bioconcentration factor BCF is used. The bioconcentration factor is determined from the concentrations in fish (C_f) and water (C_w) at steady state, or from the uptake (k_1) and elimination (k_2) rate constants by:

$$BCF = k_1 / k_2 = C_f / C_w \qquad (5)$$

Results of the bioconcentration tests with AHTN and HHCB are presented in Table 10.

Bioconcentration of ^{14}C-AHTN and ^{14}C-HHCB has been tested using two concentrations in a flow-through system. AHTN and HHCB were tested with bluegill sunfish (*Lepomis macrochirus*) as test organism according to OECD Guideline 305E (Van Dijk, 1996a,b). In both tests a solubilizer (DMF, Tween 80) was used to dissolve AHTN and HHCB. The tests were carried out with radio-labelled material that was identified as AHTN (78.8% radiochemical purity, impurities due to radiolabelling) and HHCB (radiochemically pure, three isomer groups), respectively. Identification of the parent compound in water and fish was performed by TLC/HPLC.

The concentration of AHTN in the fish reached plateau levels after 3-7 days (low dose) and 3 days (high dose) of exposure and fluctuated hereafter. According to Van Dijk (1996a) an uptake rate could not be determined due to rapid stabilization of the concentration.

Elimination followed first order kinetics. Depuration half-lives were 0.8 - 2.1 days indicating that the uptake of AHTN was highly reversible. The bioconcentration factor was derived from C_f/C_w, with C_f derived from the plateau level (days 21 and 28) and C_w as the overall mean. The uptake rate constant was calculated from $k_1 = BCF * k_2$.

Besides the parent compound AHTN at least two polar radio-active fractions were found in the water (see Table 10).

In the organic extracts of fish edibles and non-edibles besides the parent compound a very polar metabolite fraction was found in the same or higher amounts. Based on actual concentrations of parent compound in exposure water and at the plateau level in fish, the BCF for the whole fish was 597.

The main metabolite fraction in water W3 and the main polar metabolite fraction in the tissue (F3) showed identical Rf values on TLC with different solvent systems and identical elution times with HPLC. Smaller fractions of metabolites with intermediate polarity and with several subfractions occurred both in tissue (F3.1 and F3.2) and in water W2, but were not clearly identical.

The concentration of HHCB reached a plateau level after 3-7 days exposure. An uptake rate could not be determined due to rapid stabilization of the concentration. Elimination followed first order kinetics. Depuration half-lives were 2-3 days indicating that the uptake of HHCB in fish was highly reversible. The bioconcentration factor was calculated as for AHTN.

In the water at least one polar radio-active fraction was found and in the organic extracts of fish edibles and non-edibles besides the parent compound a polar metabolite fraction was found in significant amounts. Based on actual concentrations of parent compound in exposure water and at the plateau level in fish, the BCF for the whole fish was 1584.

Based on Rf values on TLC with different solvent systems and elution times on HPLC, the parent compound occurred in 3 subfractions identical to the isomers in the unpurified sample of the stock solution. The polar fraction of metabolite in tissue proved to be identical with that in water.

For substances with a log Kow of < 6 the BCF can be estimated using the following QSAR according to the TGD (Veith et al., 1979):

$$\log BCF(wet\ weight) = 0.85 * \log Kow - 0.70 \qquad (6)$$

The estimated BCF is 13,964 l/kg for AHTN and 20,654 l/kg for HHCB. These theoretical values exceed the measured BCF values by more than one order of a magnitude. This may be explained by metabolism of the parent substances in the fish to more polar metabolites that will be eliminated by the fish at a higher rate.

Table 10. Bioconcentration of AHTN and HHCB in bluegill sunfish Lepomis macrochirus in a flow-through system (Van Dijk, 1996a,b)

	AHTN	HHCB
Initial fish weight [g]	0.35	1.2-1.4
Low dose [µg/l][1]	0.99 ± 0.12	0.91 ± 0.10
High dose [µg/l]	9.81 ± 0.85	8.84 ± 0.89
Period of exposure [d]	28	28
Period of elimination [d]	28	28
Plateau level low dose [mg/kg][1]	0.49[ed], 2.12[ne], 1.30[wf]	0.45[ed], 1.98[ne], 1.49[wf]
Depuration residue low [mg/kg]	0.029[ed], 0.096[ne], 0.049[wf]	0.015[ed], 0.031[ne], 0.023[wf]
Plateau level high dose [mg/kg]	5.17[ed], 20.60[ne], 12.99[wf]	4.82[ed], 22.16[ne], 14.26[wf]
Depuration residue high [mg/kg]	0.431[ed], 1.265[ne], 1.118[wf]	0.109[ed], 0.221[ne], 0.105[wf]
Uptake rate constant k_1 [l/kg/d]	442[3] (low) 765[3] (high)	352[3] (low) 421[3] (high)
Elimination rate constant k_2 [d^{-1}]	0.337 (low), $r^2=0.99$ 0.577 (high), $r^2=0.96$	0.215 (low), $r^2=0.93$ 0.261 (high), $r^2=0.99$
Bioconcentration factor (whole fish, wet weight) [l/kg]	1320[1] 597[2]	1624[1] 1584[2]
Radioactivity in water (depuration phase)	AHTN 91-93% Polar metab. 2-8%	HHCB 81-90% Polar metab. 10-19%
Radioactivity in fish edibles (depuration phase)	AHTN 41-49% Polar metab. 33-48%	HHCB 79-88% Polar metab. 9-16%
Radioactivity in fish non-edibles (depuration phase)	AHTN 31-42% Polar metab. 44-60%	HHCB 72-87% Polar metab. 11-24%

[1] Based on total radio-activity

[2] BCF based on actual concentration of parent compound

[3] Uptake constant was calculated from BCF*k_2

[ed] in edibles

[ne] in non-edibles

[wf] in whole fish

In the bioconcentration studies with AHTN and HHCB unidentified water soluble metabolites are reported in fish tissue and water. Although the fraction of metabolite in the water in relation to the parent substance is small, the absolute amount of this quantity is high in relation to the absolute amount of parent substance present in the fish tissue. In the bioaccumulation study report this matter was not addressed, but from the data presented in the report a mass balance for the dynamic flow-through system can be made which is presented in Appendix 3. It is concluded that both AHTN and HHCB are metabolized to one or more polar metabolites in a relatively short time. Therefore it is considered justified that the BCF based on the actual concentration of the parent compound (Van Dijk, 1996a,b) is used for assessing the risk for fish-eating predators.

3.5.2 Aquatic food chain

Fish-eating predators are exposed through the fish they feed on. Consequently, $PEC_{oral,fish}$ is the level of AHTN and HHCB in fish. In the TGD it is assumed that a fraction of the diet of predators is taken from an area under the influence of a local source, while another fraction comes from an area with background levels only. Subsequently, $PEC_{oral,fish}$ is an average of the local and regional levels in fish:

$$PEC_{oral,fish} = BCF_{fish} * [(PEClocal_{water} + PECregional_{water}) / 2] \tag{7}$$

Results of the calculations for AHTN and HHCB are presented in Table 11. All input and output data of the EUSES calculations are presented in Appendix 1.

Table 11. Derivation of PECpred for fish-eating predators

	AHTN	HHCB
Fish		
Clocalwater [mg/l] dissolved	0.00097	0.0023
PECregionalwater [mg/l] dissolved	$5.4 * 10^{-5}$	$1.2 * 10^{-4}$
BCF [l/kg wet weight]	597	1584
PECoral,fish [mg/kg wet weight fish]	0.32	2.0

3.5.3 Terrestrial food chain

Also a terrestrial food chain via the route soil ⇒ earthworm ⇒ worm-eating birds or mammals is used for assessing the risk for predators. As for the aquatic food chain the exposure of this predator is based on 50% local and 50% regional sources:

$$PEC_{oral,worm} = BCF_{worm} * [(PEClocal_{soil} + PECregional_{soil}) / 2] \tag{8}$$

In EUSES the regional and local concentration in agricultural soil are used. $PEClocal_{soil}$ represents the concentration after 10 consecutive sludge applications (see §3.3). The $PECregional_{soil}$ is a steady-state concentration: concentrations have become constant in time. In EUSES the non-equilibrium steady-state ('level III') solution of the model SimpleBox (Brandes et al., 1996) is used. For substances like AHTN and HHCB, which can only disappear from the soil-system in the regional model via volatilisation, leaching or run-off (as no biodegradation is assumed; see Table 1), half-lifes for reaching steady state will be in the order of 1000-10,000 years (pers. com. D. v.d. Meent, RIVM).

Due to the lack of experience with this approach the assessment is considered as provisional (TGD).

According to the TGD the BCF_{worm} has to be calculated applying the following QSAR:

$$K_{worm\text{-}porew} = 0.25 * Kow * 0.16 \qquad (9)$$

and:

$$BCF_{worm} = K_{worm\text{-}porew} (RHO_{soil} / K_{soil\text{-}water}) \qquad (10)$$

where:

$K_{worm\text{-}porew}$	worm-pore water partition coefficient
RHO_{soil}	bulk density of soil
$K_{soil\text{-}water}$	soil-water partition coefficient

This relation is based on a data set with log Kow ranging between 1.0 and 6.0 and is based on a study of Connell and Markwell (1990). However, a critical evaluation of the data used by Connell and Markwell (1990) showed that the relationship for $K_{worm\text{-}porew}$ leads to an overestimation of this value (Jager and Hamers, 1997; Jager, in prep.). Jager (in prep.) shows that the relation should be:

$$K_{worm\text{-}porew} = 0.01 * Kow \qquad (11)$$

This relation is used in the calculations with EUSES. Results are presented in Table 12. All input and output data of the EUSES calculations are presented in Appendix 1.

Table 12. Derivation of PECoral,worm for predators in a terrestrial food chain

	AHTN	HHCB
Earthworm		
$PEClocal_{agric}$ [mg/kg ww]	0.23	0.34
$PECregional_{agric}$ [mg/kg ww]	0.12	0.20
$K_{worm\text{-}porew}$ [l/kg]	$5 * 10^3$	$7.9 * 10^3$
$K_{soil\text{-}water}$[1] [m^3/m^3]	1890	2170
BCF_{worm} [kg ww/kg ww]	4.5	6.2
$PEC_{oral,worm}$ [mg/kg ww]	0.78	1.7

[1] for the derivation of $K_{soil\text{-}water}$ see § 4.2

The calculation of $PECregional_{agric}$ is based on measured concentrations in sewage sludge as has been done for the $Clocal_{agric}$ (see Table 8). However, a measured concentration in sludge (C_{sludge} in Table 8) cannot be entered in the model calculations with EUSES. Therefore, the emission to agricultural soil is lowered with the ratio of the calculated C_{sludge} to the measured C_{sludge}, being 15 and 8.3 for HHCB and AHTN, respectively. This leads to a lowering of the emission to agricultural soil for the regional scale for AHTN from 36.6 to 4.4 kg/day and for HHCB from 93.1 to 6.2 kg/day. For the continental scale these figures are for AHTN from 879 to 106 kg/day and for HHCB from 2260 to 151 kg/day.

3.6 Monitoring data on AHTN and HHCB

Recently the presence of polycyclic musks in the environment has been investigated in several countries. The extraction method of polycyclic musks from environmental samples consists of several steps. Detailed information on analytical methods and detection limits is presented in Appendix 3. Polycyclic musks in water are concentrated with C_{18}-solid phase and/or extracted with organic solvents. Water containing suspended material (sewage, waste water) is directly extracted with n-hexane or other organic solvents. Fish samples are prepared by soxhlet extraction with n-hexane, elution in multiple organic solvents and clean-up is carried out by gel permeation chromatography (GPC) and adsorption chromatography on silicagel. Separation and detection is carried out with gas chromatography connected to a mass spectrometer (GC/MS). The reported detection limits are 0.03 µg/l and 10 µg/kg fresh weight for both substances (Eschke et al., 1994, 1995a).

For the bioaccumulation studies, separation and detection have been carried out by thin layer silicagel chromatography (TLC) with spot visualisation in UV (254 nm) and by high pressure liquid chromatography (HPLC) with UV (254 nm) detection. In studies with radioactive material, the reported detection limits with LSC are 1.2 - 1.7 ppb for water samples and 6.8 ppb for fish tissue (Van Dijk, 1996 a,b).

Samples of suspended solids were extracted by soxtec extraction with hexane/acetone, whereas sludge samples were extracted with dichloromethane. Analysis was by GC/MS in SIM mode. Reported detection limits for suspended solids were 0.05 mg/kg whereas the lower limit for reporting in sludge was 1 mg/kg (Breukel and Balk, 1996, Omegam, 1997).

Effluent concentrations were calculated from biomimetric extractions on an Empore disk formore than a week. The detection was by GC/MS. The detection limit was not reported but the lowest reported value is 0.0005 µg/l (Verbruggen, 1997).

Tables 12, 14 and 15 present concentrations of AHTN and HHCB measured in waste water, surface water, sludge, sediment and aquatic organisms. The tables include median or mean values and ranges, as well as the 90th percentile of the data, wherever possible. The median and the 90th percentile include the samples with concentrations below the detection limit. The data are presented graphically in figures 3 to 6 in § 3.7.

Influent and effluent concentrations were determined in three STPs of the German Ruhrverband during one week. According to the author (pers. comm., 1996) figures on the influent in Eschke et al.(1994) are indicative only and not representative[3]. Effluent samples were 24-h time-proportional samples. The median concentration in the effluent was 1.6 µg/l

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[3] Sampling of influent streams is complicated: to be representative sampling should be both time- and volume-proportional, it should cover both dry weather and rainy periods and the volume needs calibration for the number of inhabitants.

for AHTN and 1.2 µg/l for HHCB, with higher levels up to 3.1 and 2.5 µg/l, respectively (Eschke et al., 1995a). More recent preliminary investigations indicate higher influent levels for HHCB between 10 and 30 µg/l and effluent levels between 1 and 3 µg/l (Eschke, pers. comm. 1996). The removal percentage of around 90% for HHCB seems to be in line with the predicted removal percentage (due to adsorption, see § 3.2, point 5). No definitive studies on the levels of AHTN and HHCB in STPs on the Ruhr are available yet.

Effluents from the three largest STPs in Sweden were analysed for the presence of a large number of organic pollutants (December 1993 and January 1994). HHCB levels in the flow-proportional daily composite samples ranged between 1 and 6 µg/l (Paxéus, 1996).

During the RIZA project on 'Whole Effluent Environmental Risk' in The Netherlands, RITOX determined the bioaccumulation of a number of substances from effluents, including AHTN and HHCB. “Free dissolved concentrations” in effluents were estimated from amounts accumulated on Empore disks and are considered by the author to be accurate within a factor of 2. These values are lower than the data from Germany by an order of magnitude. After 28 days incubation with an inoculum from Lake Markermeer (no further specification), concentrations of HHCB were reduced by 98% or more, whereas concentrations of AHTN were reduced by 80 to 96% (Verbruggen, 1997). It should be remarked that adding suspended matter through the inoculum can influence the estimated concentrations (pers. com. Verbruggen, 1997).

Van Loon et al. (1997) reported on results of the application of the ‘TBR-procedure’ to environmental samples in the Netherlands. In this procedure Total Body Residues are estimated after exposure to complex mixtures of organic chemicals using a biomimetic extraction procedure. In these biomemetic extracts, the concentration of major chemicals were identified. In the 3 effluent samples from STPs AHTN and HHCB contributed 19 and 46% of the total amount of major components. The contribution to the TBR is probably lower because not all components could be identified. No results were presented in which TBRs were compared with No-Effect Body Residues. Therefore, these results cannot be interpreted in the framework of the present environmental risk assessment.

Sludge was sampled in 6 STPs in The Netherlands (Blok, 1997). One of the STPs had no combined thickener or anareobic digester. Another one had no anareobic digester but a thickener with a retention time of several days. These STPs were also involved in an earlier monitoring study in the Netherlands for four surfactants (Feijtel and Van de Plassche, 1995) and can be considered as representative for the Dutch situation. In addition samples were taken from a compost facility treating digested activated sludge from several STPs. Two grab samples were taken with an interval of one week. Concentrations of AHTN and HHCB varied in time as well as per location. Concentrations in primary, activated and digested sludge did not seem to be different (see figures 4 and 5). Taking into account that the amount of organic matter decreases during the anaerobic digestion by 36%, it is estimated that approximately 40% of AHTN and HHCB is eliminated (see Appendix V).

Surface water samples were taken along a stretch of 160 km in the Ruhr. The concentrations were generally at a level of 0.2 µg/l for AHTN and 0.5 µg/l for HHCB. Higher levels were found where tributaries enter the main stream, up to 1.2 µg/l for both AHTN and HHCB. Under dry weather conditions these tributaries are fed between 50 to 90% from effluents from STPs (Eschke et al., 1995a). Based on these figures, the mean dilution factor for effluents in the Ruhr seems to be between 2 and 8. It was confirmed by Eschke (pers. comm. 1996) that in dry periods as much as 25% of the water in the River Ruhr may be effluent water, implying a dilution factor of 4, whereas the mean dilution factor is approximately 10.

In the Netherlands surface water concentrations in the main rivers have been determined routinely by the Netherlands Institute for Inland Water Management (RIZA) from 1994 to 1996. Sampling points were at Lobith and Eysden where the rivers enter the country. Median concentrations for AHTN were 0.05 and 0.07 µg/l in the rivers Rhine and Meuse, respectively, with a maximum of 0.40 µg/l in the Meuse in 1995. Median concentrations for HHCB were 0.06 and 0.08 µg/l in the rivers Rhine and Meuse, respectively with a maximum of 0.26 µg/l in the Meuse in 1996. 90th Percentile concentrations for both rivers are 0.11 and 0.18 µg/l for AHTN and HHCB, respectively. The authors conclude that there seems to be an increasing trend, especially for the river Meuse. Considering the peaks measured earlier in time, this can only be substantiated by further measurements.

Suspended matter was analysed in the same programme. Median concentrations for AHTN were 0.24 and 0.84 mg/kg in the Rivers Rhine and Meuse, with a maximum of 1.2 mg/kg in the Meuse in 1994 and 1995. Median concentrations for HHCB were 0.06 and 0.20 mg/kg in both rivers with a maximum of 0.58 mg/kg in the Meuse in 1995 (Breukel and Balk, 1996).

Based on these results there seems to be a discrepancy in the sorptive behaviour measured in laboratory tests compared to the field. Based on batch experiments with activated sludge there is almost no difference between both substances (see § 2.2). Using the 90th percentiles for surface water and suspended solids for the Rhine and Meuse as presented in Tables 10 and 11 the sorption coefficient of AHTN is a factor 5 higher, being 8700 and 1700 l/kg for AHTN and HHCB, respectively. Calculated Kp_{susp} values for suspended matter are 6310 and 7240 l/kg for AHTN and HHCB, respectively (see § 3.2).

Concentrations in surface water in The Netherlands and Belgium were estimated from biomimetric extractions on Empore disks as described for effluents. Median concentrations were 0.028 and 0.051 µg/l for AHTN and HHCB, respectively, but concentrations were below 1 ng/l for AHTN and up to 2.7 ng/l for HHCB in four relatively unpolluted areas. In the Scheldt (Antwerp) and the Eem (Baarn), surface water concentrations were at the level observed for STP effluents (from Verbruggen, 1997).

In Switzerland, concentrations were measured in the river Glatt in Dübendorf which is 3 km downstream of the outlet of an STP. The levels were 0.075 µg/l for AHTN and 0.136 µg/l for HHCB (Müller et al., 1996).

In Japan, a stretch of the Tama River was monitored. Upstream concentrations of HHCB were 0.0007 and 0.0025 µg/l, whereas further downstream concentrations ranged between 0.08 and 0.1 µg/l. It was suggested that HHCB could be used as an indicator of domestic waste water (Yun et al., 1994).

Table 13. Concentrations in influent, effluent and surface water. Median and 90th percentile values calculated from data presented by the different auhors.

Sample	n	AHTN [µg/l]	HHCB [µg/l]	Reference
Influent[4] STPs Ruhr	7	mean 2.24 0.8-4.4	mean 1.46 0.5-2.9 10 - 30	Eschke et al., 1994 pers.com. 1996
Effluent STPs Ruhr	7	mean 1.4 0.8-2.4	mean 1.09 0.6-2.0 1 - 3	Eschke et al., 1994 pers.com. 1996
Effluent STPs Ruhr	21[1]	median 1.6[1] 0.8-3.1 90th percentile 3.0	median 1.2[1] 0.6-2.5 90th percentile 2.4	from Eschke et al., 1995a
River Ruhr	23[2]	mean 0.2 <0.03-0.3	mean 0.37 <0.03-0.5	Eschke et al., 1994
Stretch along River Ruhr, February 1994	30	median 0.2 0.1-0.3 90% 0.3	median 0.5 0.1-0.5 90% 0.5	Eschke et al., 1995a
Ruhr, entry tributaries, Feb. 94[3]		max. 1.2	max. 1.2	Eschke et al., 1995a
River Rhine 1994-96	32	median 0.05[5] 0.01-0.13 90th percentile 0.10	median 0.06[5] 0.01-0.22 90th percentile 0.16	Breukel and Balk, 1996
River Meuse 1994-96	35	median 0.07[5] 0.01-0.4 90th percentile 0.11	median 0.08[5] 0.01-0.26 90th percentile 0.19	
90th perc. Rhine and Meuse 1994-1996	67	0.11	0.18	
Effluent STPs The Netherlands	3	mean 0.23 0.11-0.42	0.23 0.17-0.29	Verbruggen, 1997
NL surface water	14	median 0.028 0.0005-0.187	median 0.051 0.001-0.174	
Effluent STPs Sweden	3	no data	1-6	Paxéus, 1996
River Glatt, Switzerland	1	0.075	0.136	Müller et al., 1996
Tama River, Japan	5	no data	geometric mean 0.017 0.0007-0.1	Yun et al., 1994

[1] Includes data from previous line (n=7)

[2] Data included in next line (n=30)

[3] Data included in previous line (n=30)

[4] Data are not representative, see text

[5] Filtered water samples. The authors present mean values for AHTN of 0.08 and 0.06 µg/l in the river Meuse and Rhine, respectively and for HHCB of 0.10 and 0.07 µg/l in the river Meuse and Rhine, respectively.

