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Environmental Exposure Assessment

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ECETOC

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European Centre for Ecotoxicology
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ENVIRONMENTAL EXPOSURE ASSESSMENT

CONTENTS

SUMMARY

In ECETOC Technical Report No. 51 (ECETOC, 1993) a process for the Environmental Risk Assessment of Substances was described which is applicable to all substances, whether new or existing, and to all environmental compartments. The scheme generally follows a stepwise approach in which, if necessary, increasingly refined estimates of the Predicted Environmental Concentrations (PECs) and the Predicted No-Effect Concentrations (PNECs) can be compared in stages.

A number of steps in the overall process could at the time not be described in detail. The main objective of the work presented in this report was to provide more detailed information on how to perform an assessment of environmental exposure on a regional and on a local scale.

Mathematical distribution and fate models are required in the screening and confirmatory phases of environmental exposure assessment. Sensitivity analyses and a critical review of parameters have shown that regional generic fugacity models of the "Mackay level III" type are, in principle, a suitable tool for performing risk characterisation on a regional scale. The model used and partly described in this report is HAZCHEM; the full description can be found in ECETOC (1994b). Such models can be used to point at environmental compartments of concern in a qualitative manner. For chemicals mainly released via diffuse sources, they may also be used quantitatively, provided that the amounts emitted into the environment can be estimated with a sufficient degree of accuracy. The model published by Mackay *et al* (1992) was used as a basis and was adapted to represent a generic European geographic scenario.

To calculate environmental concentrations in local scenarios, approaches for the water, soil and air compartments are proposed. For the water compartment the discharge (direct or via a WWTP) into a river can adequately be modelled with RIVMODEL which is included in the HAZCHEM package. Two scenarios have been proposed, a lowland river scenario with low flow rate and a mountain area river scenario with higher flow rate. A scenario for local air and soil modelling is presented which includes the most relevant exposure routes. Details on indirect human exposure are given in ECETOC (1994a).

Reliable data on release and emission of a substance are the key elements for the calculation of realistic PECs for the different environmental compartments. In the majority of cases release of a substance is determined by the process involved including dedicated treatment and not by the physico-chemical data of the substance. Emission estimation requires scenarios which cover

release, elimination and dilution processes. As could be demonstrated for e.g. chemical intermediates, it is important to use process-oriented release data, to consider all dilution processes (internal and external) and to use reliable elimination data e.g. in a biological waste water treatment plant. For emission scenarios default values for process data, elimination and dilution should be given which cover an average (generic) situation and which can be overwritten when substance-specific data are available. Using only worst case data would lead to unrealistically high PECs.

Furthermore, for the calculation of PECs information on the kinetics of primary biodegradation (degradation of the parent compound) is needed. It is difficult or almost impossible to derive kinetic biodegradation data directly from simple screening tests on ready biodegradation as they are normally available at base set level of the notification of new chemicals. Since ready biodegradation tests are based on the measurement of ultimate biodegradation, no direct correlation between the results from these tests and primary biodegradation exists. Therefore - as a first step - default half-life times/rate constants have to be assigned to substances according to the results obtained in screening tests.

For the prediction of biodegradation rates in the waste water treatment plant a tiered approach including three steps is proposed, whereby steps 2 and 3 are required only if the PEC needs to be refined. At the screening phase a default rate constant of 3 h^{-1} can be assigned to ready biodegradable compounds and to those which reached the corresponding pass level after acclimatisation. At the confirmatory phase rate constants should be directly determined from measurement of primary biodegradation or based on respirometric methods whereas at the investigative phase comparative measurements of influent and effluent concentrations replace the use of default values or calculated rate constants.

An attempt was made to derive biodegradation half-life times for surface waters and soil by evaluating a biodegradation database and industry biodegradation data but due to the limitations of the available data no recommendations on scientifically based default values to be used at screening level could be given although the data suggest that the default values used within existing risk assessment schemes may be overly conservative. At the confirmatory phase the biodegradation rates in soil and surface waters will have to be derived from primary biodegradation testing requiring specific analytical methods or radiolabelled materials. For soil, standard simulation tests are available.