Table 14. Concentrations in sewage sludge, suspended matter and sediment

Sample	n	AHTN [mg/kg dw]	HHCB [mg/kg dw]	Reference
Sludge STP Ruhr	1	42	45	Eschke, pers. comm.
Sludge STPs NL				Omegam, 1997
primary	11	mean 8.3, 3.3-14	mean 13.9, 5.4-27	
activated	12	mean 16.0, 2.3-34	mean 27.9, 4.4-63	
digested[1]	8	mean 14.8, 6.2-21	mean 23.0, 11-31	
digested[2]	10	mean 12.8, 4.9-21	mean 20.3, 9.0-31	
digested[3]	13	mean 13.5, 4.9-21	mean 19.9, 9.0-31	
digested[3]	13	median 16[6], 4.9-22	median 23[6], 9.0-31	
River sediment[4] Ruhr	1	indicative 0.15 - 0.3	indicative 0.15 - 0.3	Eschke, pers. comm.
Suspended matter Rhine 1994-1996	14	median 0.24[5] 0.10-0.54	median 0.06[5] 0.05(d.l.)-0.16	Breukel and Balk, 1996
Suspended matter Meuse 1994-1996	14	median 0.84[5] 0.06-1.2	median 0.20[5] 0.05-0.58	
90th percentile Rhine and Meuse 1994-1996	28	0.96	0.31	

[1] Concentrations in digested sewage sludge except the compost facility and thickener.

[2] Concentrations in digested sewage sludge except the compost facility.

[3] Concentrations in digested, thickened and composted sludge.

[4] From settling area in river.

[5] Median recalculated from data given by the authors who present mean values for AHTN of 0.71 and 0.27 mg/kg in the river Meuse and Rhine, respectively and for HHCB of 0.21 and 0.08 mg/kg in the river Meuse and Rhine, respectively.

[6] Used in the calculations with EUSES (see Table 8).

Table 15 summarizes the concentrations found in fish in the Ruhr by Eschke et al. (1995a). Concentrations were determined in edible parts (muscle), in adipose tissue and in the liver. The results were expressed as the concentration in fat. As the fat content for each fish was included in the publication, it was possible to recalculate the concentrations to fresh weight.

A distinction is made between eel and other fish species because the fat content of eel is considerably higher than for the other species. Therefore, even though the concentrations of AHTN and HHCB in fat sometimes seems to be lower for the eel than for the other species, the total body burden of the eel (fresh weight) is always higher.

Median concentrations in species other than eel from natural waters in Germany were 0.029 and 0.018 mg/kg fw for AHTN and HHCB, respectively. Mean concentrations in eel were approximately 5 times higher: 0.13 and 0.11 mg/kg fw for AHTN and HHCB, respectively. Concentrations in adipose tissue were comparable to the concentrations in the edible parts expressed as mg/kg fat. Concentrations in the liver fat seemed to be lower than in the edible parts for HHCB but not for AHTN (Eschke et al., 1995a).

As an indication of the bioconcentration under natural conditions, bioconcentration was estimated for eel and non-eel in the River Ruhr (see Table 16). Ratios were calculated for both median and maximum concentrations in fish muscle and in water (median total concentrations). The results are a rough indication only, since it is not known whether the fish were caught in the same area where surface water samples were taken, the amount of suspended solids in the water is unknown (relates to the bioavailability of the substances; water samples including suspended matter were directly extracted) and whether a steady state was reached in the fish. The ratio is slightly underestimated by using the total concentration in water instead of the dissolved concentration. The resulting ratios for non-eel fish are a factor of 5 below the experimentally determined BCF for AHTN and at least a factor of 18 below the value for HHCB. For eel, the ratios for HHCB are at least a factor 5 below the experimentally determined BCF. For AHTN and eel, the ratios correspond very well to the BCF.

Table 15. Concentrations in fish

Sample	n	AHTN	HHCB	Reference
Fish River Ruhr, non-eel	7	edible (muscle) med. 3.5 mg/kg fat 2.2 - 7.1, 0.36-1.56% fat --> med. 0.029 mg/kg fw 0.018-0.034	edible (muscle) med. 2.8 mg/kg fat 1.4 - 3.8, 0.36-1.56% fat --> med. 0.018 mg/kg fw 0.010-0.045	Eschke et al., 1995a
eel	2	edible (muscle) mean 0.6 mg/kg fat 0.5 - 0.7, 20.9-23.7% fat --> mean 0.13 mg/kg fw 0.119-0.146	edible (muscle) mean 0.5 mg/kg fat 0.4 - 0.6, 20.9-23.7% fat --> mean 0.11 mg/kg fw 0.095-0.125	
Fish from effluent pond, non-eel	8	edible (muscle) med. 15.3 mg/kg fat 3.0 - 37.2, 0.87-2.8% fat --> med. 0.29 mg/kg fw 0.07 - 0.647	edible (muscle) med. 8 mg/kg fat 1.0 - 19.8, 0.87-2.8% fat --> med. 0.15 mg/kg fw 0.023 - 0.344	Eschke et al., 1995a
eel	5	edible (muscle) mean 36 mg/kg fat 10.1 - 57.9, 16.5-30.2% fat --> mean 10 mg/kg fw 2.39 - 17.49	edible (muscle) mean 35 mg/kg fat 6.1 - 63.6, 16.5-30.2% fat --> mean 10 mg/kg fw 1.26 - 19.20	

Table 16. Comparison of experimentally determined bioconcentration factors to ratios of C_{fish} and C_{water} for fish caught in the River Ruhr (based on data in Eschke et al., 1995a)

Ratio based on measured data in Ruhr		AHTN C_{fish}, [mg/kg]	AHTN C_{water} [µg/l]	AHTN ratio	HHCB C_{fish} [mg/kg]	HHCB C_{water} [µg/l]	HHCB ratio
non-eel	med.	0.029	0.2	145	0.018	0.37	48.6
	max.	0.034	0.3	113	0.045	0.50	90
eel	med.	0.130	0.2	650	0.110	0.37	297
	max.	0.146	0.3	487	0.125	0.50	250
Experimental BCF				597			1584

3.7 Selection of exposure concentrations to be used for the risk characterization

3.7.1 Comparison of the PECs with concentrations measured in the environment

The predicted environmental concentrations were compared to concentrations actually measured in the environment (influent, effluent, sewage sludge, surface water, suspended matter and aquatic organisms). Figures 3 to 8 (effluents; primary, activated and digested sludge; surface water; suspended matter and fish) present the distribution frequencies and/or median (mean) and 90th percentiles or maximum measured values.

Predicted concentrations in the influent are much higher than the indicative influent concentrations in the STP in Germany cited in Eschke et al. (1994): predicted concentrations are 66 for AHTN and 160 µg/l for HHCB while the mean measured concentrations are 2.24 for AHTN and 1.46 µ/l. Maximum measured concentrations are 4.4 and 2.9 µg/l. More recently measured influent levels for HHCB of 10-30 µg/l are however only a factor of 5 below the predicted influent concentrations (Eschke, pers. com., 1996).

A frequency distribution of measured effluent levels is given in figure 3. Comparison with $C_{effluent}$ indicates that the prediction is a factor of 3.7 above the 90th percentile for AHTN and a factor of 11 for HHCB. It should be remarked that the 90th percentile is slightly underestimated as the data by Verbruggen (1997), which are included, represent dissolved concentrations.

The frequency distribution of concentrations measured in sewage sludge (figures 4 and 5) shows that the mean measured concentrations in digested sludge are lower than C_{sludge} by a factor of 11 for AHTN and a factor of 19 for HHCB. C_{sludge} is a factor of 6.3 higher than the highest concentration of AHTN in digested sludge and a factor of 11 higher for HHCB.

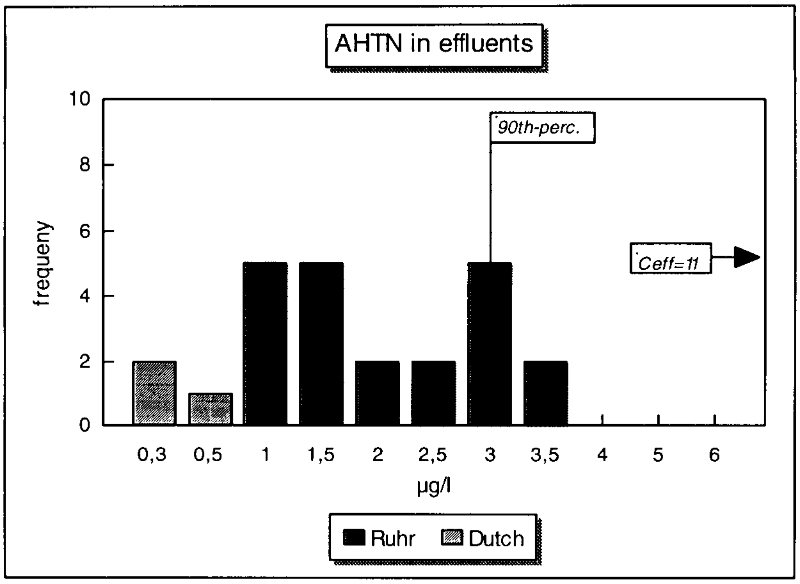
The concentrations in surface water are presented in figure 6. For AHTN $PEClocal_{water}$ is a factor of 5.0 above the 90th percentile of all samples. The maximum concentrations measured in three tributaries of the river Ruhr are close to the $PEClocal_{water}$ of 1.0 μg/l, being 0.3-1.2 μg/l. Probably these tributaries have low dilution factors. For HHCB $PEClocal_{water}$ is more than a factor of 4.8 above the 90th percentile. All other surface water samples for both substances (see also Table 13) are lower than $PEClocal_{water}$, sometimes by more than a factor of 100. These surface waters, however, where known, have a dilution factor higher than 10.

The concentrations in suspended matter in the Rhine and Meuse rivers are presented in figure 7. These concentrations are converted to concentrations in sediment by dividing the concentration in suspended matter by 2, which is a standard procedure according to RIZA based on empiricism. $PEClocal_{sed}$s for AHTN and HHCB are much higher than the 90th percentiles, while the latter concentrations are in the same range as the $PECregional_{sed}$s for both substances. It should be remarked that the river Meuse is probably more comparable to a local than a regional siuation due to discharges from the city Luik in Belgium.

The concentrations measured in fish in the River Ruhr are presented in figure 8. These concentrations should be compared to predicted concentrations for the local environment, because the Ruhr has a relatively low dilution factor. Maximum measured recalculated fresh weight concentrations in species other than eel are a factor of 9.4 lower for AHTN than the predicted concentrations and for HHCB a factor of 44 lower. Maximum measured recalculated fresh weight concentrations in eel are a factor of 2.2 lower than predicted for AHTN and a factor of 11 lower than predicted for HHCB.

It can be concluded that in general the model overestimates the actual levels of AHTN and HHCB in the environment. This is to be expected since the model in the TGD attempts to describe a 'realistic worst case'. Several aspects in the calculations according to the TGD lead probably to an overestimation of the actual concentrations:

- multiplication of the influent concentrations based on consumption per capita by a factor of 3;
- overestimation of the use volume because the use volume is not corrected for export from the EU for both substances. Also, not all consumer products in which either AHTN or HHCB are used are ‘down the drain products’;
- in the predictions no biodegradation of AHTN and HHCB is assumed, while there are indications that both substances may be biodegraded either aerobically or anaerobically. Actual degradation rates are not available, however;
- several defaults are assumed in the TGD and EUSES, e.g. for sewage flow, surplus sludge production, sorption to sludge and the dilution factor in surface water. In reality these figures vary.



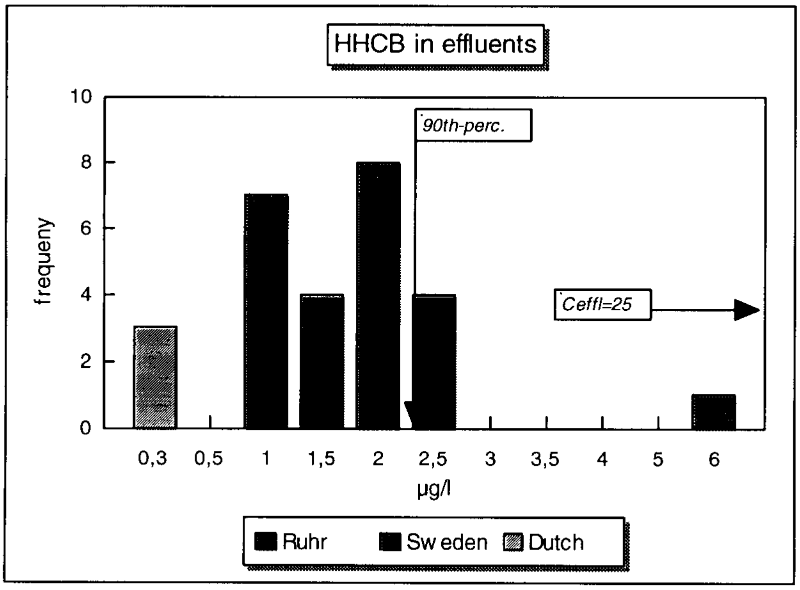


Figure 3. Concentrations in effluents (Eschke, 1995a; Paxéus, 1996; Verbruggen, 1997). The arrows indicate the 90th percentile.

AHTN: $C_{effluent}$: 11 µg/l; 90th percentile: 3.0 µg/l; n = 24;

HHCB: $C_{effluent}$: 25 µg/l; 90th percentile: 2.3 µg/l; n = 27.

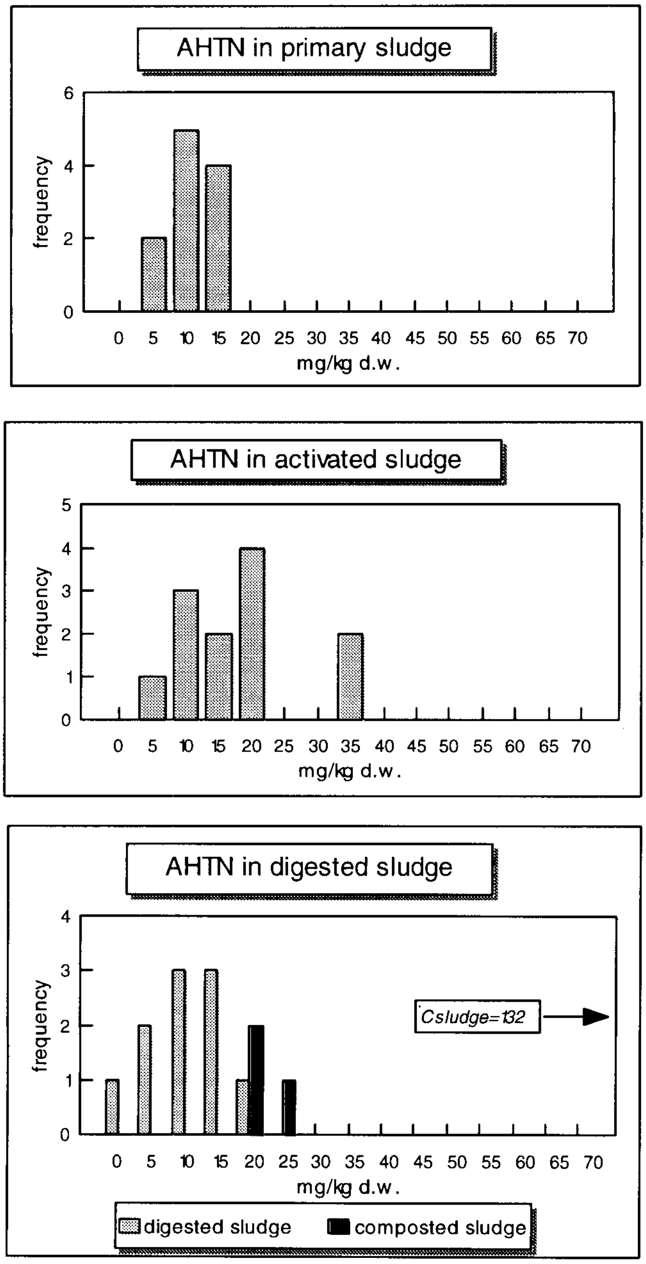


Figure 4. Concentrations in sewage sludge for AHTN (Blok, 1997).
C_{sludge} = 132 mg/kg dw;
mean measured concentration in:
- primary sludge: 8.3 mg/kg dw; n = 11;
- activated sludge: 16 mg/kg dw; n = 12;
- digested sludge is 13.5 mg/kg dw (median 16 mg/kg dw); n = 13.

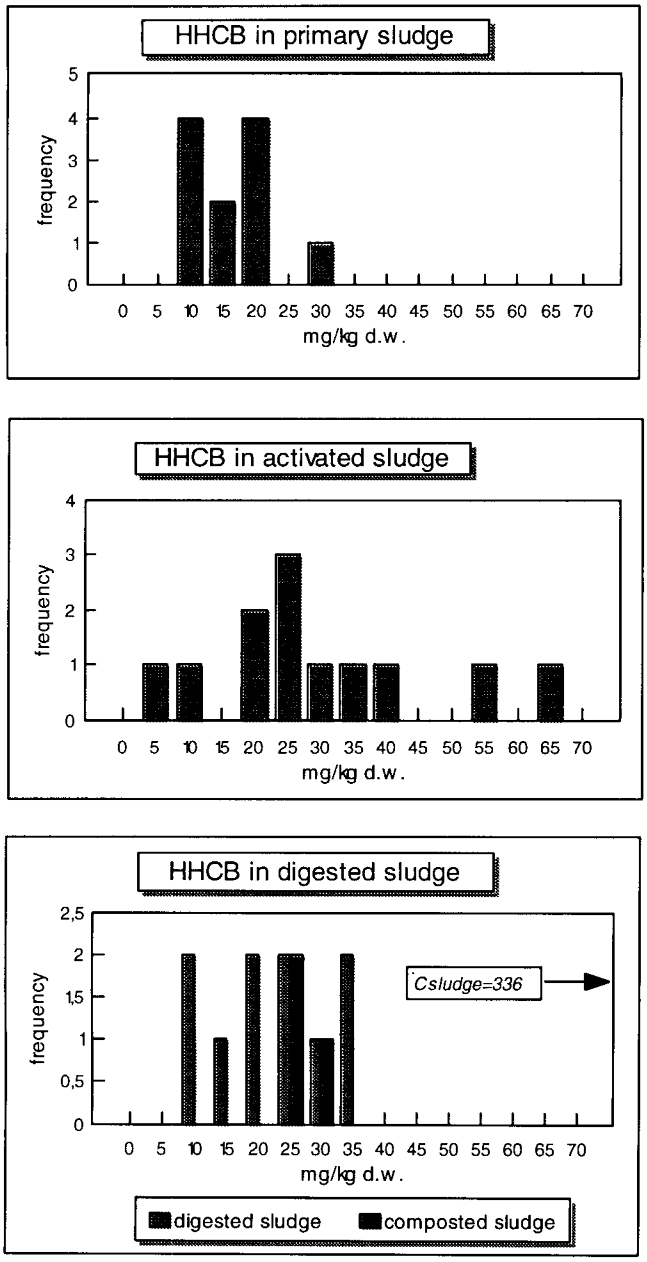
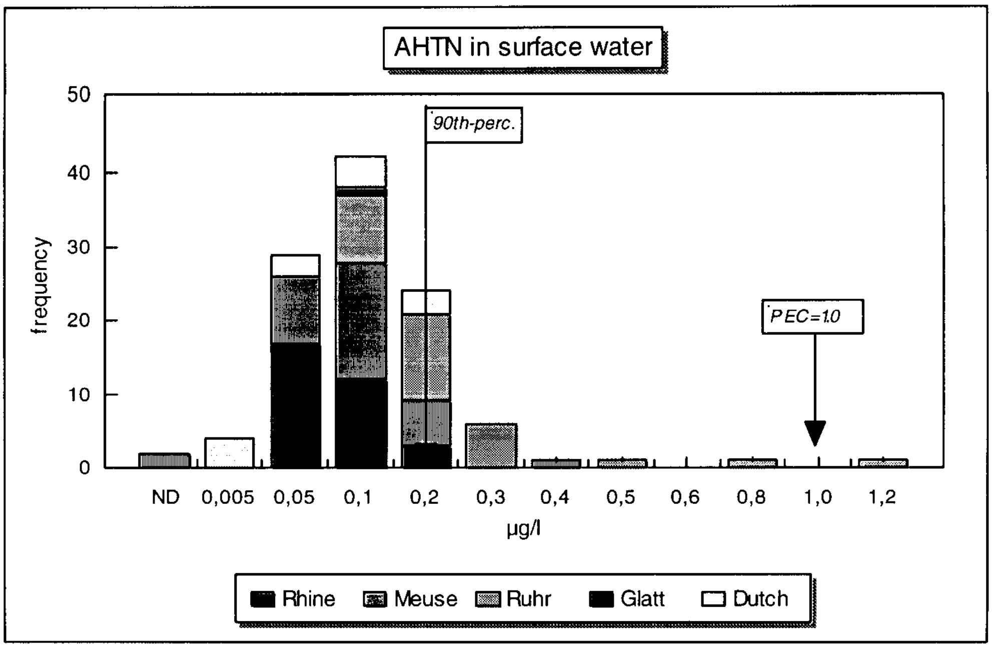


Figure 5. Concentrations in sewage sludge for HHCB (Blok, 1997).
C_{sludge} = 336 mg/kg dw;
mean measured concentration in:
- primary sludge: 13.9 mg/kg dw; n = 11;
- activated sludge: 27.9 mg/kg dw; n = 12
- digested sludge is 19.9 mg/kg dw (median 23 mg/kg dw); n = 13.



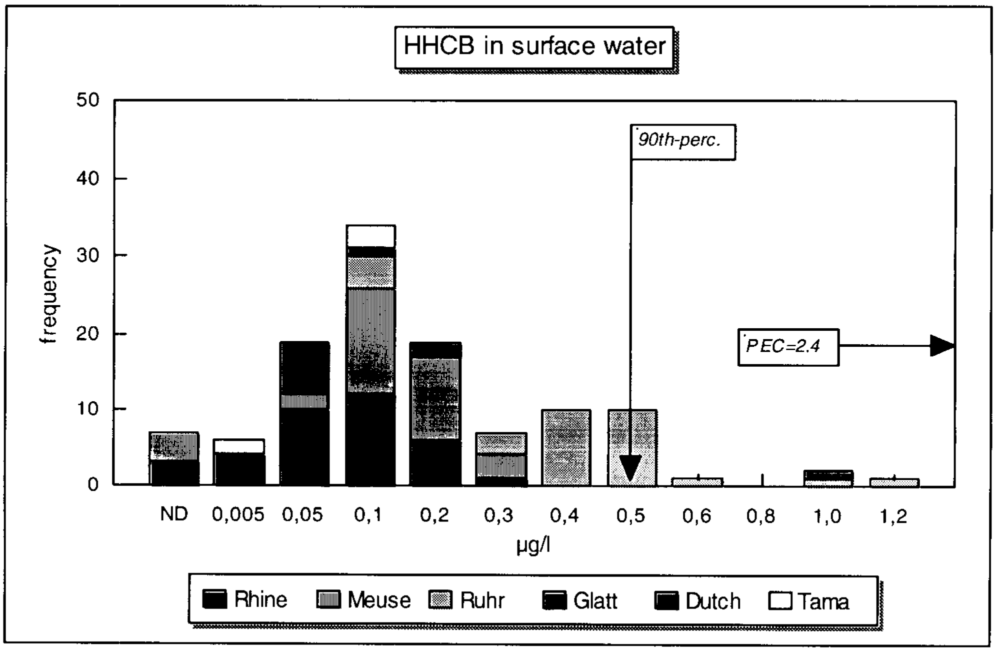
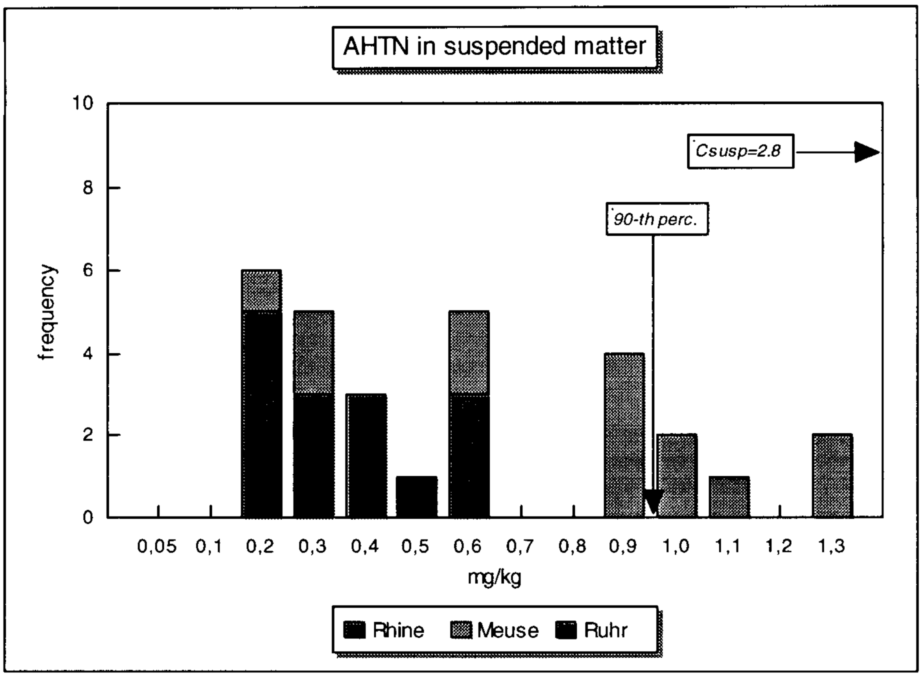


Figure 6. Concentrations in surface water (Eschke, 1995a; Breukel and Balk, 1996; Verbruggen, 1997; Müller et al., 1996; Yun et al., 1994). The arrow indicates the 90th percentile.

AHTN: $PEClocal_{water}$: 1.0 µg/l; 90th percentile: 0.2 µg/l; n = 111;

HHCB: $PEClocal_{water}$: 2.4 µg/l; 90th percentile: 0.5 µg/l; n = 116.



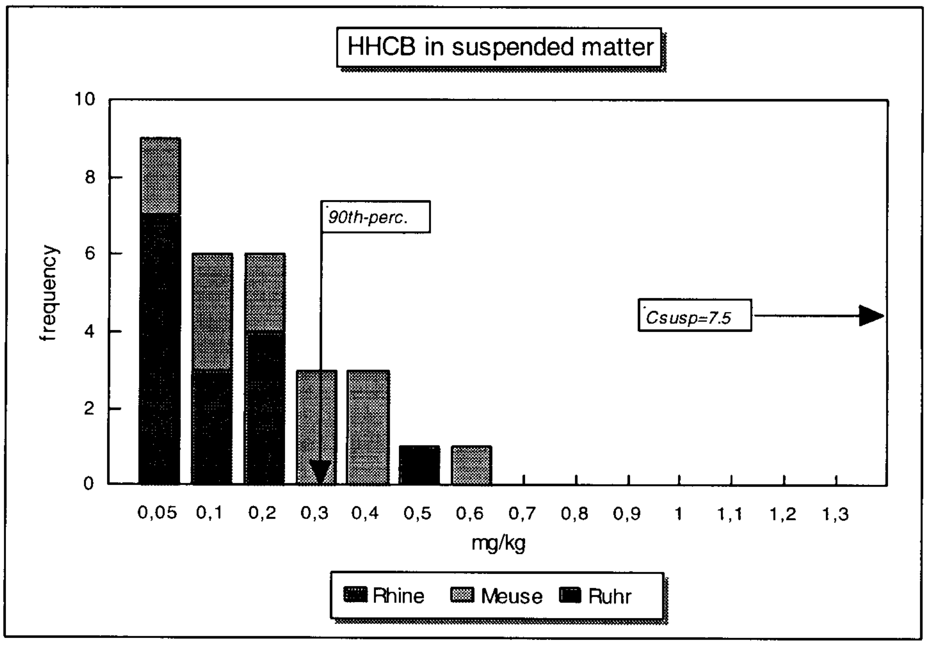
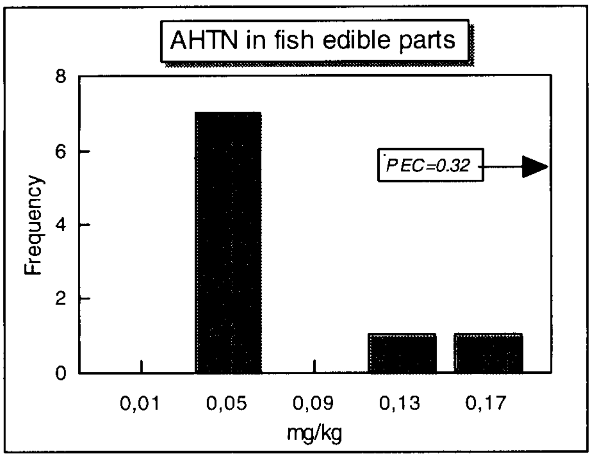


Figure 7. Concentrations in suspended matter (Eschke, pers. com.; Breukel and Balk, 1996). AHTN: C_{susp}: 2.8 mg/kg dw (PEClocal$_{sed}$ * 2); 90th precentile Rhine and Meuse: 0.96 mg/kg dw; n = 28;

HHCB: C_{susp}: 7.5 mg/kg dw (PEClocal$_{sed}$ * 2); 90th precentile Rhine and Meuse: 0.31 mg/kg dw; n = 28.



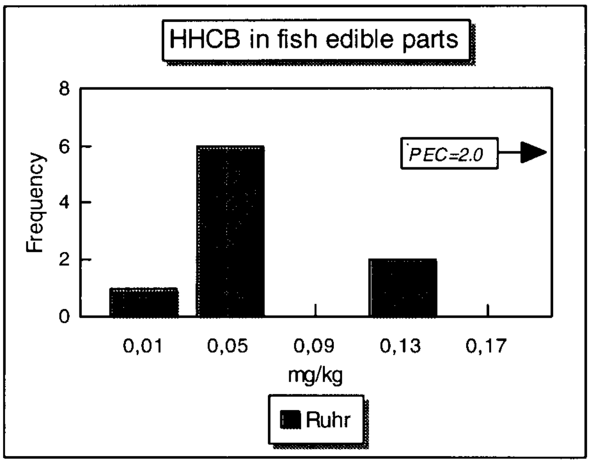


Figure 8. Concentrations in fish in mg/kg fw (Eschke et al., 1995a).

AHTN: $PEC_{oral,\ fish}$: 0.32 mg/kg fw; maximum concentration: 0.146 mg/kg fw (non-eel: 0.029; eel: 0.146 mg/kg fw); n = 9.

HHCB: $PEC_{oral,\ fish}$: 2.0 mg/kg fw; maximum concentration: 0.125 mg/kg fw (non-eel: 0.045; eel: 0.125 mg/kg fw); n = 9.

Measured concentrations expressed on fw basis were recalculated from data expressed on muscle fat basis by Eschke et al., 1995a.

The use volume of HHCB is 2.5 times higher than for AHTN. The higher use volume of HHCB is reflected in higher levels in sludge for HHCB than for AHTN, although not proportional to the use volume. Cconcentrations in primary sludge should especially reflect the difference in use volumes. The mean concentration of HHCB is a factor 1.7 higher than the concentration of AHTN: 8.3 and 13.9 mg/kg, respectively. The levels actually found in influent, effluent, surface water are in the same range for both substances. The concentrations in suspended matter of AHTN are considerably higher than HHCB, however (90th percentiles differ by a factor of 3).

The slight discrepancy between measured concentrations for AHTN and HHCB and their use volumes may be explained by differences in environmental behaviour e.g. in-sewer removal, biodegradation in sewage sludge and metabolism in fish. For surfactants it has been shown that in-sewer removal occurs (Feijtel and Van de Plassche, 1995). The reverse relation found in suspended matter is hard to explain.

3.7.2 Selection of exposure concentrations

For the risk characterization the concentration in the environment is compared with a PNEC for several selected endpoints (water organisms, sediment dwelling organisms etc). As measured as well as calculated concentrations are present or have been derived a choice between both has to be made. It should be stated that measured as well as predicted concentrations can have a considerable uncertainty associated with them. Measured concentrations should include both temporal and spatial variations, whereas predicted concentrations include uncertainties connected to assumptions in the models applied.

For surface water a large number of measured data are available. Most data come from Germany and the Netherlands, countries with an average use in detegents and cosmetics (see § 3.1), and from high as well as low dilution systems. Therefore, the 90th percentile concentrations based on over 100 measured samples, are preferred over the calculated PEC_{water} values for AHTN and HHCB.

It must be considered whether in the monitoring data presented in Table 13 local and regional situations are included. Data from Breukel and Balk (1996) for the river Rhine and maybe for the river Meuse should be regarded as regional situations. However, the data from Eschke (1994; 1995a) should be regarded as local situations as the river Ruhr and its tributaries are low dilution situations. It must be stated that the assignment of measured concentrations to a local or regional scale for substances with a wide dispersive use like AHTN and HHCB can probably not be done unequivocally. Low dilution systems are often not affected by background concentrations, while the opposite is true for high dilution systems. Also, background concentrations are, for the most part, caused by direct discharge without treatment. Based on these considerations the 90th percentile of all measurements is used without distinguishing between the local and regional scale. The 90th percentiles coincide with the Ruhr data, which are of a local character.

A risk characterization for the sediment compartment can only be carried out if measured concentrations in sediment or if toxiciy data for sediment dwelling organisms are available. For example, if both the PEC_{sed} as well as the $PNEC_{sed}$ are derived from the related values for the water compartment (deriving the PEC_{sed} from the PEC_{water} using the $K_{susp\text{-}water}$ and the $PNEC_{sed}$ from the $PNEC_{water}$ using equilibrium partitioning), calculating a PEC/PNEC ratio is of no relevance as this would lead to the same results as for aquatic organisms (TGD). Therefore, the measured concentrations for suspended matter are used, which are converted to concentrations in the sediment. As the equilibrium partitioning method is used to derive the $PNEC_{sed}$ and the log Kow value for both substances is higher than 5, the measured concentrations are multiplied by a factor of 10 (TGD).

For the soil compartment no measured concentrations are available in the soil itself. The starting point for the calculation is the concentration in digested sludge, which is applied to agricultural land. Measured concentrations in digested sludge are available and are preferred over calculated concentrations. These measured concentrations are median values in sludge from 6 representative STPs and a compost treating facility in the Netherlands.

For fish some measured data are available from Germany. Fish were sampled in the river Ruhr, which is a low dilution system. Measured concentrations are preferred over predicted ones even though not that many data are available. To compensate for the small amount of data, maximum concentrations are used rather than the 90th percentiles.

For worms no measured concentrations are available so the predicted concentrations have to be used. The predicted concentrations are based on the local and regional concentrations in agricultural soil, for which the measured concentrations in digested sludge are used as starting-point, and on the calculated BCFs for earthworms.

In Table 17 the exposure concentrations are presented which are used for the risk characterization in chapter 5.

Table 17. Exposure concentrations used for the risk characterization.

	AHTN	HHCB
surface water [µg/l]	0.2 (m)[1]	0.5 (m)
sediment [mg/kg dw]	0.48 (m) * 10^1	0.16 (m) * 10^1
soil [mg/kg dw]	0.26 (p)	0.38 (p)
fish-eating predators [mg/kg fw]	0.146 (m)	0.125 (m)
worm-eating predators [mg/kg fw]	0.78 (p)	1.7 (p)

(p) predicted concentration

(m) measured concentration

[1] As the equilibrium partitioning method is applied to derive the $PNEC_{sed}$ (see § 4.3) and the log Kow of AHTN is above 5 the PEC_{sed} is multiplied with a factor 10 according to the TGD. The value presented is derived from measured concentrations in suspended matter by dividing the concentration in suspended matter by 2.

4 EFFECT ASSESSMENT

4.1 Aquatic organisms

AHTN

For AHTN toxicity tests were carried out with algae, *Daphnia magna* and fish (Table 18). In these tests stock solutions wereprepared using either DMF as a solvent and Tween 80 as a dispersant or using triethylene glycol as a solvent. Final concentrations in water were analyzed by HPLC and the test concentrations are expressed as measured concentrations. Except for the highest concentration in the fish growth test, the tested concentrations did not exceed the water solubility limit.

The toxicity to algae was studied according to OECD Test Guideline 201 with *Pseudokirchneriella subcapitata*. Two tests were carried out and both produced valid results. Nominal concentrations both for test A and B ranged from 0.0625 to 1.0 mg/l, mean measured concentrations were 0.035, 0.088, 0.204, 0.438 and 0.797 mg/l for test A and 0.0679, 0.140, 0.170, 0.374 and 0.835 mg/l for test B[4]. The NOEC is based on growth rate and biomass production after 72 hours. For both parameters an EC50 was determined as well. Growth was not significantly inhibited in concentrations up to (A) 0.438 and (B) 0.374 mg/l. In the next higher concentration, the LOEC, (A) 0.797 and (B) 0.835 mg/l, the biomass production was inhibited by (A) 82 % and (B) 54%, measured as Area Under the Curve, whereas growth rate (μ) was inhibited by (A) 22 % and (B) 16%. The geometric mean NOEC for both tests was 0.276 mg/l. The EC50 for biomass production was (A) 0.468 and (B) approximately 0.835 μg/l[5], whereas the EC50 for growth rate was (A) >0.797 and (B) >0.835 mg/l.

For *Daphnia magna* a 21-d toxicity test was carried out according to OECD Test Guideline 202, part II, proposed updated version of June 1993. Nominal concentrations ranged between 0.062 and 1.0 mg/l, and mean measured concentrations were 0.054, 0.113, 0.196, 0.401 and 0.804 mg/l. Immobility of the parent generation was 80% at 0.401 mg/l and the 21d-EC50 was 0.341 mg/l. The mean reproduction in test concentrations up to 0.196 mg/l ranged between 80 and 114% as compared to the solvent control. In the next higher test concentration of 0.401 mg/l, reproduction of the surviving adults was inhibited almost completely.

A 21-d prolonged toxicity test was carried out with bluegill sunfish (*Lepomis macrochirus*) according to OECD Test Guideline 204. The mean fish weight at the start of the experiment was 1.6 g, the mean length was 4.9 cm. Nominal concentrations ranged from 0.125 to 2.0 mg/l, mean measured concentrations were 0.089, 0.184, 0.392, 1.00 and 2.22

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[4] Maintenance of test concentrations proved to be difficult. Concentrations not only decreased, but in the lower range of test B, concentrations after 72 h were almost double the initial concentrations. in addition, pH rose to values above 10, indicating an insufficient buffering capacity of the growth medium.

[5] Van Dijk (1997a) reports an E_bC_{50} of 0.801 mg/l (extrapolated between 0.374 and 0.835 mg/l, corresponding to 0 (but actually -12.4%) and 54% inhibition, respectively). As the extrapolation method is not indicated, this value is not included here.

mg/l. Concentrations up to 0.184 mg/l did not significantly affect survival of the fish. Mortality was 70% at the next higher concentration of 0.392 mg/l, and 100% in 1.00 mg/l after 11 days and in 1.94 mg/l after 4 days. The 21-d LC50 was 0.314 mg/l. Clinical signs such as loss of equilibrium, enhanced and/or irregular respiration and cessation of food intake were observed before the onset of death. Fish growth was significantly reduced at 0.184 mg/l (Wüthrich, 1996b).

An early life stage test was carried out with fathead minnow (*Pimephales promelas*) according to OECD Test Guideline 210. Eggs, less than 24 h old were exposed to nominal concentrations ranging from 0.0125 to 0.2 mg/l. Mean measured concentrations were 0.0081, 0.018, 0.035, 0.067 and 0.140 mg/l. Hatchability was not significantly affected in any of the test concentrations. Larval survival after 32 days was not affected in concentrations of 0.067 mg/l and below. In 0.14 mg/l larval survival was 18%. Larval growth was not affected in concentrations of 0.035 mg/l. At 0.067 and 0.14 mg/l, standard lengths were reduced by 7 and 38%, whereas weights were reduced by 7 and 75%, respectively, as compared to the solvent control. In these higher concentrations, physical abnormalities were recorded in the surviving larvae. For the majority (84%) of the larvae surviving in 0.067 mg/l, and in all survivors in 0.14 mg/l, the caudal (tail) fin was absent. The relative tail length of 16% of the larvae in 0.067 mg/l was not affected at all as compared to the control. These effects were completely absent at lower concentrations.

HHCB

For HHCB the same tests were carried out as for AHTN (Table 19). Test solutions were prepared with DMF as a solvent and Tween 80 as a dispersant or with triethylene glycol. Final concentrations in water were analyzed by HPLC and the test concentrations are expressed as measured concentrations. The tested concentrations probably did not exceed the water solubility limit.

The toxicity to algae was studied according to OECD Test Guideline 201 with *Pseudokirchneriella subcapitata*. Nominal concentrations ranged from 0.0625 to 1.0 mg/l and mean measured concentrations were 0.042, 0.084, 0.201, 0.466 and 0.854 mg/l[6]. The NOEC is based on growth rate and biomass. Both biomass production and growth rate were not significantly inhibited up to 0.201 mg/l. The inhibition based on Area Under the Curve was 35% in 0.466 mg/l and 56% in 0.854 mg/l. The NOEC was 0.201 mg/l. Growth rate was inhibited by 9 and 20% in the highest concentrations.

The toxicity to *Daphnia magna* in a 21-d toxicity test was tested according to OECD Test Guideline 202, part II (version June 1993). Nominal concentrations ranged between 0.063 and 1.0 mg/l, and mean measured concentrations were 0.049, 0.111, 0.205, 0.419 and 0.842 mg/l. Mobility of the parent generation was not affected at concentrations up to 0.205 mg/l, whereas 100% was immobile in the next higher concentration 0.419 mg/l. The 21d-EC50 was 0.293 mg/l. From the report 95% confidence limits are derived: 0.205 and 0.419 mg/l. The NOEC for reproduction was 0.111 mg/l. At the level of the NOEC, the mean

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[6] see footnote 4.

Table 18. Toxicity data for AHTN

Species	Test	Results[1] [mg/l]	Remarks[2]	Reference
Alga: *Pseudokirchneriella subcapitata*[3]	72-h static	Test A NOECg = 0.438 NOECb = 0.204, LOECb = 0.438 EgC50 > 0.797 EbC50 = 0.468 <0.434 - 0.508> Test B NOEC = 0.374 LOEC = 0.835 EgC50 > 0.835 EbC50 ≈ 0.835 geom.mean NOEC = 0.276	carrier: 0.005% DMF and 0.005% Tween 80 n=5 Test A HPLC identification start conc. 81-90% of nominal end conc. 31-85% of nominal mean 57-88% Test B start conc. 77-90% of nominal end conc. 53-142% of nominal mean 75-112%	Van Dijk 1997a
Daphnia magna	21-d semi-static	NOEC(rep) = 0.196, LOEC = 0.401 ErC50-21d = 0.244 <0.239 - 0.249> 21d-IC50 = 0.341 (mobility), <0.243 - 0.433>	carrier: 0.008% DMF and 0.002% Tween 80 n=5 HPLC identification conc.fresh 84-103% of nominal conc.used 70-85% of nominal mean 78-90%	Wüthrich, 1996a
Bluegill sunfish *Lepomis macrochirus*	21-d flow-through	NOECgrowth = 0.089, LOEC = 0.184 21d-LC50 = 0.314 <0.226 - 0.448>	carrier: 0.005% DMF and 0.005% Tween 80 n=5 HPLC identification conc. 57-109% of nominal mean 71-100%	Wüthrich, 1996b
Fathead minnow *Pimephales promelas*	32 days post hatch, 36 days overall	LOEChatch > 0.140 NOECsurv. = 0.067, LOECsurv. = 0.140 32d-LC50 = 0.100 <0.097 - 0.100> NOECgrowth = 0.035, LOECgrowth = 0.067 NOECdevelop.= 0.035, LOECdevelop.= 0.067	solvent triethylene glycol GC identification conc. 55-108% of nominal mean 65-73%	Croudace, 1997a

[1] <95% confidence limits>

[2] The number of concentrations tested (n) excludes control and solvent control

[3] Former name *Selenastrum capricornutum*

reproduction was inhibited by 21% as compared to the solvent control. At the next higher concentration, 0.205 mg/l (LOEC) the mean reproduction was inhibited by 26%. In the next higher test concentration of 0.419 mg/l, reproduction of the surviving adults was inhibited almost completely (Wüthrich, 1996c).