SECTION 1. INTRODUCTION

In environmental exposure assessment the concentration of a substance in the different environmental compartments is estimated based on physico-chemical properties, the production and emission processes, the use and disposal patterns and the properties of the environmental compartments. The 'Predicted Environmental Concentration' (PEC) can therefore be calculated based on knowledge of the quantity of the substance that will enter the environment and the distribution and degradation processes occurring in the environment using generic, representative model environments.

An alternative to such calculations is measuring (monitoring) the environmental concentrations in the relevant environmental compartments according to a pre-planned sampling strategy. This is only possible for substances which are released in quantities large enough to be detectable by appropriate analytical methods after dilution in the environment. In those cases where reliable high quality monitoring data are available, they should take precedence over the predicted PECs.

In ECETOC (1993) a number of steps in the overall process could at the time not be described in detail. Based on the recommendations of this report, a Task Force was established with the following Terms of Reference:

- verify and if necessary refine the ECETOC risk assessment scheme and use product "Release Scenarios" as input for the scheme by applying them to selected well-documented representative substances;

- define generic regional and local environments and recommend mathematical models for the prediction of realistic worst case exposure levels in the environmental compartments of concern;

- recommend approaches for deriving the kinetic constants required for the application of models for the simulation of (bio)degradation in all the relevant environmental compartments and in waste water treatment plants from available test results and verify waste water treatment plant models;

- seek collaboration with the regulatory authorities for the development of a transparent and consistent computerised mathematical model in line with current and evolving guidelines for environmental risk assessment.

In relation to these Terms of Reference, in this report special attention is given to:

- environmental exposure assessment in the context of risk assessment;
- data requirements and the applicability of generic local and regional models;
- release scenarios including background information;
- (bio)degradation kinetics;
- a number of examples for a local and a regional scale.

This report deals with the environmental exposure assessment whereas the exposure assessment for man as a consumer or to substances released to the environment is described in ECETOC Technical Report No. 58 (ECETOC, 1994a).

The purpose of this report is to present the current "state of the art" knowledge on the above topics supplementing the definitions and processes as described by ECETOC (1993), aiming at the development of scientifically based, pragmatic approaches for environmental exposure assessment for both "existing" and "new" substances.

As in ECETOC (1993) most emphasis is placed on the aquatic environment which is generally regarded as the main compartment at risk.

SECTION 2. BACKGROUND

2.1 LEGISLATION

On 30th April 1992 the European Council adopted the "7th Amendment" of Directive 67/548/EEC (EEC, 1992), which came into force on 31th October 1993. Article 3.2 of this Council Directive requires that risk assessment for notified new substances be carried out according to principles laid down in Commission Directive 93/67/EEC (EEC, 1993a) which came into force 20 July 1993.

In the Council Regulation 793/93/EEC on the evaluation and control of risks of existing substances, which came into force 4th June 1993, a risk assessment is required according to Article 10(4) (EEC, 1993b). It will be amended by a Commission Regulation describing the principles of the assessment of risks to man and the environment of existing substances (EEC, 1993c).

Additionally several national authorities and international organisations have developed hazard and risk assessment concepts for new and/or existing substances (e.g. Germany, The Netherlands, UK, Switzerland, USA and the OECD), as documented by ECETOC (1993).

2.2 EXISTING HAZARD ASSESSMENT SCHEMES

In 1990, the Commission of the European Communities, Directorate General XI, organised a workshop on "Environmental Hazard and Risk Assessment in the Context of Directive 79/831/EEC" (EEC, 1990) in collaboration with the Environmental Institute of the Joint Research Centre Ispra. This workshop discussed and identified common principles for the environmental risk assessment of substances to achieve a harmonised and transparent procedure for the evaluation of new substances within the Community.

At the request of the Commission the conclusions of the "Ispra workshop" were discussed by various interested organisations. ECETOC (1991) concluded that the outcome of the Ispra workshop formed a good basis for further discussions. The main points of agreement were that the hazard assessment process should be iterative, that exposure scenarios should be developed for "use-categories" (surfactants, dye-stuffs, solvents, etc.) and that there was a need for differentiation in the assessment process between the exposure from limited point sources and exposure from diffuse release.