The toxicity to fish was studied in a 21-d prolonged test with bluegill sunfish (*Lepomis macrochirus*) according to OECD Test Guideline 204. The mean fish weight at the start of the experiment was 1.4 g, the mean length was 4.9 cm. Nominal concentrations ranged from 0.125 to 2.0 mg/l and mean measured concentrations were 0.093, 0.182, 0.393, 0.830 and 1.566 mg/l. Survival of the fish was not significantly affected up to 0.182 mg/l. Mortality was 10% at the next higher concentration of 0.393 mg/l and coincided with reduced growth. In 0.830 mg/l, mortality reached 100% after 14 days and in 1.566 mg/l at day 2. The 21-d LC50 was 0.452 mg/l with 95% confidence limits of 0.316 and 0.911 mg/l. From the LC50-time relationship, it is not clear whether this value represents the incipient LC50. Clinical signs such as loss of equilibrium, enhanced and/or irregular respiration and cessation of food intake were observed before the onset of death. Fish growth was significantly reduced at 0.393 mg/l. The overall NOEC of the test was 0.093 mg/l as determined by the onset of clinical signs (Wüthrich, 1996d).

For the early life stage test according to OECD Test Guideline 210, fathead minnows (*Pimephales promelas)* were used. Eggs, less than 24 h old were exposed to nominal concentrations ranging from 0.0125 to 0.2 mg/l. Mean measured concentrations were 0.0091, 0.019, 0.037, 0.068 and 0.140 mg/l. Hatchability was not significantly affected in any of the test concentrations. Larval survival after 32 days was not affected in concentrations of 0.068 mg/l and below. In the highest concentration of 0.14 mg/l mean larval survival was 78%. Larval growth was not affected in concentrations of 0.068 mg/l. At 0.140 mg/l, lengths and weight were reduced by 20 and 54%, respectively, as compared to the solvent control. Larvae surviving in the highest concentration (0.140 mg/l) were recorded to be generally smaller, less well developed and appeared less active, exhibiting some erratic swimming behaviour and loss of balance.

General considerations

In all toxicity studies, carrier solvents were used to prepare stock solutions. With the use of solvent aids, the actual bioavailability of the substances to the test organisms is unknown. Since the solvent aids caused no negative effects on the test organisms, and the concentration remained below the levels advised in the test guidelines, the results of the toxicity studies are considered valid. The tests have been carried out and inspected according to the principles of Good Laboratory Practice (OECD, 1981).

In the Chapter 4 of the TGD QSARs are given for base-line or minimum toxicity for chronic endpoints for fish (*Brachydanio rerio/Pimephales promelas*, *Daphnia magna* and *Selenastrum capricornutum*). Applying these QSARs leads to 28-32 d NOECs for fish of 9.6 and 6.3 μg/l, to 16 d NOECs for *D. magna* of 3.8 and 2.3 μg/l and 72-96 h EC50 for *S. capricornutum* of 30 and 19 μg/l for AHTN and HHCB, respectively. The QSAR estimations are lower than the experimental data, probably because of uncertainty in the QSAR estimation itself (especially for hydrophobic substances like AHTN and HHCB) and due to metabolism of AHTN and HHCB (see § 3.5.1).

The tested species represent three trophic levels (primary producer: algae; primary consumer: *D. magna*; secondary consumer: *L. macrochirus* and *Pimephales promelas*), three taxonomic groups (green algae, crustaceans and bone fish) and three feeding strategies (phototrophic, herbivorous filter feeding and carnivorous). Fish seems to be only slightly more sensitive than the other species. Comparison of the results of the 21d-growth test and the 36d-ELS test for fish shows that the development of fish early life stages seem only marginally more sensitive to these substances than growth.

Table 19. Toxicity data for HHCB

Species	Test	Results [1] [mg/l]	Remarks [2]	Reference
Alga: *Pseudokirchneriella subcapitata* [3]	72-h static	NOEC = 0.201 LOEC = 0.466 EgC50 > 0.854 EbC50 = 0.723 <0.678-0.778>	carrier: 0.005% DMF and 0.005% Tween 80 n=6 HPLC identification start conc. 71-102% of nominal end conc. 54-85% of nominal mean 67-93%	Van Dijk 1997b
Daphnia magna	21-d semi-static	NOEC(rep) = 0.111, LOEC = 0.205 ErC50-21d = 0.282 <0.260-0.312> IC50-21d = 0.293 (mobility), <0.204-0.419>[4]	carrier: 0.008% DMF and 0.002% Tween 80 n=5 HPLC identification conc.fresh 82-104% of nominal conc.used 63-91% of nominal mean 79-89%	Wüthrich, 1996c
Bluegill sunfish *Lepomis macrochirus*	21-d flow-through	NOEC = 0.093 (clinical signs), LOEC = 0.182 NOEC(growth) = 0.182 LC50-21d = 0.452 <0.316-0.911>	carrier: 0.005% DMF and 0-.005% Tween 80 n=5 HPLC identification conc. 66-86% of nominal mean 73-83%	Wüthrich, 1996d
Fathead minnow *Pimephales promelas*	32 days post hatch, 36 days overall	LOEChatch > 0.140 NOECsurv. = 0.068, LOECsurv. = 0.140 32d-LC50 > 0.140 NOECgrowth = 0.068, LOECgrowth = 0.140 NOECdevelop.= 0.068, LOECdevelop.= 0.140	solvent triethylene glycol GC identification conc. 50-104% of nominal mean 68-75%	Croudace, 1997b

[1] <95% confidence limits>

[2] The number of concentrations tested (n) excludes control and solvent control

[3] Former name *Selenastrum capricornutum*

[4] estimated 95% confidence limits after data reported by Wüthrich (1996c)

Derivation of the $\text{PNEC}_{\text{water}}$

The values used to determine the $\text{PNEC}_{\text{water}}$ are presented in Table 20. $\text{PNEC}_{\text{water}}$ is obtained using the assessment factors as described in the TGD. If three or more chronic studies are available, an assessment factor of 10 may be applied to the lowest NOEC to derive $\text{PNEC}_{\text{water}}$. For AHTN and HHCB, studies of a chronic nature are available for algae, *Daphnia* and fish. Application of an assessment factor of 10 to the 36d-NOEC of the fish early-life stage tests results in PNECs of 0.0035 mg/l for AHTN and 0.0068 mg/l for HHCB.

Table 20. Derivation of PNECwater

Species	AHTN [mg/l]		HHCB [mg/l]	
Algae	72h-NOEC	0.374	72h-NOEC	0.201
Daphnia	21d-NOEC	0.196	21d-NOEC	0.111
Fish	36d-NOEC	**0.035**	32d-NOEC	**0.068**
assessment factor	10		10	
PNECwater	0.0035		0.0068	

4.2 Soil organisms

AHTN

For AHTN toxicity tests were carried out with earthworms and springtails (Table 21). The earthworm test was carried out according to ISO 11268. Adult earthworms (*Eisenia fetida*) were exposed to nominal concentrations in soil of 8, 19, 45, 105 and 250 mg/kg. The test medium was an artificial soil according to ISO-Standard 11268-1 and OECD Test Guideline 207, containing 10% *Sphagnum* peat, 20% kaolinite clay, aproximately 70% fine quartz-sand (grain size 0.1-0.5 mm) and 0.5% calcium carbonate to adjust to pH 6.0±0.5. After preparation of the test concentrations, and an equilibrium period of one week, the test organisms were added to the soil. Weights of the adult worms ranged between 340 and 540 mg, but did not differ more than 100 mg within this range in each test container. The worms were fed weekly with finely ground cattle manure. Adult worms were removed after 4 weeks of exposure, counted and weighed. The remaining offspring remained in the test containers for another four weeks.

No mortality nor growth inhibition of the adults was observed after 4 weeks in concentrations up to 250 mg/kg. In the range finding test 100% mortality occurred after 14 days exposure to 1000 mg/kg. Reproduction was not significantly affected up to concentrations of 105 mg/kg (14% inhibition). At the level of the LOEC (250 mg/kg), the reproduction was 39% of the control and food consumption was reduced.

The springtail test was carried out according to the draft ISO/CD 11267. Juvenile springtails of the species *Folsomia candida*, 10 to 12 days of age were placed in an artificial soil and survival and reproduction after 28 days were determined. The artificial soil was the same as used in the earthworm study. Nominal test concentrations were 1,3,8,19,45 and 105 mg/kg soil. After prepration of the test concentrations and an equilibrium period of one week, the test organisms were added to the soil. The animals were fed with granulated dry yeast.

No significant mortality nor effects on reproduction were observed in concentrations up to 45 mg/kg. Mortality was significant (18%) in the highest concentration of 105 mg/kg. The reproduction, expressed as the number of juveniles per container, was also significantly reduced (51%) in 105 mg/kg.

Table 21. Toxicity data for AHTN and HHCB

Species	Test	Results	Reference
Earthworm *Eisenia foetida*	ISO 11268 (OECD 207) inital weight adults 0.34-0.54 g test range 8-250 mg/kg solvent: acetone artificial soil pH 6.1, 10% sphagnum DIN[1] temp. 17-23°C	AHTN 8wk-NOEC = 105 mg/kg, LOEC = 250 mg/kg, reproduction and food consumption 4wk-NOEC ≥ 250 mg/kg, mortality and growth	Gossmann1 997a
		HHCB 8wk-NOEC = 45 mg/kg, LOEC = 105 mg/kg, reproduction and food consumption 4wk-$NOEC_{growth}$ = 105 mg/kg, LOEC = 250 mg/kg 4wk-$NOEC_{survival}$ ≥ 250 mg/kg	Gossmann1 997b
Springtail *Folsomia candida*	ISO /CD 11267 10-12 d old juveniles test range 1-105 mg/kg solvent: acetone temperature 17-25°C artificial soil, 10% sphagnum DIN[1]	AHTN 4wk-NOEC = 45 mg/kg, LOEC = 105 mg/kg, mortality and reproduction	Klepka, 1997a
		HHCB 4wk-NOEC = 45 mg/kg, LOEC = 105 mg/kg, mortality and reproduction	Klepka, 1997b

[1] Sphagnum DIN standard: organic material minimum 90%, organic carbon 52%

HHCB

For HHCB the same tests were carried out (Table 21). In the earthworm test mortality of the adults was not affected after 4 weeks in concentrations up to 250 mg/kg. In the range finding test mortality was 100% after 14 days exposure to 1000 mg/kg. Growth was significantly inhibited (15%) in the highest concentration of 250 mg/kg. Reproduction was not significantly affected up to concentrations of 45 mg/kg (7% inhibition). At the level of the LOEC (105 mg/kg), the reproduction was 57% of the control, whereas in the highest concentration reproduction was inhibited commpletely. Food consumption was reduced in the highest concentration as well.

In the test on springtails, no significant mortality was observed in soils containing up to 45 mg/kg, but mortality was 72% in 105 mg/kg. Reproduction was inhibited by 23% in 45 mg/kg. This inhibition was however not significantly different from the control. The reproduction in 105 mg/kg was 16% of the control.

Derivation of the $PNEC_{soil}$

For the derivation of $PNEC_{soil}$, the results from an experiment are first normalized using relationships that describe the bioavailability of a chemical in the soil. The defined standard soil of the TGD contains 3.4% organic matter, whereas the tests were carried out in the standard OECD soil with an organic matter content of 10%. Subsequenlty for organic substances like HHCB and AHTN, the test results are normalized according to the formula (TGD):

$$NOEC_{standard\ soil} = NOEC_{experiment} * Fom_{standard\ soil} / Fom_{experiment} \qquad (12)$$

where:

$NOEC_{standard\ soil}$:	normalized NOEC for the defined standard soil with 3.4% organic matter;
$NOEC_{experiment}$:	NOEC from experiment (see Table 21);
$Fom_{standard\ soil}$:	weight fraction organic matter in soil solids of the standard soil, being 3.4% assuming $Fom_{soil} = 1.7\ Foc_{soil}$ (TGD);
$Fom_{experiment}$:	weight fraction organic matter in experimental soil, being 10% for tests with AHTN and HHCB (see Table 21).

For both substances, standard long-term toxicity studies for two trophic levels are available, implying that an assessment factor of 50 should be applied to the lowest of the two NOECs (see Table 22).

Table 22. Derivation of PNECsoil

Species	AHTN [mg/kg]		HHCB [mg/kg]	
earthworm	8wk-NOEC	105	8 wk-NOEC	**45**
springtail	4wk-NOEC	**45**	4 wk-NOEC	**45**
lowest NOEC normalized for organic matter standard soil (Fomexperiment/Fomstandard = 0.1/0.034)	16		16	
assessment factor	50		50	
PNECsoil [mg/kg dw]	0.32		0.32	

For comparison, the $PNEC_{soil}$ was also derived on the basis of equilibrium partitioning. According to the equilibrium partitioning theory it is assumed that test organisms are exposed only through the pore water and that soil organisms and aquatic organisms are equally sensitive to the test substances. In the soil, AHTN and HHCB partition between the solid phase and the aqueous phase.

The general applicability of the equilibrium partitioning method has been tested less for soil than for sediment-dwelling organisms. The approach is considered as a screening for assessment of the risk both organisms (TGD).

The pore water concentration can be calculated from the concentration in soil using the sorption coefficient (Kp or $K_{soil-water}$). The other way around, $PNEC_{water}$ can be taken to calculate the corresponding no-effect-concentration in soil, $PNEC_{soil, ep}$. This value is not based on direct experimental data from soil. The calculation of $PNEC_{soil, ep}$ is presented in Table 23.

Table 23. Derivation of PNECsoil according to the equilibrium partition method

Step	Parameter	AHTN	HHCB
1	log Koc [-]	4.8	4.86
2	Kp [l/kg]	1260	1450
3	Ksoil-water [-]	1890	2170
4	PNEClocalwater [mg/l]	0.0035	0.0068
5	PNECsoil, ep [mg/kg ww]	3.9	8.7
6	PNECsoil, ep [mg/kg dw]	4.4	9.8

ad 1
See § 2.2 and Table 1 on physico-chemical properties.

ad 2
Kp is estimated from Koc:
for AHTN: Kp = Koc * foc = $10^{4.8}$ * 0.02 = 1260 l/kg, where foc is the fraction of organic carbon;
for HHCB: Kp = $10^{4.86}$ * 0.02 = 1450 l/kg.

ad 3
The partition coefficient $K_{soil-water}$ between the entire bulk of the soil and water (total compartment-water partitioning coefficient) is derived from Kp:
for AHTN: $K_{soil-water}$ = $Fwater_{soil}$ * RHOwater + $Fsolid_{soil}$ * Kp * RHOsolid =
= 0.2 * 1.0 + 0.6 * 1260 * 2.5 = 1890 where F stands for fraction and RHO is bulk density;
for HHCB: $K_{soil-water}$ = 0.2 * 1.0 + 0.6 * 1450 * 2.5 = 2170.

ad 4
Values derived in § 4.1.

ad 5
$K_{soil-water}$ is used to derive $PNEC_{soil, ep.}$ from $PNEC_{water}$.

$$PNEC_{soil,\,ep} = PNEC_{water} * K_{soil\text{-}water} / RHO_{soil} \qquad (13)$$

For AHTN: $PNEC_{soil,\,ep}$ = 0.0035 * 1890 / 1.7 = 3.9 mg/kg ww.
For HHCB: $PNEC_{soil,\,ep}$ = 0.0068 * 2170 / 1.7 = 8.7 mg/kg ww.

ad 6
Concentrations in mg/kg ww are converted to mg/kg dw by multiplying the wet weight values with a factor 1.13 using formula 2 presented in §3.3.

Comparison of both approaches (Table 24) reveals that $PNEC_{soil}$ based on terrestrial toxicity data is lower than $PNEC_{soil.ep}$ calculated from $PNEC_{water}$ by equilibrium partitioning by factors of 14 and 31 for AHTN and HHCB, respectively. This may be explained by the higher assessment factor (50) used for the terrestrial data compared to the aquatic data (10). If the ratios of 11 and 31 are subsequently lowered by a factor 5, i.e. the difference between the assessment factors 50 and 10, it can be concluded that both methods give comparable results, considering also that the equilibrium partitioning does not take the contribution of food ingestion into account.

Table 24. Comparison of PNECsoil based on terrestrial toxicity data with PNECsoil based on equilibrium partitioning

Parameter	AHTN	HHCB
PNECsoil [mg/kg dw]	0.32	0.32
PNECsoil, ep [mg/kg dw]	4.4	9.8

4.3 Sediment organisms

No data are available on the toxicity of AHTN and HHCB to sediment-dwelling organisms. Therefore $PNEC_{sed}$ is calculated from $PNEC_{water}$ using equilibrium partitioning (TGD), taking into account the same assumptions as for terrestrial organisms. As this PNEC-value is not based on direct experimental data from sediment organisms, the reliability is considered lower and an indication of $PNEC_{sed}$ only. The calculation of $PNEC_{sed,\,ep}$ is presented in Table 25. Associated with the use of $PNEC_{sed,\,ep}$ for AHTN and HHCB, both having a log Kow value of more than 5, is the increase of PEC_{sed} by a factor of 10 for the calculation of the PEC/PNEC ratio in order to take ingestion via food into account (see also § 3.7.2).

Table 25. Derivation of PNECsed, ep according to equilibrium partition method

Step	Parameter	AHTN	HHCB
1	log Koc	4.72	4.88
2	Kpsed (foc=0.05) [l/kg]	3160	3620
3	Ksed-water	1580	1810
4	PNECwater [mg/l], dissolved	0.0035	0.0068
5	PNECsed, ep [mg/kg ww]	4.3	9.5
6	PNECsed, ep [mg/kg dw]	11	25

ad 1
See § 2.2 and Table 1 on physico-chemical properties.

ad 2
Kp is calculated from the indirect measured Koc with Kp = Koc * foc, where foc is the fraction organic carbon (0.05):
for AHTN: log Koc = 4.8, and Kp = 3160 l/kg;
for HHCB: log Koc = 4.86, and Kp = 3620.

ad 3
The partition coefficient $K_{sed\text{-}water}$ between suspended solids and water is derived from the Kp:
for AHTN: $K_{sed\text{-}water}$ = $Fwater_{sed}$ * RHOwater + $Fsolid_{sed}$ * Kp * RHOsolid = 0.8 * 1.0 + 0.2 * 3160 * 2.5 = 1580;
for HHCB: $K_{sed\text{-}water}$ = 0.8 * 1.0 + 0.2 * 3620 * 2.5 = 1810.

ad 4
$K_{sed\text{-}water}$ is used to derive $PNEC_{sed,\,ep}$ from $PNEC_{water}$ (§ 4.1) and corrected for density differences:

$$PNEC_{sed,\,ep} = K_{sed\text{-}water} * PNEC_{water} / RHO_{sed} \qquad (14)$$

For AHTN: $PNEC_{sed,\,ep}$ = 1580 * 0.0035 / 1.3 = 4.3 mg/kg ww;
for HHCB: $PNEC_{sed,\,ep}$ = 1810 * 0.0068 / 1.3 = 9.5 mg/kg ww.

ad 5
Concentrations in mg/kg ww are converted to mg/kg dw by multiplying the wet weight values with a factor 2.6 using formula 3 presented in §3.4.

4.4 Predators

Toxicity studies with AHTN and HHCB on predators present in the environment like fish-eating birds and mammals are not available. Therefore toxicity data for laboratory mammals are used to derive a PNEC. For AHTN and HHCB, subchronic oral studies are available for rats.

AHTN was administered in the diet of rats (15 males and 15 females per group) at daily doses of 1.5, 5, 15 and 50 mg/kg for 13 weeks (Hopkins et al., 1996a). On completion of the treatment period, three males and three females from the high dose and controls were maintained for a treatment free period of 4 weeks before sacrifice. Bodyweight gain was decreased in males and females at the highest dose but this response improved during the treatment free period. The liver weights of females at 15 mg/kg and of both sexes at 50 mg/kg were increased but there were no histopathological findings at either dose indicating that this may represent an increased demand for liver function. There were no differences in liver weights at the end of the treatment free period. It can be concluded, therefore, that a no-adverse-effect-level of 15 mg/kg for AHTN has been demonstrated.

HHCB was tested by an identical protocol but at doses of 5, 15, 50 and 150 mg/kg/day (Hopkins et al., 1996b). There was a slightly higher mean absolute but not relative liver weight in males in all doses groups but there was no dose response, no histopathology and no similar effects in the females. These effects were not seen at the end of the treatment free period. Since increased relative and absolute liver weights for males and females and an adverse effect on bodyweight gain was seen at 341 mg/kg in the 2-week range finding test, it can be concluded that the no-adverse-effect-level in the diet is 150 mg/kg.

Derivation of the $PNEC_{oral}$

The estimation of $PNEC_{oral}$ for fish- and worm-eating birds and mammals is presented in Table 26. For the conversion of the NOEC determined for mammals from daily doses [mg per kg body weight] to a level in the food [mg per kg food] a factor of 20 is used for a rat > 6 weeks old. According to the TGD the assessment factor for extrapolation from a 90-day toxicity test is 30. Therefore $PNEC_{oral}$ is 10 mg/kg for AHTN and 100 mg/kg for HHCB.

Table 26. Derivation of PNECoral

Parameter	AHTN	HHCB
NOEC mammal [mg/kg bw]	15	150
NOEC mammal [mg/kg food]	300	3000
Assessment factor	30	30
$PNEC_{pred}$ [mg/kg food]	10	100

5 RISK CHARACTERIZATION

5.1 Results

The end product of the risk assessment are the Risk Characterization Ratios (RCRs) of the exposure to no-effect concentrations. In Tables 27 and 28 RCRs are presented for aquatic organisms in surface water, sediment dwelling organisms, soil organisms, fish-eating predators and worm-eating predators. Exposure concentrations are taken from Table 17 while the PNEC values are taken from Tables 20, 22, 25 and 26.

Table 27. Risk Characterization Ratios (RCRs) for AHTN

AHTN	exposure concentrations	PNEC	RCR
aquatic organisms (μg/l)	0.2 (m)	3.5	0.057
sediment organisms (mg/kg dw)	0.48 (m) * 10[1]	11	0.44
soil organisms (mg/kg dw)	0.26 (p)	0.32	0.81
fish-eating predators (mg/kg)	0.146 (m)	10	0.015
worm-eating predators (mg/kg)	0.78 (p)	10	0.078

Table 28. Risk Characterization Ratios (RCRs) for HHCB

HHCB	exposure concentrations	PNEC	RCR
aquatic organisms (μg/l)	0.5 (m)	6.8	0.074
sediment organisms (mg/kg dw)	0.16 (m) * 10[1]	25	0.064
soil organisms (mg/kg dw)	0.38 (p)	0.32	1.2
fish-eating predators (mg/kg)	0.125 (m)	100	0.0013
worm-eating predators (mg/kg)	1.7 (p)	100	0.017

(m): measured concentration
(p): predicted concentration
[1]: measured concentration multiplied by 10 as log Kow of AHTN and HHCB is above 5 (TGD)

Surface water

Based on measured concentrations, the RCR is less than 0.1 for AHTN and HHCB. Even comparing the maximum measured concentration of 1.2 μg/l for both substances with the $\mathrm{PNEC}_{\mathrm{water}}$ gives ratios considerably below 1: 0.34 and 0.18 for AHTN and HHCB, respectively. Also if predicted concentrations presented in Table 6, are used the PEC/PNEC ratios are below 1: 0.29 and 0.35 for AHTN and HHCB, respectively.

Sediment

The resulting ratios based on measured concentrations in suspended matter are 0.44 for AHTN and 0.06 for HHCB. Improved reliability can be obtained by determination of the toxicity to sediment-dwelling organisms or by validating the extrapolated concentrations in the sediment by measurements since degradation of the substances in sediment might contribute to a lower concentration in sediment than predicted.

Soil

PEC/PNEC ratios for the terrestrial environment are 0.81 and 1.2 for AHTN and HHCB, respectively. An assessment factor of 50 has been used to derive the $PNEC_{soil}$, because long term toxicity data are available for two species. Testing an additional species will lower the assessment factor to 10. Moreover, a major refinement could be obtained on the side of PEC_{soil} by replacement of the conservative estimate where both AHTN and HHCB are not degraded in soil by measured degradation rate constants.

Predators

Based on measured data the RCRs for fish-eating predators are less than 0.1 for both substances: 0.015 and 0.0013 for AHTN and HHCB, respectively. Also based on predicted concentrations presented in Table 11 all ratios arebelow 1: 0.032 and 0.20 for AHTN and HHCB, respectively.

For worm-eating predators no measured exposure concentrations are available. PEC/PNEC ratios are less than 0.1: 0.078 and 0.017 for AHTN and HHCB, respectively. The lower ratio for HHCB is a reflection of the lower toxicity to predators of HHCB compared to AHTN since the BCF_{worm} values are almost equal.

5.2 Further refinement of the environmental risk assessment

There are several options for refinement of the environmental risk assessment for AHTN and HHCB. On the effects side:

- aquatic organisms: in the ELS test for AHTN with fathead minnows absence of the caudal tail fin occurred at concentrations of 67 µg/l and higher. Physical abnormalities are found for more substances in ecotoxicological tests with fish. From a risk assessment point of view other tests are not considered necessary as the RCR is below 0.1. However, it might be relevant to investigate whether this effect is reproducible and whether it occurs also in tests with other fish species.
- soil organisms: long-term tests are available for springtails and earthworms. Testing another species, e.g. plants, would lead to a lower assessment factor in deriving the $PNEC_{soil}$.
- sediment dwelling organisms: presently $PNEC_{sed}$ is derived from aquatic toxicity data with the equilibrium partitioning method and applying a factor of 10 on the exposure side. A test with a sediment dwelling organism might be considered leading to a derivation of the $PNEC_{sed}$ using assessment factors.
- predators: considering the low risks for predators tests with species other than rats, e.g. birds, are not considered necessary.

On the exposure side:

- although there are strong indications that biodegradation of AHTN and HHCB occurs, aerobically as well as anaerobically, this could not be incorporated into the risk assessment as no rate constants were available. So, tests could be carried out to determine these constants.
- since in the sludge monitoring study in the Netherlands grab samples were taken, no complete mass balance in the STPs could be determined (Blok, 1997). A mass balance for

one or more STPs, determined with time proportional samplers, will give more insight into the environmental fate of AHTN and HHCB.

- monitoring data for fish are scarce: all data come from one site in Germany. Although from a risk assessment point of view this is not considered necessary, gathering more data will give a more representative picture.
- no measured concentrations are available for the sediment and soil compartment. As RCRs are close to one or above one for soil a sludge-amended soil study might be considered.

At the moment the Institute for Inland Water Management and Waste Water Treatment (RIZA) is monitoring polycyclic musks in surface water, sludge, suspended matter and fish in the Netherlands. A mass balance will be determined for several STPs. Results will become available in 1998.

From a risk assessment point of view priority should be given to elements in the risk assessment with the highest uncertainty, for the compartment with the highest RCR. Therefore, additional tests on the exposure side for the soil compartment are considered more relevant than on the effects side.

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Appendix 1 EUSES Full reports for AHTN and HHCB

AHTN

(21 pages)

EUSES Full report	**Single substance**
Printed on	**8/26/97 4:30:48 PM**
Study	**AHTN**
Substance	**AHTN**
Defaults	**Standard**
Assessment types	**1A, 1B, 2**
Base set complete	**No**
Explanation status column	**'O' = Output; 'D' = Default; 'S' = Set; 'I' = Imported**

Name	Reference	Value	Units	Status
STUDY				
STUDY IDENTIFICATION				
Study name	AHTN	AHTN		S
Study description	environmental risk assessment	environmental risk assessment		S
Author	E. v.d. Plassche	E. v.d. Plassche		S
Institute	RIVM	RIVM		S
Address	PO Box 1	PO Box 1		S
Zip code	3720 BA	3720 BA		S
City	Bilthoven	Bilthoven		S
Country	The Netherlands	The Netherlands		S
Telephone	+31-(0)30-2743658	+31-(0)30-2743658		S
Telefax	+31-(0)30-2744401	+31-(0)30-2744401		S
Email	Erik.van.de.Plassche@rivm.nl	Erik.van.de.Plassche@rivm.nl		S
Calculations checksum	C1CBE4CE	C1CBE4CE		S

EUSES Full report	**Single substance**
Printed on	**8/26/97 4:30:48 PM**
Study	**AHTN**
Substance	**AHTN**
Defaults	**Standard**
Assessment types	**1A, 1B, 2**
Base set complete	**No**

Name	Reference	Value	Units	Status
DEFAULTS				
DEFAULT IDENTIFICATION				
General name	Standard	Standard		D
Description	According to TGDs	According to TGDs		D
RELEASE ESTIMATION				
Fraction of EU production volume for region	0.1	0.1	[-]	D
Fraction connected to sewer systems	0.7	0.7	[-]	D
CHARACTERISTICS OF COMPARTMENTS				
GENERAL				
Density of solid phase	2.5	2.5	[kg.l-1]	D
Density of water phase	1	1	[kg.l-1]	D
Density of air phase	1.3E-03	1.3E-03	[kg.l-1]	D
Environmental temperature	12	12	[oC]	D
Constant of Junge equation	0.01	0.01	[Pa.m]	D
Surface area of aerosol particles	0.01	0.01	[m2.m-3]	D
Gas constant (8.314)	8.314	8.314	[Pa.m3.mol-1.K-1]	D
SUSPENDED MATTER				
Volume fraction solids in suspended matter	0.1	0.1	[m3.m-3]	D
Volume fraction water in suspended matter	0.9	0.9	[m3.m-3]	D
Weight fraction of organic carbon in suspended matter	0.1	0.1	[kg.kg-1]	D
Wet bulk density of suspended matter	1.15E+03	1.15E+03	[kg.m-3]	O
SEDIMENT				
Volume fraction solids in sediment	0.2	0.2	[m3.m-3]	D
Volume fraction water in sediment	0.8	0.8	[m3.m-3]	D
Weight fraction of organic carbon in sediment	0.05	0.05	[kg.kg-1]	D
Bulk density of sediment	1.3E+03	1.3E+03	[kgwwt.m-3]	O
Conversion factor wet-dry sediment	2.6	2.6	[kgwwt.kgdwt-1]	O
SOIL				
Volume fraction solids in soil	0.6	0.6	[m3.m-3]	D
Volume fraction water in soil	0.2	0.2	[m3.m-3]	D
Volume fraction air in soil	0.2	0.2	[m3.m-3]	D
Weight fraction of organic carbon in soil	0.02	0.02	[kg.kg-1]	D
Bulk density of soil	1.7E+03	1.7E+03	[kgwwt.m-3]	O
Conversion factor wet-dry soil	1.13	1.13	[kgwwt.kgdwt-1]	O
STP SLUDGE				
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D

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Study	**AHTN**
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Assessment types	**1A, 1B, 2**
Base set complete	**No**

Name	Reference	Value	Units	Status
DEGRADATION AND TRANSFORMATION RATES				
Concentration of OH-radicals in atmosphere	5E+05	5E+05	[molec.cm-3]	D
Rate constant for abiotic degradation in STP	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk soil	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk sediment	0	0	[d-1]	D
Rate constant for anaerobic biodegradation in sediment	0	0	[d-1]	D
Fraction of sediment compartment that is aerated	0.1	0.1	[m3.m-3]	D
SEWAGE TREATMENT				
GENERAL				
Number of inhabitants feeding one STP	1E+04	1E+04	[eq]	D
Sewage flow	200	200	[l.eq-1.d-1]	D
Effluent discharge rate of local STP	2E+06	2E+06	[l.d-1]	O
Temperature dependency correction	No	No		D
Temperature of air above aeration tank	15	15	[oC]	D
Temperature of water in aeration tank	15	15	[oC]	D
Height of air column above STP	10	10	[m]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Windspeed in the system	3	3	[m.s-1]	D
RAW SEWAGE				
Mass of O2 binding material per person per day	54	54	[g.eq-1.d-1]	D
Dry weight solids produced per person per day	0.09	0.09	[kg.eq-1.d-1]	D
Density solids in raw sewage	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
PRIMARY SETTLER				
Depth of primary settler	4	4	[m]	D
Hydraulic retention time of primary settler	2	2	[hr]	D
Density suspended and settled solids in primary settler	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
ACTIVATED SLUDGE TANK				
Depth of aeration tank	3	3	[m]	D
Density solids of activated sludge	1.3	1.3	[kg.l-1]	D
Concentration solids of activated sludge	4	4	[kg.m-3]	D
Steady state O2 concentration in activated sludge	2E-03	2E-03	[kg.m-3]	D
Mode of aeration	Surface	Surface		D
Aeration rate of bubble aeration	1.31E-05	1.31E-05	[m3.s-1.eq-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Sludge loading rate	0.15	0.15	[kg.kg-1.d-1]	D
Hydraulic retention time in aerator (9-box STP)	6.9	6.9	[hr]	O
Hydraulic retention time in aerator (6-box STP)	10.8	10.8	[hr]	O
Sludge retention time of aeration tank	9.2	9.2	[d]	O

EUSES Full report	Single substance
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Study	AHTN
Substance	AHTN
Defaults	Standard
Assessment types	1A, 1B, 2
Base set complete	No

Name	Reference	Value	Units	Status
SOLIDS-LIQUIDS SEPARATOR				
Depth of solids-liquid separator	3	3	[m]	D
Density suspended and settled solids in solids-liquid separator	1.3	1.3	[kg.l-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Hydraulic retention time of solids-liquid separator	6	6	[hr]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D
REGIONAL AND CONTINENTAL DISTRIBUTION				
CONTINENTAL				
Area of EU	3.56E+06	3.56E+06	[km2]	D
Area of continental system	3.52E+08	3.52E+08	[km2]	O
Number of inhabitants in the EU	3.7E+08	3.7E+08	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Area fraction of water of the continental system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from global scale to continent	0	0	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of continental system	25	25	[mg.l-1]	D
Residence time of water in system	166	166	[d]	O
Residence time of air in system	6.41	6.41	[d]	O
Net sedimentation rate	2.59	2.59	[mm.yr-1]	O
REGIONAL				
Area of regional system	4E+04	4E+04	[km2]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Area fraction of water of the regional system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from continental scale to region	0.034	0.034	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of regional system	15	15	[mg.l-1]	D
Residence time of water in system	40.1	40.1	[d]	O
Residence time of air in system	0.684	0.684	[d]	O
Net sedimentation rate	3.13	3.13	[mm.yr-1]	O
AIR				
Atmospheric mixing height	1000	1000	[m]	D
Windspeed in the system	3	3	[m.s-1]	D
Aerosol deposition velocity	1E-03	1E-03	[m.s-1]	D
Aerosol collection efficiency	2E+05	2E+05	[-]	D
Average annual precipitation	700	700	[mm.yr-1]	D

Name	Reference	Value	Units	Status
WATER AND SEDIMENT				
Concentration biota	1	1	[mg.l-1]	D
Sediment mixing depth	0.03	0.03	[m]	D
Settling velocity of suspended solids	2.5	2.5	[m.d-1]	D
(biogenic) production of suspended solids in water	0	0	[kg.d-1]	D
Sewage flow	200	200	[l.eq-1.d-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Fraction connected to sewer systems	0.7	0.7	[-]	D
SOIL				
Mixing depth natural soil	0.05	0.05	[m]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Mixing depth industrial/urban soil	0.05	0.05	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D
Fraction of rain water running off soil	0.25	0.25	[-]	D
Soil erosion rate of regional system	0.03	0.03	[mm.yr-1]	D
MASS TRANSFER				
Air-film PMTC (air-water interface)	1.39E-03	1.39E-03	[m.s-1]	D
Water-film PMTC (air-water interface)	1.39E-05	1.39E-05	[m.s-1]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Water-film PMTC (sediment-water interface)	2.78E-06	2.78E-06	[m.s-1]	D
Pore water PMTC (sediment-water interface)	2.78E-08	2.78E-08	[m.s-1]	D
LOCAL DISTRIBUTION				
AIR AND SURFACE WATER				
Concentration in air at source strength 1 [kg.d-1]	2.78E-04	2.78E-04	[mg.m-3]	D
Standard deposition flux of aerosol-bound compounds	0.01	0.01	[mg.m-2.d-1]	D
Standard deposition flux of gaseous compounds	4E-04	4E-04	[mg.m-2.d-1]	O
Suspended solids concentration of regional system	15	15	[mg.l-1]	D
Dilution factor	10	10	[-]	D
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	D
Calculate dilution from river flow rate	No	No		D
SOIL				
Mixing depth of grassland soil	0.1	0.1	[m]	D
Dry sludge application rate on agricultural soil	5E+03	5E+03	[kg.ha-1.yr-1]	D
Dry sludge application rate on grassland	1000	1000	[kg.ha-1.yr-1]	D
Averaging time soil (for terrestrial ecosystem)	30	30	[d]	D
Averaging time agricultural soil	180	180	[d]	D
Averaging time grassland	180	180	[d]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D

Printed on	**8/26/97 4:30:48 PM**
Study	**AHTN**
Substance	**AHTN**
Defaults	**Standard**
Assessment types	**1A, 1B, 2**
Base set complete	**No**

Name	Reference	Value	Units	Status
SOIL (Continued)				
Average annual precipitation	700	700	[mm.yr-1]	D
CHARACTERISTICS OF PLANTS AND CATTLE				
PLANTS				
Volume fraction of water in plant tissue	0.65	0.65	[m3.m-3]	D
Volume fraction of lipids in plant tissue	0.01	0.01	[m3.m-3]	D
Volume fraction of air in plant tissue	0.3	0.3	[m3.m-3]	D
Correction for differences between plant lipids and octanol	0.95	0.95	[-]	D
Bulk density of plant tissue (wet weight)	0.7	0.7	[kg.l-1]	D
Rate constant for metabolism in plants	0	0	[d-1]	D
Rate constant for photolysis in plants	0	0	[d-1]	D
Leaf surface area	5	5	[m2]	D
Conductance	1E-03	1E-03	[m.s-1]	D
Shoot volume	2	2	[l]	D
Rate constant for dilution by growth	0.035	0.035	[d-1]	D
Transpiration stream	1	1	[l.d-1]	D
CATTLE				
Daily intake for cattle of grass (dryweight)	16.9	16.9	[kg.d-1]	D
Conversion factor grass from dryweight to wetweight	4	4	[kg.kg-1]	D
Daily intake of soil (dryweight)	0.41	0.41	[kg.d-1]	D
Daily inhalation rate for cattle	122	122	[m3.d-1]	D
Daily intake of drinking water for cattle	55	55	[l.d-1]	D

EUSES Full report	Single substance
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Study	**AHTN**
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Assessment types	**1A, 1B, 2**
Base set complete	**No**

Name	Reference	Value	Units	Status
SUBSTANCE				
SUBSTANCE IDENTIFICATION				
General name	AHTN	AHTN		S
Description				D
CAS-No	1222-05-5	1222-05-5		S
EC-notification no.				D
EINECS no.				D
PHYSICO-CHEMICAL PROPERTIES				
Molecular weight	258.4	258.4	[g.mol-1]	S
Melting point	54.5	54.5	[oC]	S
Boiling point	??	??	[oC]	D
Vapour pressure at 25 [oC]	0.0608	0.0608	[Pa]	S
Octanol-water partition coefficient.	5.7	5.7	[log10]	S
Water solubility	1.25	1.25	[mg.l-1]	S

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Base set complete	No

Name	Reference	Value	Units	Status
RELEASE ESTIMATION				
CHARACTERIZATION AND TONNAGE				
High Production Volume Chemical	Yes	Yes		S
Production volume of chemical in EU	0	0	[tonnes.yr-1]	D
Volume of chemical imported to EU	585	585	[tonnes.yr-1]	S
Volume of chemical exported from EU	0	0	[tonnes.yr-1]	D
Intermittent release	No	No		D
INTERMEDIATE RESULTS PRODUCTION VOLUMES				
Tonnage of substance in Europe	585	585	[tonnes.yr-1]	S
Regional production volume of substance	0	0	[tonnes.yr-1]	O
Continental production volume of substance	0	0	[tonnes.yr-1]	O
USE PATTERNS				
EMISSION INPUT DATA				
Industry category	5 Personal / domestic use	5 Personal / domestic use		S
Use category	9 Cleaning/washing agents and additives	9 Cleaning/washing agents and additives		S
Emission scenario document available	Yes	Yes		O
Extra details on use category	No extra details necessary	No extra details necessary		D
Extra details on use category	No extra details necessary	No extra details necessary		D
Fraction of tonnage for application	1	1	[-]	O
Fraction of chemical in formulation	1	1	[-]	D
Production	No	No		S
Formulation	No	No		S
Processing	No	No		S
Private use	Yes	Yes		D
Recovery	No	No		S
Main category production	III Multi-purpose equipment	III Multi-purpose equipment		D
Main category formulation	III Multi-purpose equipment	III Multi-purpose equipment		D
Main category processing	III Non-dispersive use	III Non-dispersive use		D
INTERMEDIATE RESULTS				
USE PATTERN 1				
INTERMEDIATE RESULTS TONNAGES PER USE PATTERN				
Relevant tonnage for application	585	585	[tonnes.yr-1]	O
Regional tonnage of substance	58.5	23.4	[tonnes.yr-1]	S
Continental tonnage of substance	526	562	[tonnes.yr-1]	O
RELEASE FRACTIONS AND EMISSION DAYS				
[PRODUCTION]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O

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Study	**AHTN**
Substance	**AHTN**
Defaults	**Standard**
Assessment types	**1A, 1B, 2**
Base set complete	**No**

Name	Reference	Value	Units	Status
RELEASE FRACTIONS AND EMISSION DAYS (Continued)				
[PRODUCTION]				
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O
[FORMULATION]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O
[PROCESSING]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	1	1	[-]	O
Source of B-table data	No applicable data found	No applicable data found		O
[PRIVATE USE]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0.99	1	[-]	S
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-02	0	[-]	S
Source of A-table data	Specific IC/UC combination	Specific IC/UC combination		O
Fraction of the main local source	2E-03	2E-03	[-]	O
Number of emission days per year	365	365	[-]	O
Source of B-table data	General table	General table		O
[RECOVERY]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	1	1	[-]	O

Name	Reference	Value	Units	Status
[RECOVERY] (Continued)				
Source of B-table data	No applicable data found	No applicable data found		O
CONTINENTAL				
[PRODUCTION]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
[FORMULATION]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
[PROCESSING]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
[PRIVATE USE]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	1.43E+03	1.54E+03	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	14.4	0	[kg.d-1]	O
[RECOVERY]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
REGIONAL				
[PRODUCTION]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
[FORMULATION]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
[PROCESSING]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O

Name	Reference	Value	Units	Status
[PROCESSING] (Continued)				
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
[PRIVATE USE]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	159	64.1	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	1.6	0	[kg.d-1]	O
[RECOVERY]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
CONTINENTAL				
Total continental emission to air	0	0	[kg.d-1]	O
Total continental emission to wastewater	1E+03	1.08E+03	[kg.d-1]	O
Total continental emission to surface water	428	462	[kg.d-1]	O
Total continental emission to industrial soil	14.4	0	[kg.d-1]	O
Total continental emission to agricultural soil	0	0	[kg.d-1]	O
REGIONAL				
Total regional emission to air	0	0	[kg.d-1]	O
Total regional emission to wastewater	111	44.9	[kg.d-1]	O
Total regional emission to surface water	47.6	19.2	[kg.d-1]	O
Total regional emission to industrial soil	1.6	0	[kg.d-1]	O
Total regional emission to agricultural soil	0	0	[kg.d-1]	O
LOCAL				
[PRODUCTION]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[FORMULATION]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[PROCESSING]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[PRIVATE USE]				
Local emission to air during episode	0	0	[kg.d-1]	O

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Name	Reference	Value	Units	Status
[PRIVATE USE] (Continued)				
Local emission to wastewater during episode	0.317	0.128	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[RECOVERY]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D