The Dutch National Institute of Public Health and Environmental Protection (RIVM) has developed on behalf of the Netherlands Ministry of Housing, Spatial Planning and the Environment (VROM) and the Ministry of Welfare, Health and Cultural Affairs (WVC) a risk assessment software package USES (Uniform System for the Evaluation of Substances) which integrates DRANC (Dutch Risk Assessment New Chemicals), PRISEC (Priority Setting Existing Chemicals) and ESPE (Evaluation System Pesticides) (RIVM, VROM, WVC, 1994; see also Vermeire *et al*, 1992). It is the intention of both DG XI, the Dutch competent authorities and industry representatives to investigate the possibilities of the development of a similar system suitable for performing risk assessments in accordance with the Technical Guidance Documents adopted for notified new substances in 1993 and the Technical Guidance Documents for existing substances (in preparation during 1994).

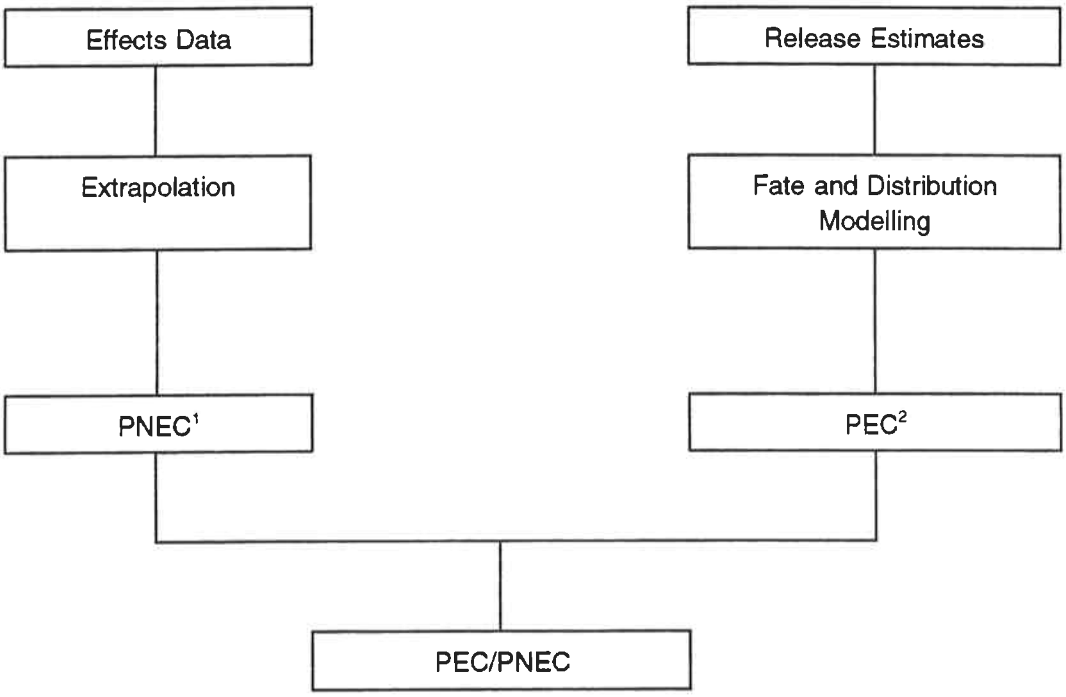
The EU has adopted the Technical Guidance documents for the risk assessment for notified new substances. At the request of DG XI, the German authorities are producing the Technical Guidance documents for the risk assessment for existing substances. Furthermore the UK Government together with UK industries have produced a risk assessment scheme for existing substances (UK, 1993) in the context of EC and OECD existing chemicals programmes.

The existing schemes for risk assessment as developed for new and existing substances by the EC DG XI, generally follow a stepwise approach in which, if necessary, increasingly refined estimates of the Predicted Environmental Concentrations (PECs) and the predicted No-Effect Concentrations (PNECs) can be compared in stages. The necessity of refinement of either PEC(s) and/or PNEC(s), when one of the PEC/PNEC ratios is greater than 1, is based on the assumption that such refinement significantly will reduce the PEC/PNEC ratios to values below 1. If it is obvious that this cannot be achieved, further refinement of either PEC or PNEC is not useful and hence should not be performed.