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Name	Reference	Value	Units	Status
DISTRIBUTION				
PARTITION COEFFICIENTS				
SOLIDS WATER PARTITIONING				
Organic carbon-water partition coefficient	5.2164E+04	6.31E+04	[l.kg-1]	S
Solids-water partition coefficient in soil	1.04E+03	1.26E+03	[l.kg-1]	O
Solids-water partition coefficient in sediment	2.61E+03	3.16E+03	[l.kg-1]	O
Solids-water partition coefficient suspended matter	5.22E+03	6.31E+03	[l.kg-1]	O
Solids-water partition coefficient in raw sewage sludge	1.56E+04	1.89E+04	[l.kg-1]	O
Solids-water partition coefficient in settled sewage sludge	1.56E+04	1.89E+04	[l.kg-1]	O
Solids-water partition coefficient in activated sewage sludge	1.93E+04	2.33E+04	[l.kg-1]	O
Solids-water partition coefficient in effluent sewage sludge	1.93E+04	2.33E+04	[l.kg-1]	O
Suspended matter-water partition coefficient	1.3E+03	1.58E+03	[m3.m-3]	O
Soil-water partition coefficient	1.57E+03	1.89E+03	[m3.m-3]	O
Sediment-water partition coefficient	1.3E+03	1.58E+03	[m3.m-3]	O
AIR-WATER PARTITIONING AND ADSORPTION TO AEROSOL PARTICLES				
Sub-cooled liquid vapour pressure	0.167	0.167	[Pa]	O
Fraction of chemical associated with aerosol particles	5.97E-04	5.97E-04	[-]	O
Henry's law constant	12.6	12.6	[Pa.m3.mol-1]	O
Air-water partitioning coefficient	5.3E-03	5.3E-03	[m3.m-3]	O
BIOTA-WATER				
Bioconcentration factor for aquatic biota	1.4E+04	1.4E+04	[l.kg-1]	O
DEGRADATION AND TRANSFORMATION RATES				
CHARACTERIZATION AND STP				
Characterization of biodegradability	Not biodegradable	Not biodegradable		D
Degradation calculation method in STP	First order, standard OECD/EU tests	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	0	[d-1]	O
Total rate constant for degradation in STP	0	0	[d-1]	O
Maximum growth rate of specific microorganisms	2	2	[d-1]	D
Half saturation concentration	0.5	0.5	[g.m-3]	D
ENVIRONMENTAL				
Specific degradation rate constant with OH-radicals	0	0	[cm3.molec-1.s-1]	D
Rate constant for degradation in air	0	0	[d-1]	O
Rate constant for hydrolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for photolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for biodegradation in surface water	0	0	[d-1]	O
Total rate constant for degradation in bulk surface water	1.39E-06	1.39E-06	[d-1]	O
Rate constant for biodegradation in bulk soil	6.93E-07	6.93E-07	[d-1]	O

Name	Reference	Value	Units	Status
ENVIRONMENTAL (Continued)				
Total rate constant for degradation in bulk soil	6.93E-07	6.93E-07	[d-1]	O
Rate constant for biodegradation in aerated sediment	6.93E-07	6.93E-07	[d-1]	O
Total rate constant for degradation in bulk sediment	6.93E-08	6.93E-08	[d-1]	O
SEWAGE TREATMENT				
CONTINENTAL				
Fraction of emission directed to air	0.0197	0.0167	[-]	O
Fraction of emission directed to water	0.182	0.167	[-]	O
Fraction of emission directed to sludge	0.798	0.816	[-]	O
Fraction of the emission degraded	0	0	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	19.7	18	[kg.d-1]	O
Indirect emission to surface water	182	180	[kg.d-1]	O
Indirect emission to agricultural soil	797.608	106	[kg.d-1]	S
REGIONAL				
Fraction of emission directed to air	0.023	0.0195	[-]	O
Fraction of emission directed to water	0.181	0.166	[-]	O
Fraction of emission directed to sludge	0.796	0.815	[-]	O
Fraction of the emission degraded	0	0	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	2.55	0.876	[kg.d-1]	O
Indirect emission to surface water	20.1	7.43	[kg.d-1]	O
Indirect emission to agricultural soil	88.4499	4.4	[kg.d-1]	S
LOCAL				
[PRIVATE USE]				
INPUT AND CONFIGURATION [PRIVATE USE]				
Use or bypass STP	Use STP	Use STP		D
Local emission to wastewater during episode	0.317	0.128	[kg.d-1]	O
Concentration in untreated wastewater	0.159	0.0641	[mg.l-1]	O
Local emission entering the STP	0.317	0.128	[kg.d-1]	O
Type of local STP	With primary settler (9-box)	With primary settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	1E+04	[eq]	O
Effluent discharge rate of this STP	2E+06	2E+06	[l.d-1]	O
Calculate dilution from river flow rate	No	No		O
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O
Dilution factor	10	10	[-]	D
OUTPUT [PRIVATE USE]				
Fraction of emission directed to air by STP	0.0242	0.0206	[-]	O
Fraction of emission directed to water by STP	0.18	0.165	[-]	O
Fraction of emission directed to sludge by STP	0.796	0.814	[-]	O
Fraction of the emission degraded in STP	0	0	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	7.68E-03	2.64E-03	[kg.d-1]	O

Name	Reference	Value	Units	Status
OUTPUT [PRIVATE USE] (Continued)				
Concentration in untreated wastewater	0.159	0.0641	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.0286	0.0106	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	319.668	16	[mg.kg-1]	S
PEC for micro-organisms in the STP	0.0286	0.0106	[mg.l-1]	O
CONTINENTAL AND REGIONAL				
CONTINENTAL				
Continental PEC in surface water (total)	1.81E-05	1.62E-05	[mg.l-1]	O
Continental PEC in surface water (dissolved)	1.58E-05	1.38E-05	[mg.l-1]	O
Continental PEC in air (total)	2.48E-06	1.29E-06	[mg.m-3]	O
Continental PEC in agricultural soil (total)	0.199	0.0317	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.16E-04	2.85E-05	[mg.l-1]	O
Continental PEC in natural soil (total)	6.91E-04	4.31E-04	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	0.0108	4.31E-04	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	0.0315	0.0333	[mg.kgwwt-1]	O
REGIONAL				
Regional PEC in surface water (total)	1.46E-04	5.02E-05	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.34E-04	4.53E-05	[mg.l-1]	O
Regional PEC in air (total)	4.68E-06	1.74E-06	[mg.m-3]	O
Regional PEC in agricultural soil (total)	1.94	0.115	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	2.11E-03	1.03E-04	[mg.l-1]	O
Regional PEC in natural soil (total)	1.3E-03	5.8E-04	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	0.1	5.8E-04	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	0.265	0.109	[mg.kgwwt-1]	O
LOCAL				
REMOVAL RATE CONSTANTS SOIL				
Total rate constant for degradation in bulk soil	6.93E-07	6.93E-07	[d-1]	O
Rate constant for volatilisation from agricultural soil	8.26E-06	6.83E-06	[d-1]	O
Rate constant for volatilisation from grassland soil	1.65E-05	1.37E-05	[d-1]	O
Rate constant for leaching from agricultural soil	1.53E-06	1.27E-06	[d-1]	O
Rate constant for leaching from grassland soil	3.06E-06	2.53E-06	[d-1]	O
Total rate constant for removal from agricultural top soil	1.05E-05	8.79E-06	[d-1]	O
Total rate constant for removal from grassland top soil	2.03E-05	1.69E-05	[d-1]	O
[PRIVATE USE]				
LOCAL CONCENTRATIONS AND DEPOSITIONS [PRIVATE USE]				
Concentration in air during emission episode	2.14E-06	7.33E-07	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	2.14E-06	7.33E-07	[mg.m-3]	O
Total deposition flux during emission episode	3.12E-06	1.07E-06	[mg.m-2.d-1]	O
Annual average total deposition flux	3.12E-06	1.07E-06	[mg.m-2.d-1]	O

Name	Reference	Value	Units	Status
[PRIVATE USE] (Continued)				
LOCAL CONCENTRATIONS AND DEPOSITIONS [PRIVATE USE]				
Concentration in surface water during emission episode	2.65E-03	9.66E-04	[mg.l-1]	O
Annual average concentration in surface water	2.65E-03	9.66E-04	[mg.l-1]	O
Concentration in agric. soil averaged over 30 days	4.62	0.232	[mg.kgwwt-1]	O
Concentration in agric. soil averaged over 180 days	4.62	0.232	[mg.kgwwt-1]	O
Concentration in grassland averaged over 180 days	1.82	0.0914	[mg.kgwwt-1]	O
Fraction of steady-state (agricultural soil)	0.0375	0.0316	[-]	O
Fraction of steady-state (grassland soil)	0.0713	0.0598	[-]	O
LOCAL PECS [PRIVATE USE]				
Annual average local PEC in air (total)	6.81E-06	2.47E-06	[mg.m-3]	O
Local PEC in surface water during emission episode	2.78E-03	1.01E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	2.78E-03	1.01E-03	[mg.l-1]	O
Local PEC in sediment during emission episode	3.16	1.39	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	4.62	0.232	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	4.62	0.232	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.82	0.092	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	5.02E-03	2.09E-04	[mg.l-1]	O
Local PEC in pore water of grassland	1.97E-03	8.26E-05	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	5.02E-03	2.09E-04	[mg.l-1]	O

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Name	Reference	Value	Units	Status
EXPOSURE				
BIOCONCENTRATION FACTORS				
Partition coefficient worm-porewater	2.00475E+04	5E+03	[l.kg-1]	S
Bioconcentration factor for earthworms	21.8	4.49	[kg.kg-1]	O
Bioconcentration factor for fish	1.39637E+04	597	[l.kg-1]	S
Partition coefficient between plant tissue and water	2.6E+03	2.6E+03	[m3.m-3]	O
Partition coefficient between leaves and air	4.9E+05	4.9E+05	[m3.m-3]	O
Transpiration-stream concentration factor	0.0378	0.0378	[-]	O
Bioaccumulation factor for meat	0.0126	0.0126	[d.kg-1]	O
Bioaccumulation factor for milk	3.98E-03	3.98E-03	[d.kg-1]	O
Purification factor for surface water	0.25	0.25	[-]	O
SECONDARY POISONING				
SECONDARY POISONING [PRIVATE USE]				
Concentration in fish from surface water for predators	20.4	0.315	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	71.4	0.78	[mg.kg-1]	O

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Name	Reference	Value	Units	Status
EFFECTS				
INPUT OF EFFECTS DATA				
MICRO-ORGANISMS				
EC50 for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
EC10 for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
NOEC for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
AQUATIC ORGANISMS				
LC50 for fish	??	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	??	[mg.l-1]	D
EC50 for algae	??	??	[mg.l-1]	D
LC50 for other aquatic species	??	??	[mg.l-1]	D
Species	other	other		D
NOEC for fish	0.035	0.035	[mg.l-1]	S
NOEC for Daphnia	0.11	0.11	[mg.l-1]	S
NOEC for algae	0.2	0.2	[mg.l-1]	S
NOEC for other aquatic species	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
TERRESTRIAL ORGANISMS				
LC50 for plants	??	??	[mg.kgwwt-1]	D
LC50 for earthworms	??	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	??	[mg.kgwwt-1]	D
Species	other	other		D
NOEC for plants	??	??	[mg.kgwwt-1]	D
NOEC for earthworms	36	36	[mg.kgdwt-1]	S
NOEC for microorganisms	??	??	[mg.kgwwt-1]	D
NOEC for other terrestrial species	16	16	[mg.kgdwt-1]	S
NOEC for other terrestrial species	16	16	[mg.kgdwt-1]	S
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
BIRDS				
LC50 in avian dietary study (5 days)	??	??	[mg.kg-1]	D
NOAEL	??	??	[mg.kg-1.d-1]	D
NOEC via food	??	??	[mg.kg-1]	O
Duration of (sub-)chronic oral test	Chronic	Chronic		D
Conversion factor NOAEL to NOEC	8	8	[kg.d.kg-1]	D

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Name	Reference	Value	Units	Status
MAMMALS				
ACUTE				
Oral LD50	??	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	??	[mg.kg-1]	D
Dermal LD50	??	??	[mg.kg-1]	O
Inhalatory LC50	??	??	[mg.m-3]	O
(SUB)CHRONIC				
Oral NOAEL	30	30	[mg.kg-1.d-1]	O
Oral LOAEL	??	??	[mg.kg-1.d-1]	O
Inhalatory NOAEL	140	140	[mg.m-3]	O
Inhalatory LOAEL	??	??	[mg.m-3]	O
Dermal NOAEL	30	30	[mg.kg-1.d-1]	O
Dermal LOAEL	??	??	[mg.kg-1.d-1]	O
NOEC via food	300	300	[mg.kg-1]	S
LOEC via food	??	??	[mg.kg-1]	D
Duration of (sub-)chronic oral test	90 days	90 days		S
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<6 weeks)	Rattus norvegicus (<6 weeks)		D
Conversion factor NOAEL to NOEC	10	10	[kg.d.kg-1]	O
ENVIRONMENTAL EFFECTS ASSESSMENT				
INTERMEDIATE RESULTS AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
Toxicological data used for extrapolation to PNEC Aqua	0.035	0.035	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	10	10	[-]	O
Toxicological data used for extrapolation to PNEC Aqua	??	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	??	[-]	O
Toxicological data used for extrapolation to PNEC micro	??	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	??	[-]	O
Toxicological data used for extrapolation to PNEC oral	300	300	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	30	30	[-]	O
INTERMEDIATE RESULTS TERRESTRIAL AND SEDIMENT ORGANISMS				
Toxicological data used for extrapolation to PNEC Terr	16	16	[mg.kgdwt-1]	O
Assessment factor applied in extrapolation to PNEC Terr	100	50	[-]	S
Equilibrium partitioning used for PNEC in soil?	No	No		O
Equilibrium partitioning used for PNEC in sediment?	Yes	Yes		O
PNECS FOR AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
PNEC for aquatic organisms	3.5E-03	3.5E-03	[mg.l-1]	O

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Defaults	**Standard**
Assessment types	**1A, 1B, 2**
Base set complete	**No**

Name	Reference	Value	Units	Status
PNECS FOR AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS (Continued)				
PNEC for aquatic organisms, intermittent releases	??	??	[mg.l-1]	O
PNEC for micro-organisms in a STP	??	??	[mg.l-1]	O
PNEC for secondary poisoning of birds and mammals	10	10	[mg.kg-1]	O
PNEC for aquatic organisms with statistical method	??	??	[mg.l-1]	O
PNECS FOR TERRESTRIAL AND SEDIMENT ORGANISMS				
PNEC for terrestrial organisms	0.141	0.282	[mg.kgwwt-1]	O
PNEC for terrestrial organisms with statistical method	??	??	[mg.kgwwt-1]	O
PNEC for sediment-dwelling organisms	3.51	4.25	[mg.kgwwt-1]	O

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Name	Reference	Value	Units	Status
RISK CHARACTERIZATION				
ENVIRONMENTAL EXPOSURE				
LOCAL				
RISK CHARACTERIZATION OF [PRIVATE USE]				
ENVIRONMENTAL				
RCR for the local water compartment	0.795	0.289	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	32.7	0.823	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	8.99	3.27	[-]	O
Extra factor 10 applied to PEC	Yes	Yes		O
RCR for the sewage treatment plant	??	??	[-]	O
PREDATORS				
RCR for fish-eating birds and mammals	2.04	0.0315	[-]	O
RCR for worm-eating birds and mammals	7.14	0.078	[-]	O
REGIONAL				
ENVIRONMENT				
RCR for the regional water compartment	0.0382	0.0129	[-]	O
RCR for the regional soil compartment	13.7	0.407	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the regional sediment compartment	0.754	0.256	[-]	O
Extra factor 10 applied to PEC	Yes	Yes		O

HHCB

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Base set complete	No
Explanation status column	'O' = Output; 'D' = Default; 'S' = Set; 'I' = Imported

Name	Reference	Value	Units	Status
STUDY				
STUDY IDENTIFICATION				
Study name	HHCB	HHCB		S
Study description	environmental risk assessment	environmental risk assessment		S
Author	E. v.d. Plassche	E. v.d. Plassche		S
Institute	RIVM	RIVM		S
Address	PO Box 1	PO Box 1		S
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Calculations checksum	4BE2D9A7	4BE2D9A7		S

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Base set complete	**No**

Name	Reference	Value	Units	Status
DEFAULTS				
DEFAULT IDENTIFICATION				
General name	Standard	Standard		D
Description	According to TGDs	According to TGDs		D
RELEASE ESTIMATION				
Fraction of EU production volume for region	0.1	0.1	[-]	D
Fraction connected to sewer systems	0.7	0.7	[-]	D
CHARACTERISTICS OF COMPARTMENTS				
GENERAL				
Density of solid phase	2.5	2.5	[kg.l-1]	D
Density of water phase	1	1	[kg.l-1]	D
Density of air phase	1.3E-03	1.3E-03	[kg.l-1]	D
Environmental temperature	12	12	[oC]	D
Constant of Junge equation	0.01	0.01	[Pa.m]	D
Surface area of aerosol particles	0.01	0.01	[m2.m-3]	D
Gas constant (8.314)	8.314	8.314	[Pa.m3.mol-1.K-1]	D
SUSPENDED MATTER				
Volume fraction solids in suspended matter	0.1	0.1	[m3.m-3]	D
Volume fraction water in suspended matter	0.9	0.9	[m3.m-3]	D
Weight fraction of organic carbon in suspended matter	0.1	0.1	[kg.kg-1]	D
Wet bulk density of suspended matter	1.15E+03	1.15E+03	[kg.m-3]	O
SEDIMENT				
Volume fraction solids in sediment	0.2	0.2	[m3.m-3]	D
Volume fraction water in sediment	0.8	0.8	[m3.m-3]	D
Weight fraction of organic carbon in sediment	0.05	0.05	[kg.kg-1]	D
Bulk density of sediment	1.3E+03	1.3E+03	[kgwwt.m-3]	O
Conversion factor wet-dry sediment	2.6	2.6	[kgwwt.kgdwt-1]	O
SOIL				
Volume fraction solids in soil	0.6	0.6	[m3.m-3]	D
Volume fraction water in soil	0.2	0.2	[m3.m-3]	D
Volume fraction air in soil	0.2	0.2	[m3.m-3]	D
Weight fraction of organic carbon in soil	0.02	0.02	[kg.kg-1]	D
Bulk density of soil	1.7E+03	1.7E+03	[kgwwt.m-3]	O
Conversion factor wet-dry soil	1.13	1.13	[kgwwt.kgdwt-1]	O
STP SLUDGE				
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D

Name	Reference	Value	Units	Status
DEGRADATION AND TRANSFORMATION RATES				
Concentration of OH-radicals in atmosphere	5E+05	5E+05	[molec.cm-3]	D
Rate constant for abiotic degradation in STP	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk soil	0	0	[d-1]	D
Rate constant for abiotic degradation in bulk sediment	0	0	[d-1]	D
Rate constant for anaerobic biodegradation in sediment	0	0	[d-1]	D
Fraction of sediment compartment that is aerated	0.1	0.1	[m3.m-3]	D
SEWAGE TREATMENT				
GENERAL				
Number of inhabitants feeding one STP	1E+04	1E+04	[eq]	D
Sewage flow	200	200	[l.eq-1.d-1]	D
Effluent discharge rate of local STP	2E+06	2E+06	[l.d-1]	O
Temperature dependency correction	No	No		D
Temperature of air above aeration tank	15	15	[oC]	D
Temperature of water in aeration tank	15	15	[oC]	D
Height of air column above STP	10	10	[m]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Windspeed in the system	3	3	[m.s-1]	D
RAW SEWAGE				
Mass of O2 binding material per person per day	54	54	[g.eq-1.d-1]	D
Dry weight solids produced per person per day	0.09	0.09	[kg.eq-1.d-1]	D
Density solids in raw sewage	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in raw sewage sludge	0.3	0.3	[kg.kg-1]	D
PRIMARY SETTLER				
Depth of primary settler	4	4	[m]	D
Hydraulic retention time of primary settler	2	2	[hr]	D
Density suspended and settled solids in primary settler	1.5	1.5	[kg.l-1]	D
Fraction of organic carbon in settled sewage sludge	0.3	0.3	[kg.kg-1]	D
ACTIVATED SLUDGE TANK				
Depth of aeration tank	3	3	[m]	D
Density solids of activated sludge	1.3	1.3	[kg.l-1]	D
Concentration solids of activated sludge	4	4	[kg.m-3]	D
Steady state O2 concentration in activated sludge	2E-03	2E-03	[kg.m-3]	D
Mode of aeration	Surface	Surface		D
Aeration rate of bubble aeration	1.31E-05	1.31E-05	[m3.s-1.eq-1]	D
Fraction of organic carbon in activated sewage sludge	0.37	0.37	[kg.kg-1]	D
Sludge loading rate	0.15	0.15	[kg.kg-1.d-1]	D
Hydraulic retention time in aerator (9-box STP)	6.9	6.9	[hr]	O
Hydraulic retention time in aerator (6-box STP)	10.8	10.8	[hr]	O
Sludge retention time of aeration tank	9.2	9.2	[d]	O

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Name	Reference	Value	Units	Status
SOLIDS-LIQUIDS SEPARATOR				
Depth of solids-liquid separator	3	3	[m]	D
Density suspended and settled solids in solids-liquid separator	1.3	1.3	[kg.l-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Hydraulic retention time of solids-liquid separator	6	6	[hr]	D
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	[kg.kg-1]	D
REGIONAL AND CONTINENTAL DISTRIBUTION				
CONTINENTAL				
Area of EU	3.56E+06	3.56E+06	[km2]	D
Area of continental system	3.52E+08	3.52E+08	[km2]	O
Number of inhabitants in the EU	3.7E+08	3.7E+08	[eq]	D
Number of inhabitants of continental system	3.5E+08	3.5E+08	[eq]	O
Area fraction of water of the continental system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from global scale to continent	0	0	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of continental system	25	25	[mg.l-1]	D
Residence time of water in system	166	166	[d]	O
Residence time of air in system	6.41	6.41	[d]	O
Net sedimentation rate	2.59	2.59	[mm.yr-1]	O
REGIONAL				
Area of regional system	4E+04	4E+04	[km2]	D
Number of inhabitants of region	2E+07	2E+07	[eq]	D
Area fraction of water of the regional system	0.03	0.03	[-]	D
Area fraction of natural soil	0.6	0.6	[-]	D
Area fraction of agricultural soil	0.27	0.27	[-]	D
Area fraction of industrial/urban soil	0.1	0.1	[-]	D
Fraction of water flow from continental scale to region	0.034	0.034	[-]	D
Water depth of system	3	3	[m]	D
Suspended solids concentration of regional system	15	15	[mg.l-1]	D
Residence time of water in system	40.1	40.1	[d]	O
Residence time of air in system	0.684	0.684	[d]	O
Net sedimentation rate	3.13	3.13	[mm.yr-1]	O
AIR				
Atmospheric mixing height	1000	1000	[m]	D
Windspeed in the system	3	3	[m.s-1]	D
Aerosol deposition velocity	1E-03	1E-03	[m.s-1]	D
Aerosol collection efficiency	2E+05	2E+05	[-]	D
Average annual precipitation	700	700	[mm.yr-1]	D

Name	Reference	Value	Units	Status
WATER AND SEDIMENT				
Concentration biota	1	1	[mg.l-1]	D
Sediment mixing depth	0.03	0.03	[m]	D
Settling velocity of suspended solids	2.5	2.5	[m.d-1]	D
(biogenic) production of suspended solids in water	0	0	[kg.d-1]	D
Sewage flow	200	200	[l.eq-1.d-1]	D
Concentration solids in effluent	30	30	[mg.l-1]	D
Fraction connected to sewer systems	0.7	0.7	[-]	D
SOIL				
Mixing depth natural soil	0.05	0.05	[m]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Mixing depth industrial/urban soil	0.05	0.05	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D
Fraction of rain water running off soil	0.25	0.25	[-]	D
Soil erosion rate of regional system	0.03	0.03	[mm.yr-1]	D
MASS TRANSFER				
Air-film PMTC (air-water interface)	1.39E-03	1.39E-03	[m.s-1]	D
Water-film PMTC (air-water interface)	1.39E-05	1.39E-05	[m.s-1]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Water-film PMTC (sediment-water interface)	2.78E-06	2.78E-06	[m.s-1]	D
Pore water PMTC (sediment-water interface)	2.78E-08	2.78E-08	[m.s-1]	D
LOCAL DISTRIBUTION				
AIR AND SURFACE WATER				
Concentration in air at source strength 1 [kg.d-1]	2.78E-04	2.78E-04	[mg.m-3]	D
Standard deposition flux of aerosol-bound compounds	0.01	0.01	[mg.m-2.d-1]	D
Standard deposition flux of gaseous compounds	4E-04	4E-04	[mg.m-2.d-1]	O
Suspended solids concentration of regional system	15	15	[mg.l-1]	D
Dilution factor	10	10	[-]	D
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	D
Calculate dilution from river flow rate	No	No		D
SOIL				
Mixing depth of grassland soil	0.1	0.1	[m]	D
Dry sludge application rate on agricultural soil	5E+03	5E+03	[kg.ha-1.yr-1]	D
Dry sludge application rate on grassland	1000	1000	[kg.ha-1.yr-1]	D
Averaging time soil (for terrestrial ecosystem)	30	30	[d]	D
Averaging time agricultural soil	180	180	[d]	D
Averaging time grassland	180	180	[d]	D
Air-film PMTC (air-soil interface)	1.39E-03	1.39E-03	[m.s-1]	D
Soil-air PMTC (air-soil interface)	5.56E-06	5.56E-06	[m.s-1]	D
Soil-water film PMTC (air-soil interface)	5.56E-10	5.56E-10	[m.s-1]	D
Mixing depth agricultural soil	0.2	0.2	[m]	D
Fraction of rain water infiltrating soil	0.25	0.25	[-]	D

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Name	Reference	Value	Units	Status
SOIL (Continued)				
Average annual precipitation	700	700	[mm.yr-1]	D
CHARACTERISTICS OF PLANTS AND CATTLE				
PLANTS				
Volume fraction of water in plant tissue	0.65	0.65	[m3.m-3]	D
Volume fraction of lipids in plant tissue	0.01	0.01	[m3.m-3]	D
Volume fraction of air in plant tissue	0.3	0.3	[m3.m-3]	D
Correction for differences between plant lipids and octanol	0.95	0.95	[-]	D
Bulk density of plant tissue (wet weight)	0.7	0.7	[kg.l-1]	D
Rate constant for metabolism in plants	0	0	[d-1]	D
Rate constant for photolysis in plants	0	0	[d-1]	D
Leaf surface area	5	5	[m2]	D
Conductance	1E-03	1E-03	[m.s-1]	D
Shoot volume	2	2	[l]	D
Rate constant for dilution by growth	0.035	0.035	[d-1]	D
Transpiration stream	1	1	[l.d-1]	D
CATTLE				
Daily intake for cattle of grass (dryweight)	16.9	16.9	[kg.d-1]	D
Conversion factor grass from dryweight to wetweight	4	4	[kg.kg-1]	D
Daily intake of soil (dryweight)	0.41	0.41	[kg.d-1]	D
Daily inhalation rate for cattle	122	122	[m3.d-1]	D
Daily intake of drinking water for cattle	55	55	[l.d-1]	D

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Name	Reference	Value	Units	Status
SUBSTANCE				
SUBSTANCE IDENTIFICATION				
General name	HHCB	HHCB		S
Description				D
CAS-No	1222-05-5	1222-05-5		S
EC-notification no.				D
EINECS no.				D
PHYSICO-CHEMICAL PROPERTIES				
Molecular weight	258.4	258.4	[g.mol-1]	S
Melting point	??	??	[oC]	D
Boiling point	??	??	[oC]	D
Vapour pressure at 25 [oC]	0.0727	0.0727	[Pa]	S
Octanol-water partition coefficient.	5.9	5.9	[log10]	S
Water solubility	1.75	1.75	[mg.l-1]	S

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Name	Reference	Value	Units	Status
RELEASE ESTIMATION				
CHARACTERIZATION AND TONNAGE				
High Production Volume Chemical	Yes	Yes		S
Production volume of chemical in EU	0	0	[tonnes.yr-1]	D
Volume of chemical imported to EU	1.482E+03	1.482E+03	[tonnes.yr-1]	S
Volume of chemical exported from EU	0	0	[tonnes.yr-1]	D
Intermittent release	No	No		D
INTERMEDIATE RESULTS PRODUCTION VOLUMES				
Tonnage of substance in Europe	1.48E+03	1.48E+03	[tonnes.yr-1]	O
Regional production volume of substance	0	0	[tonnes.yr-1]	O
Continental production volume of substance	0	0	[tonnes.yr-1]	O
USE PATTERNS				
EMISSION INPUT DATA				
Industry category	5 Personal / domestic use	5 Personal / domestic use		S
Use category	9 Cleaning/washing agents and additives	9 Cleaning/washing agents and additives		S
Emission scenario document available	Yes	Yes		O
Extra details on use category	No extra details necessary	No extra details necessary		D
Extra details on use category	No extra details necessary	No extra details necessary		D
Fraction of tonnage for application	1	1	[-]	O
Fraction of chemical in formulation	1	1	[-]	D
Production	No	No		S
Formulation	No	No		S
Processing	No	No		S
Private use	Yes	Yes		D
Recovery	No	No		S
Main category production	III Multi-purpose equipment	III Multi-purpose equipment		D
Main category formulation	III Multi-purpose equipment	III Multi-purpose equipment		D
Main category processing	III Non-dispersive use	III Non-dispersive use		D
INTERMEDIATE RESULTS				
USE PATTERN 1				
INTERMEDIATE RESULTS TONNAGES PER USE PATTERN				
Relevant tonnage for application	1.48E+03	1.48E+03	[tonnes.yr-1]	O
Regional tonnage of substance	148.2	58.6	[tonnes.yr-1]	S
Continental tonnage of substance	1.33E+03	1.42E+03	[tonnes.yr-1]	O
RELEASE FRACTIONS AND EMISSION DAYS [PRODUCTION]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O

Name	Reference	Value	Units	Status
RELEASE FRACTIONS AND EMISSION DAYS (Continued)				
[PRODUCTION]				
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O
[FORMULATION]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	General table	General table		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	300	300	[-]	O
Source of B-table data	General table	General table		O
[PROCESSING]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	1	1	[-]	O
Source of B-table data	No applicable data found	No applicable data found		O
[PRIVATE USE]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0.99	1	[-]	S
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	1E-02	0	[-]	S
Source of A-table data	Specific IC/UC combination	Specific IC/UC combination		O
Fraction of the main local source	2E-03	2E-03	[-]	O
Number of emission days per year	365	365	[-]	O
Source of B-table data	General table	General table		O
[RECOVERY]				
Fraction of tonnage released to air	0	0	[-]	O
Fraction of tonnage released to waste water	0	0	[-]	O
Fraction of tonnage released to surfacewater	0	0	[-]	O
Fraction of tonnage released to industrial soil	0	0	[-]	O
Source of A-table data	No applicable data found	No applicable data found		O
Fraction of the main local source	0	0	[-]	O
Number of emission days per year	1	1	[-]	O

Name	Reference	Value	Units	Status
[RECOVERY] (Continued)				
Source of B-table data	No applicable data found	No applicable data found		O
CONTINENTAL				
[PRODUCTION]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
[FORMULATION]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
[PROCESSING]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
[PRIVATE USE]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	3.62E+03	3.9E+03	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	36.5	0	[kg.d-1]	O
[RECOVERY]				
Continental release to air	0	0	[kg.d-1]	O
Continental release to waste water	0	0	[kg.d-1]	O
Continental release to surface water	0	0	[kg.d-1]	O
Continental release to industrial soil	0	0	[kg.d-1]	O
REGIONAL				
[PRODUCTION]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
[FORMULATION]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
[PROCESSING]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O

Name	Reference	Value	Units	Status
[PROCESSING] (Continued)				
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
[PRIVATE USE]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	402	161	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	4.06	0	[kg.d-1]	O
[RECOVERY]				
Regional release to air	0	0	[kg.d-1]	O
Regional release to waste water	0	0	[kg.d-1]	O
Regional release to surface water	0	0	[kg.d-1]	O
Regional release to industrial soil	0	0	[kg.d-1]	O
CONTINENTAL				
Total continental emission to air	0	0	[kg.d-1]	O
Total continental emission to wastewater	2.53E+03	2.73E+03	[kg.d-1]	O
Total continental emission to surface water	1.09E+03	1.17E+03	[kg.d-1]	O
Total continental emission to industrial soil	36.5	0	[kg.d-1]	O
Total continental emission to agricultural soil	0	0	[kg.d-1]	O
REGIONAL				
Total regional emission to air	0	0	[kg.d-1]	O
Total regional emission to wastewater	281	112	[kg.d-1]	O
Total regional emission to surface water	121	48.2	[kg.d-1]	O
Total regional emission to industrial soil	4.06	0	[kg.d-1]	O
Total regional emission to agricultural soil	0	0	[kg.d-1]	O
LOCAL				
[PRODUCTION]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[FORMULATION]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[PROCESSING]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D
[PRIVATE USE]				
Local emission to air during episode	0	0	[kg.d-1]	O

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Name	Reference	Value	Units	Status
[PRIVATE USE] (Continued)				
Local emission to wastewater during episode	0.804	0.321	[kg.d-1]	O
Show this step in further calculations	Yes	Yes		O
Intermittent release	No	No		D
[RECOVERY]				
Local emission to air during episode	0	0	[kg.d-1]	O
Local emission to wastewater during episode	0	0	[kg.d-1]	O
Show this step in further calculations	No	No		O
Intermittent release	No	No		D

Name	Reference	Value	Units	Status
DISTRIBUTION				
PARTITION COEFFICIENTS				
SOLIDS WATER PARTITIONING				
Organic carbon-water partition coefficient	7.57479E+04	7.24E+04	[l.kg-1]	S
Solids-water partition coefficient in soil	1.51E+03	1.45E+03	[l.kg-1]	O
Solids-water partition coefficient in sediment	3.79E+03	3.62E+03	[l.kg-1]	O
Solids-water partition coefficient suspended matter	7.57E+03	7.24E+03	[l.kg-1]	O
Solids-water partition coefficient in raw sewage sludge	2.27E+04	2.17E+04	[l.kg-1]	O
Solids-water partition coefficient in settled sewage sludge	2.27E+04	2.17E+04	[l.kg-1]	O
Solids-water partition coefficient in activated sewage sludge	2.8E+04	2.68E+04	[l.kg-1]	O
Solids-water partition coefficient in effluent sewage sludge	2.8E+04	2.68E+04	[l.kg-1]	O
Suspended matter-water partition coefficient	1.89E+03	1.81E+03	[m3.m-3]	O
Soil-water partition coefficient	2.27E+03	2.17E+03	[m3.m-3]	O
Sediment-water partition coefficient	1.89E+03	1.81E+03	[m3.m-3]	O
AIR-WATER PARTITIONING AND ADSORPTION TO AEROSOL PARTICLES				
Sub-cooled liquid vapour pressure	0.0727	0.0727	[Pa]	O
Fraction of chemical associated with aerosol particles	1.37E-03	1.37E-03	[-]	O
Henry's law constant	10.7	10.7	[Pa.m3.mol-1]	O
Air-water partitioning coefficient	4.53E-03	4.53E-03	[m3.m-3]	O
BIOTA-WATER				
Bioconcentration factor for aquatic biota	2.07E+04	2.07E+04	[l.kg-1]	O
DEGRADATION AND TRANSFORMATION RATES				
CHARACTERIZATION AND STP				
Characterization of biodegradability	Not biodegradable	Not biodegradable		D
Degradation calculation method in STP	First order, standard OECD/EU tests	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	0	[d-1]	O
Total rate constant for degradation in STP	0	0	[d-1]	O
Maximum growth rate of specific microorganisms	2	2	[d-1]	D
Half saturation concentration	0.5	0.5	[g.m-3]	D
ENVIRONMENTAL				
Specific degradation rate constant with OH-radicals	0	0	[cm3.molec-1.s-1]	D
Rate constant for degradation in air	0	0	[d-1]	O
Rate constant for hydrolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for photolysis in surface water	6.93E-07	6.93E-07	[d-1]	O
Rate constant for biodegradation in surface water	0	0	[d-1]	O
Total rate constant for degradation in bulk surface water	1.39E-06	1.39E-06	[d-1]	O
Rate constant for biodegradation in bulk soil	6.93E-07	6.93E-07	[d-1]	O

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Name	Reference	Value	Units	Status
ENVIRONMENTAL (Continued)				
Total rate constant for degradation in bulk soil	6.93E-07	6.93E-07	[d-1]	O
Rate constant for biodegradation in aerated sediment	6.93E-07	6.93E-07	[d-1]	O
Total rate constant for degradation in bulk sediment	6.93E-08	6.93E-08	[d-1]	O
SEWAGE TREATMENT				
CONTINENTAL				
Fraction of emission directed to air	0.0124	0.0129	[-]	O
Fraction of emission directed to water	0.155	0.158	[-]	O
Fraction of emission directed to sludge	0.833	0.829	[-]	O
Fraction of the emission degraded	0	0	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	31.4	35.2	[kg.d-1]	O
Indirect emission to surface water	392	431	[kg.d-1]	O
Indirect emission to agricultural soil	2.10908E+03	151	[kg.d-1]	S
REGIONAL				
Fraction of emission directed to air	0.0145	0.0151	[-]	O
Fraction of emission directed to water	0.154	0.157	[-]	O
Fraction of emission directed to sludge	0.832	0.828	[-]	O
Fraction of the emission degraded	0	0	[-]	O
Total of fractions	1	1	[-]	O
Indirect emission to air	4.07	1.69	[kg.d-1]	O
Indirect emission to surface water	43.3	17.6	[kg.d-1]	O
Indirect emission to agricultural soil	234.027	6.2	[kg.d-1]	S
LOCAL				
[PRIVATE USE]				
INPUT AND CONFIGURATION [PRIVATE USE]				
Use or bypass STP	Use STP	Use STP		D
Local emission to wastewater during episode	0.804	0.321	[kg.d-1]	O
Concentration in untreated wastewater	0.402	0.161	[mg.l-1]	O
Local emission entering the STP	0.804	0.321	[kg.d-1]	O
Type of local STP	With primary settler (9-box)	With primary settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	1E+04	[eq]	O
Effluent discharge rate of this STP	2E+06	2E+06	[l.d-1]	O
Calculate dilution from river flow rate	No	No		O
Flow rate of the river	1.8E+04	1.8E+04	[m3.d-1]	O
Dilution factor	10	10	[-]	D
OUTPUT [PRIVATE USE]				
Fraction of emission directed to air by STP	0.0153	0.0159	[-]	O
Fraction of emission directed to water by STP	0.153	0.156	[-]	O
Fraction of emission directed to sludge by STP	0.831	0.828	[-]	O
Fraction of the emission degraded in STP	0	0	[-]	O
Total of fractions	1	1	[-]	O
Local indirect emission to air from STP during episode	0.0123	5.11E-03	[kg.d-1]	O

Name	Reference	Value	Units	Status
OUTPUT [PRIVATE USE] (Continued)				
Concentration in untreated wastewater	0.402	0.161	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.0617	0.0251	[mg.l-1]	O
Concentration in effluent exceeds solubility	No	No		O
Concentration in dry sewage sludge	845.991	23	[mg.kg-1]	S
PEC for micro-organisms in the STP	0.0617	0.0251	[mg.l-1]	O
CONTINENTAL AND REGIONAL				
CONTINENTAL				
Continental PEC in surface water (total)	5.21E-05	4.47E-05	[mg.l-1]	O
Continental PEC in surface water (dissolved)	4.31E-05	3.72E-05	[mg.l-1]	O
Continental PEC in air (total)	5.96E-06	2.96E-06	[mg.m-3]	O
Continental PEC in agricultural soil (total)	0.81	0.0572	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	6.06E-04	4.47E-05	[mg.l-1]	O
Continental PEC in natural soil (total)	3.61E-03	1.72E-03	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	0.0439	1.72E-03	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	0.125	0.103	[mg.kgwwt-1]	O
REGIONAL				
Regional PEC in surface water (total)	4.07E-04	1.35E-04	[mg.l-1]	O
Regional PEC in surface water (dissolved)	3.59E-04	1.2E-04	[mg.l-1]	O
Regional PEC in air (total)	1.12E-05	3.96E-06	[mg.m-3]	O
Regional PEC in agricultural soil (total)	7.89	0.203	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	5.9E-03	1.59E-04	[mg.l-1]	O
Regional PEC in natural soil (total)	6.79E-03	2.3E-03	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	0.401	2.3E-03	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	1.04	0.33	[mg.kgwwt-1]	O
LOCAL				
REMOVAL RATE CONSTANTS SOIL				
Total rate constant for degradation in bulk soil	6.93E-07	6.93E-07	[d-1]	O
Rate constant for volatilisation from agricultural soil	4.87E-06	5.1E-06	[d-1]	O
Rate constant for volatilisation from grassland soil	9.75E-06	1.02E-05	[d-1]	O
Rate constant for leaching from agricultural soil	1.05E-06	1.1E-06	[d-1]	O
Rate constant for leaching from grassland soil	2.11E-06	2.21E-06	[d-1]	O
Total rate constant for removal from agricultural top soil	6.62E-06	6.9E-06	[d-1]	O
Total rate constant for removal from grassland top soil	1.26E-05	1.31E-05	[d-1]	O
[PRIVATE USE]				
LOCAL CONCENTRATIONS AND DEPOSITIONS [PRIVATE USE]				
Concentration in air during emission episode	3.41E-06	1.42E-06	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	3.41E-06	1.42E-06	[mg.m-3]	O
Total deposition flux during emission episode	5.07E-06	2.11E-06	[mg.m-2.d-1]	O
Annual average total deposition flux	5.07E-06	2.11E-06	[mg.m-2.d-1]	O

Name	Reference	Value	Units	Status
[PRIVATE USE] (Continued)				
LOCAL CONCENTRATIONS AND DEPOSITIONS [PRIVATE USE]				
Concentration in surface water during emission episode	5.54E-03	2.27E-03	[mg.l-1]	O
Annual average concentration in surface water	5.54E-03	2.27E-03	[mg.l-1]	O
Concentration in agric. soil averaged over 30 days	12.3	0.334	[mg.kgwwt-1]	O
Concentration in agric. soil averaged over 180 days	12.3	0.334	[mg.kgwwt-1]	O
Concentration in grassland averaged over 180 days	4.87	0.132	[mg.kgwwt-1]	O
Fraction of steady-state (agricultural soil)	0.0239	0.0249	[-]	O
Fraction of steady-state (grassland soil)	0.0448	0.0467	[-]	O
LOCAL PECS [PRIVATE USE]				
Annual average local PEC in air (total)	1.46E-05	5.38E-06	[mg.m-3]	O
Local PEC in surface water during emission episode	5.9E-03	2.38E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	5.9E-03	2.38E-03	[mg.l-1]	O
Local PEC in sediment during emission episode	9.72	3.76	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	12.3	0.337	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	12.3	0.336	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	4.88	0.135	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	9.21E-03	2.63E-04	[mg.l-1]	O
Local PEC in pore water of grassland	3.65E-03	1.05E-04	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	9.21E-03	2.63E-04	[mg.l-1]	O

EUSES Full report	**Single substance**
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Name	Reference	Value	Units	Status
EXPOSURE				
BIOCONCENTRATION FACTORS				
Partition coefficient worm-porewater	3.17731E+04	7.9E+03	[l.kg-1]	S
Bioconcentration factor for earthworms	23.8	6.18	[kg.kg-1]	O
Bioconcentration factor for fish	2.06538E+04	1.584E+03	[l.kg-1]	S
Partition coefficient between plant tissue and water	4.03E+03	4.03E+03	[m3.m-3]	O
Partition coefficient between leaves and air	8.89E+05	8.89E+05	[m3.m-3]	O
Transpiration-stream concentration factor	0.0378	0.0378	[-]	O
Bioaccumulation factor for meat	0.02	0.02	[d.kg-1]	O
Bioaccumulation factor for milk	6.31E-03	6.31E-03	[d.kg-1]	O
Purification factor for surface water	0.25	0.25	[-]	O
SECONDARY POISONING				
SECONDARY POISONING [PRIVATE USE]				
Concentration in fish from surface water for predators	64.6	1.98	[mg.kg-1]	O
Local concentration in earthworms from agricultural soil	240	1.67	[mg.kg-1]	O

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Name	Reference	Value	Units	Status
EFFECTS				
INPUT OF EFFECTS DATA				
MICRO-ORGANISMS				
EC50 for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
EC10 for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
NOEC for micro-organisms in a STP	??	??	[mg.l-1]	D
Specific bacterial population?	No	No		D
AQUATIC ORGANISMS				
LC50 for fish	??	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	??	[mg.l-1]	D
EC50 for algae	??	??	[mg.l-1]	D
LC50 for other aquatic species	??	??	[mg.l-1]	D
Species	other	other		D
NOEC for fish	0.068	0.068	[mg.l-1]	S
NOEC for Daphnia	0.11	0.11	[mg.l-1]	S
NOEC for algae	0.2	0.2	[mg.l-1]	S
NOEC for other aquatic species	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
Additional aquatic NOEC	??	??	[mg.l-1]	D
TERRESTRIAL ORGANISMS				
LC50 for plants	??	??	[mg.kgwwt-1]	D
LC50 for earthworms	??	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	??	[mg.kgwwt-1]	D
Species	other	other		D
NOEC for plants	??	??	[mg.kgwwt-1]	D
NOEC for earthworms	16	16	[mg.kgdwt-1]	S
NOEC for microorganisms	??	??	[mg.kgwwt-1]	D
NOEC for other terrestrial species	16	16	[mg.kgdwt-1]	S
NOEC for other terrestrial species	16	16	[mg.kgdwt-1]	S
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
Additional terrestrial NOEC	??	??	[mg.kgwwt-1]	D
BIRDS				
LC50 in avian dietary study (5 days)	??	??	[mg.kg-1]	D
NOAEL	??	??	[mg.kg-1.d-1]	D
NOEC via food	??	??	[mg.kg-1]	O
Duration of (sub-)chronic oral test	Chronic	Chronic		D
Conversion factor NOAEL to NOEC	8	8	[kg.d.kg-1]	D

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Name	Reference	Value	Units	Status
MAMMALS				
ACUTE				
Oral LD50	??	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	??	[mg.kg-1]	D
Dermal LD50	??	??	[mg.kg-1]	O
Inhalatory LC50	??	??	[mg.m-3]	O
(SUB)CHRONIC				
Oral NOAEL	300	300	[mg.kg-1.d-1]	O
Oral LOAEL	??	??	[mg.kg-1.d-1]	O
Inhalatory NOAEL	1.4E+03	1.4E+03	[mg.m-3]	O
Inhalatory LOAEL	??	??	[mg.m-3]	O
Dermal NOAEL	300	300	[mg.kg-1.d-1]	O
Dermal LOAEL	??	??	[mg.kg-1.d-1]	O
NOEC via food	3E+03	3E+03	[mg.kg-1]	S
LOEC via food	??	??	[mg.kg-1]	D
Duration of (sub-)chronic oral test	90 days	90 days		S
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<6 weeks)	Rattus norvegicus (<6 weeks)		D
Conversion factor NOAEL to NOEC	10	10	[kg.d.kg-1]	O
ENVIRONMENTAL EFFECTS ASSESSMENT				
INTERMEDIATE RESULTS AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
Toxicological data used for extrapolation to PNEC Aqua	0.068	0.068	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	10	10	[-]	O
Toxicological data used for extrapolation to PNEC Aqua	??	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	??	[-]	O
Toxicological data used for extrapolation to PNEC micro	??	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	??	[-]	O
Toxicological data used for extrapolation to PNEC oral	3E+03	3E+03	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	30	30	[-]	O
INTERMEDIATE RESULTS TERRESTRIAL AND SEDIMENT ORGANISMS				
Toxicological data used for extrapolation to PNEC Terr	14.1	14.1	[mg.kgwwt-1]	O
Assessment factor applied in extrapolation to PNEC Terr	100	50	[-]	S
Equilibrium partitioning used for PNEC in soil?	No	No		O
Equilibrium partitioning used for PNEC in sediment?	Yes	Yes		O
PNECS FOR AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS				
PNEC for aquatic organisms	6.8E-03	6.8E-03	[mg.l-1]	O

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Name	Reference	Value	Units	Status
PNECS FOR AQUATIC ORGANISMS, MICRO-ORGANISMS AND PREDATORS (Continued)				
PNEC for aquatic organisms, intermittent releases	??	??	[mg.l-1]	O
PNEC for micro-organisms in a STP	??	??	[mg.l-1]	O
PNEC for secondary poisoning of birds and mammals	100	100	[mg.kg-1]	O
PNEC for aquatic organisms with statistical method	??	??	[mg.l-1]	O
PNECS FOR TERRESTRIAL AND SEDIMENT ORGANISMS				
PNEC for terrestrial organisms	0.141	0.282	[mg.kgwwt-1]	O
PNEC for terrestrial organisms with statistical method	??	??	[mg.kgwwt-1]	O
PNEC for sediment-dwelling organisms	9.91	9.47	[mg.kgwwt-1]	O

Printed on	**8/26/97 4:34:31 PM**
Study	**HHCB**
Substance	**HHCB**
Defaults	**Standard**
Assessment types	**1A, 1B, 2**
Base set complete	**No**

Name	Reference	Value	Units	Status
RISK CHARACTERIZATION				
ENVIRONMENTAL EXPOSURE				
LOCAL				
RISK CHARACTERIZATION OF [PRIVATE USE]				
ENVIRONMENTAL				
RCR for the local water compartment	0.867	0.351	[-]	O
Intermittent release	No	No		D
RCR for the local soil compartment	87.2	1.19	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the local sediment compartment	9.8	3.96	[-]	O
Extra factor 10 applied to PEC	Yes	Yes		O
RCR for the sewage treatment plant	??	??	[-]	O
PREDATORS				
RCR for fish-eating birds and mammals	0.646	0.0198	[-]	O
RCR for worm-eating birds and mammals	2.4	0.0167	[-]	O
REGIONAL				
ENVIRONMENT				
RCR for the regional water compartment	0.0528	0.0176	[-]	O
RCR for the regional soil compartment	55.9	0.719	[-]	O
Extra factor 10 applied to PEC	No	No		O
RCR for the regional sediment compartment	1.05	0.348	[-]	O
Extra factor 10 applied to PEC	Yes	Yes		O

Appendix 2 Use of detergents and cosmetics in Europe (3 pages)

In the tables below the use of detergents and cosmetics in Europe is presented based on information from:

- A.I.S.E. (1996). 1994/1995 statistical tables.
- Colipa (1996). The European cosmetic, toiletry & perfumery market 1995. The European Cosmetic Toiletry and Perfumery Association.

				fabric washing		hard (household)		fabric washing		fabric washing -		fabric rinsing				machine dish		surface cleaning -	
country	inhabitants	toilet soaps		powders		soaps		liquids		auxiliary products		products		hand dish cleaning		cleaning		general purpose	
	million	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita
Belgium and Luxemburg	10.50	5.40	0.51	96.00	9.14	0.40	0.04	13.00	1.24	3.10	0.30	21.00	2.00	460.00	4.38	included in hand dish		32.20	3.07
Denmark	5.20	1.70	0.33	27.10	5.20	na	na	4.10	0.79	3.00	0.58	10.00	1.92	6.00	1.15	3.40	0.65	5.10	0.97
Germany	81.50	30.00	0.37	610.60	7.47	1.70	0.02	30.10	0.37	6.80	0.08	140.30	1.72	117.00	1.43	54.20	0.66	72.00	0.88
Spain	39.70	11.10	0.28	503.60	**12.67**	5.90	0.15	32.00	0.81	na	na	300.00	**7.55**	200.00	**5.03**	16.00	0.40	125.00	3.15
France	58.00	56.70	0.97	572.90	9.83	11.70	0.20	144.80	2.49	na	na	142.70	2.45	110.20	1.89	56.60	0.97	152.40	2.62
Greece	10.40	4.60	0.44	87.30	8.33	1.00	0.10	1.70	**0.16**	5.80	0.55	24.80	2.37	29.70	2.83	2.70	**0.26**	21.10	2.01
Ireland	3.50	2.60	0.74	29.90	8.54	0.30	0.09	3.60	1.03	0.10	**0.03**	7.20	2.06	6.80	1.94	1.80	0.51	4.20	1.20
Italy	57.10	47.10	0.82	450.20	7.86	21.00	0.37	149.80	**2.62**	39.50	0.69	178.10	3.11	257.00	4.49	29.00	0.51	167.40	2.92
Netherlands	15.30	12.30	0.80	106.50	6.90	0.60	0.04	14.00	0.91	1.40	0.09	24.30	1.58	30.70	1.99	9.60	0.62	23.60	1.53
Norway	4.30	3.10	0.72	21.20	4.85	0.10	**0.02**	na	na	na	na	14.70	3.36	5.70	1.30	3.60	0.82	9.90	2.28
Austria	7.70	3.10	0.39	57.50	7.28	0.80	0.10	3.70	0.47	2.10	0.27	17.00	2.15	9.60	1.22	6.30	0.80	4.60	0.58
Portugal	9.90	19.10	**1.91**	110.60	11.12	28.40	**2.85**	2.40	0.24	5.40	0.55	4.80	**0.48**	34.20	3.43	3.30	0.33	40.20	**4.04**
Schwitzerland	7.00	1.70	**0.24**	58.70	8.31	3.80	0.54	10.40	1.47	18.10	**2.56**	6.20	0.88	15.40	2.18	20.20	**2.86**	7.80	1.11
Finland	5.10	1.60	0.31	16.40	**3.20**	na	na	1.90	0.37	0.60	0.12	5.30	1.04	56.00	**1.09**	4.10	0.80	5.50	1.07
Sweden	8.80	na	na	33.70	3.81	na	na	6.80	0.77	na	na	15.40	1.74	113.00	1.28	6.40	0.72	7.90	0.89
UK	58.20	49.60	0.85	440.90	7.55	0.90	0.02	137.60	2.36	8.80	0.15	199.80	3.42	159.60	2.73	31.40	0.54	37.30	**0.64**
total per capita			9.68		122.06		4.54		16.10		5.97		37.83		38.36		11.45		28.96
total volume or mean per capita		249.70	0.65	3223.10	7.63	76.60	0.35	555.90	1.07	94.70	0.50	1111.60	2.36	1610.90	2.40	248.60	0.76	716.20	1.81
fraction of total volume		0.03		0.38		0.01		0.07		0.01		0.13		0.19		0.03		0.08	
total volume	8481.40	ktonnes																	
maximum/minimum			7.96		3.96		142.50		16.38		85.33		15.73		4.61		10.77		6.31
maximum/mean			2.96		1.66		8.16		2.44		5.15		3.19		2.10		3.75		2.23
mean/minimum			2.69		2.38		1.57		6.71		16.58		4.93		2.20		2.94		2.83
minimum and maximum are printed in bold																			
na = not available																			

surface cleaning -		surface cleaning -		surface cleaning -				
lavatory cleaners		special purpose		scourers		total		country
kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	kilotonnes	per capita	
na	na	1.70	0.16	11.80	**1.12**	230.60	21.96	Belgium and Luxemburg
2.30	0.44	na	na	0.50	0.09	63.20	12.12	Denmark
60.00	**0.73**	28.00	0.34	28.60	0.35	1179.30	14.42	Germany
17.60	0.44	na	na	12.20	0.31	1223.40	**30.79**	Spain
na	na	94.10	**1.60**	47.70	0.82	1389.80	23.85	France
na	na	9.10	0.87	3.80	0.36	191.60	18.28	Greece
1.90	0.54	2.70	0.77	0.40	0.11	61.50	17.56	Ireland
19.30	0.34	56.50	0.98	47.40	0.82	1462.30	25.53	Italy
included special purpose		10.40	0.67	9.30	0.60	242.70	15.73	Netherlands
0.00	**0.00**	5.30	1.22	1.70	0.39	65.30	14.96	Norway
5.50	0.70	5.50	0.70	4.20	0.53	119.90	15.19	Austria
0.90	**0.09**	4.20	0.42	8.60	0.86	262.10	26.32	Portugal
na	na	8.00	1.13	4.00	0.56	154.30	21.84	Schwitzerland
0.50	0.10	1.50	0.30	0.10	**0.02**	43.10	**8.42**	Finland
1.40	0.16	1.30	**0.15**	1.30	0.15	85.50	9.67	Sweden
25.90	0.44	22.80	0.39	26.10	0.45	1140.70	19.54	UK
	3.98		9.70		7.54		296.18	total per capita
135.30	0.36	251.10	0.69	207.70	0.47	7915.30	18.51	total volume or mean per capita
0.02		0.03		0.02				fraction of total volume
								total volume
	8.11		10.67		56.00		3.66	maximum/minimum
	2.02		2.31		2.38		1.66	maximum/mean
	4.02		4.62		23.56		2.20	mean/minimum
								minimum and maximum are printed in bold
								na = not available

	perfumes		decorative		skin		hair					
country	& fragrances		cosmetics		care		care		toiletries		total	
	ECU RSP	per capita	ECU RSP	per capita	ECU RSP	per capita	ECU RSP	per capita	ECU RSP	per capita	ECU RSP	per capita
Germany	1.28	15.72	0.72	**15.72**	1.95	8.85	2.45	23.91	2.73	30.09	9.13	94.28
France	1.52	**26.19**	0.83	14.34	1.81	**31.17**	1.68	28.95	1.42	24.53	7.26	**125.19**
UK	0.65	11.12	0.71	12.20	0.79	13.57	1.23	21.13	1.51	26.00	4.89	84.02
Italy	0.54	9.53	0.63	10.95	1.11	19.44	1.12	19.65	1.34	23.45	4.74	83.01
Spain	0.74	18.51	0.20	**5.06**	0.63	15.77	0.73	18.41	0.68	17.05	2.97	74.81
Netherlands	0.22	14.51	0.15	9.93	0.34	22.42	0.45	29.08	0.46	30.20	1.62	106.14
Belgium and Luxemburg	0.20	19.05	0.14	13.43	0.22	21.33	0.37	**35.52**	0.20	18.67	1.13	108.00
Austria	0.07	8.44	0.07	8.96	0.16	21.30	0.26	33.64	0.29	**38.05**	0.85	110.39
Greece	0.12	11.44	0.07	6.35	0.20	19.04	0.22	21.54	0.13	**12.69**	0.74	71.06
Sweden	0.06	6.36	0.09	10.00	0.11	12.61	0.17	19.09	0.19	21.59	0.61	69.66
Portugal	0.14	14.14	0.03	2.63	0.10	9.70	0.18	17.88	0.17	16.67	0.60	**61.01**
Finland	0.03	5.10	0.06	11.37	0.10	20.00	0.18	34.31	0.11	21.76	0.47	92.55
Denmark	0.02	**3.85**	0.03	5.19	0.03	**6.54**	0.11	21.35	0.17	31.73	0.36	68.65
Ireland	0.05	13.43	0.05	14.00	0.05	15.14	0.05	**15.43**	0.11	30.57	0.31	88.57
total ECU or per capita	5.62	177.38	3.77	140.13	7.61	236.88	9.20	339.90	9.50	343.05		1237.35
mean per capita		12.67		10.01		16.92		24.28		24.50		88.38
maximum/minimum		6.81		3.10		4.77		2.30		3.00		2.05
maximum/mean		2.07		1.57		1.84		1.46		1.55		1.42
mean/minimum		3.29		1.98		2.59		1.57		1.93		1.45
minimum and maximum are printed in bold												

Appendix 3 Analytics for AHTN and HHCB

reference	phase	extraction	detection	detection limit
Eschke, 1994 and Eschke, 1995	surface water	C_{18}-solid phase/acetone elution	GC/MS: DB5 and HT8 columns	0.03 µ g/l, 10 µ g/kg ww
	sewage water	n-hexane extraction		
	fish tissue	soxhlet extraction with hexane cyclohexane/ethylacetate elution cleanup: GPC and silicagel		
Van Dijk, 1996a and b	water	dichloromethane/ethylacetate	TLC: UV (254 nm), qualitative detection HPLC: lichrocart and lichrospher RP18 Baker columns UV (254 nm)	
	fish tissue	homogenate extraction in acetonitrile and acetonitrile/methanol soxhlet extraction with methanol methanol elution		
	water, organic phases	diluted in scintillation fluid	LSC	1.2-1.7 ppb
	silicagel from TLC spots	in acetonitrile/acetone		6.8 ppb
	fish tissue	homogenates solubilised in Soluene 350		
Verbruggen, 1997	water, effluent	empore disk extraction without depletion	direct injection in GC/MS	lower than 0.0006 µg/l

reference	phase	extraction	detection	detection limit
Breukel en Balk, 1996	suspended solids	freeze-dried samples, soxtec boiling, soxtec extraction with hexane/acetone,	GC/MS (SIM mode)	0.05 mg/kg
	water	solid-phase extraction (XAD)/dichloromethane elution	GC/MS	0.01 µg/l
Omegam, 1997	sludge	fresh samples, extraction with dichloromethane, dried and concentrated	GC/MS (SIM mode)	lower limits for reporting: 1 mg/kg

Appendix 4 Mass balances for metabolites in BCF studies

AHTN

The curves in figures 6 and 7 of the BCF study report (Van Dijk, 1996a) allows estimation of the rate at which the total radioactivity expressed as parent compound concentrations in tissue, decreases after termination of the dosing at day 28. This "loss" is 0.3 mg/kg/day from an average level of 2 mg/kg and 2.5 mg/kg/day from an average level of 21 mg/kg for the low and high dose, respectively. If the "loss" is multiplied with the average fish to water loading rate given in the report (0.12 g/l/day), the nominal concentration in the water leaving the system can be calculated. This figure can be compared to the concentration of polar metabolite in the water averaged for the 28 days exposure period (Van Dijk, 1996a: Tables 11 and 12) which is calculated from the percentage parent material and the dose level.

Concentration	nominal concentration in water by loss of parent compound from tissue	measured concentration of metabolite on average
0.99 μg/l	0.036 μg/l	0.059 μg/l
9.81 μg/l	0.3 μg/l	0.8 μg/l

It can be concluded that the concentrations of polar metabolite exceed the loss of total radioactivity from the tissue. From the beginning of the exposure, the daily amount of metabolite leaving the system is about 25 to 32 % of the average radioactivity present in the tissue. Thus the parent substance is metabolised with a turnover rate of about one third per day. Fluctuations in percentage metabolite in the water may be caused by fluctuations of fish loading as a combined result of growth, sampling and mortality. The high turnover rate with formation of polar metabolites explains the presence of metabolite in fish tissue (up to 50 %), but fractions of metabolites in tissue cannot be used for mass balance calculation.

Impurities

Although purity of the test material was high according to TLC, HPLC measurements indicated about 20% impurities with HPLC detection times similar to those of the parent substance. These impurities may be homologues that behave rather similar in the total extraction procedure. The variable high percentage of metabolite F3 in edible and non-edible tissue (from 33 up to 60%) clearly behaves differently in TLC and HPLC as compared to the parent substance and impurities, see figure 2 and 40 in the study report (Van Dijk, 1996a).

HHCB

The curves in figures 6 and 7 of the BCF study report (Van Dijk, 1996b) allows an estimation of the rate at which total radioactivity expressed as parent compound leaves the tissue after termination of the exposure at day 28. This "loss" is 0.33 mg/kg/day from an average level of 2 mg/kg for the low dose and 2.5 mg/kg/day from an average level of 23 mg/kg for the high dose. If the "loss" is multiplied with the average fish to water loading rate given in the report (0.4 g fish /liter/day), the nominal concentration in the water leaving the system can be calculated. This figure can be compared to the measured concentration of polar metabolite in the water, averaged for the 28 day exposure period (Van Dijk: 1996b, Tables 12 and 13).

Test concentration	nominal concentration in water by loss of parent compound from tissue	measured concentration of metabolite on average
0.91 µg/l	0.132 µg/l	0.097 µg/l
8.84 µg/l	1.0 µg/l	1.03 µg/l

It can be concluded that the concentrations of metabolite roughly match the fast loss of radioactivity from the tissue. During the 28 days of exposure the parent substance is metabolised with a turnover rate of about one third per day. Fluctuations of percentage metabolite in water may be caused by fluctuations of fish loading as a combined result of growth, sampling and mortality. This high turnover rate with formation of polar metabolites explains the presence of metabolite in the tissues, although the fractions of metabolite in tissues (20 to 30 % of total radioactivity) cannot be used for mass balance calculations.

BCF_{total} versus BCF_{parent}

The BCF is based on average plateau levels in fish (days 21 and 28) and in water (day 7,14,21,28): $BCF = C_{fish} / C_{water}$. The average level of the parent substance in total fish is 83% of the total radioactivity, whereas the average level of the parent substance in water is 85%. This explains, in spite of the high metabolic rate, the minor difference between BCF_{total} of 1624 and BCF_{parent} of 1584 for HHCB.

Appendix 5 Partial mass balance for the Sewage Treatment Plant

A tentative mass balance was made for the amounts of AHTN and HHCB in the *digested sludge process* based on the operation characteristics of STPs (data for 1991). It should be remarked that this is an indication based on *mean* measured concentrations and *mean* values for operation characteristics for all sewage treatment plants in The Netherlands. Moreover, elimination in the activated sludge tank due to degradation or evaporation is neglected.

Production of activated sludge 40 g/day per i.e. (Table 4.4 in CBS, 1993).
Production of digested sludge 37 g/day per i.e. (Table 4.10 in CBS, 1993).
Efficiency of sludge digestion: 36% (Table 4.6 in CBS, 1993).

With the efficiency and amount of digested sludge, the sum of primary plus activated sludge can be calculated: 37/0.64 = 58 g/day per i.e. This implies that the amount of primary sludge is 18 g/day per i.e. In April 1997 samples were taken in six STPs in The Netherlands. This was a dry weather period. Samples were grab samples of the primary sludge, the secondary sludge and the digested sludge. Each STP was sampled twice with a one week interval.

The incoming and outgoing streams in a sludge composting facility was sampled during three consecutive weeks. The efficiency of the composting process is 12%. The results were not included in the mass balance below. However, they were included in the overall estimation of the concentration of sludge deposited on land, see Table 14, which was used for the estimation of PEC_{soil}.

Mean concentrations in sludges of the 6 STPs are:

	production per i.e. [g/d]	AHTN [mg/kg]	HHCB [mg/kg]
primary sludge (C_{prim})	18	8.6	13.9
activated sludge (C_{act})	40	16	27.6
digested sludge (C_{dig})	37	12.8	20.3

The input of AHTN per i.e. in the STP is $0.018*C_{prim} + 0.040*C_{act} = 0.795$ mg/d.
The output per i.e. is $0.037*C_{dig} = 0.474$ mg/d.
The removal of AHTN is estimated as (0.795-0.474)/0.795 * 100% = 40%.

The input of HHCB per i.e. in the STP is $0.018*C_{prim} + 0.040*C_{act} = 1.354$ mg/d.
The output per i.e. is $0.037*C_{dig} = 0.751$ mg/d.
The removal of HHCB is estimated as (1.354-0.751)/1.354 * 100% = 45%.