SECTION 3. ENVIRONMENTAL EXPOSURE ASSESSMENT IN RELATION TO RISK ASSESSMENT

The process of environmental risk assessment was defined and described in ECETOC Technical Report No. 51 (ECETOC, 1993). It was related to production, distribution, use and disposal of substances on a localised scale as well as on a more widespread, 'regional' scale. The risk assessment procedure involves comparison of the PEC of the substance with the best estimate of the concentration which causes no effect to the organisms resident in the environmental compartment of concern (PNEC) (see Figure 1).

Figure 1 **Basic Elements of the Hazard Assessment Scheme Resulting in PEC/PNEC Comparisons**



1 PNEC = Predicted No-Effect Concentration
2 PEC = Predicted Environmental Concentration

The process therefore includes the derivation of:

- predicted (or measured) environmental concentrations (i.e. exposure assessment);
- predicted no-effect concentrations in the environment (i.e. effects assessment).

It is important to take the PEC and the PNEC into account in a risk assessment, although for the process it is necessary to differentiate between fate (e.g. degradation/persistence) and effects (e.g. acute or chronic toxicity) of the substance. The risk assessment should not be based either on environmental concentrations or effects. Quite often persistence, for instance, is regarded as an undesirable property (effect). Strictly speaking it only relates to the fate of a substance in a particular environment. There are many situations in which persistence is seen as a desirable property, e.g. in polymers, paints, varnishes for construction purposes. Therefore, persistence *per se* should not drive the risk assessment, specifically in the absence of adverse effects.

The risk assessment is conducted as an iterative process. The phases of the exposure assessment can be called screening, confirmatory and investigative and are related to the level of detail of the data used. In the effects assessment the phases are characterised by data from acute, chronic or ecosystem tests from which PNECs are derived by using application factors.

The PEC values needed for the above-mentioned risk assessment can be measured or predicted by applying mathematical models (Section 4). Environmental concentrations depend on the total release and its pattern as well as on the distribution and fate of the substance in the environment. Therefore, important aspects of the environmental exposure assessment are the methods to derive or estimate the total release (Section 5) and methods to estimate degradation (fate) in the different environmental compartments (Section 6).

Discontinuous releases should be treated differently from the continuous releases. The result of discontinuous releases lead to time-dependent concentrations in the environment (variable PECs). To compare these PECs with appropriate PNEC values, the latter will have to be derived from either acute or chronic toxicity tests using a different set of application factors to take into account the temporal variation in PEC values. In the absence of proper tests to account for this variation, acute toxicity tests seem to be most appropriate for deriving PNECs.

SECTION 4. GENERIC ENVIRONMENTAL EXPOSURE MODELS

4.1 INTRODUCTION

Computer models are valuable tools for estimating the concentration of substances in different environmental compartments and to predict the chemical fate of a substance. Input parameters for these estimations are the physico-chemical properties of the substance evaluated and the characteristics of the receiving environmental compartment(s). While physico-chemical parameters are inherent properties of the substance, the nature and properties of the environment may vary widely depending on the location. Moreover, even small ecosystems like a tributary are very complex and are difficult to characterise. In order to decrease the complexity inherent to 'real' environments, the use of a 'generic' or 'evaluative' environment with standard properties has been suggested (Baughman and Lassiter, 1978) and developed (Mackay *et al*, 1992).

By using these 'generic' environments the fate of different substances can be compared under standard conditions. Moreover it is easier to evaluate results for a given substance obtained for different locations. However, it is important to understand that the use of 'generic' environments is no attempt to simulate the 'real' environment, but simply a concept to predict the behaviour of the substance under standard conditions. The inherent disadvantage of these 'generic' environments is that the estimations are difficult to validate. Therefore, figures obtained with these models must be used with great care.

4.2 GENERIC REGIONAL MODEL

The regional generic model may be used to determine the 'compartment of concern' and to estimate the background levels of substances that enter the environment via a diffuse release.

As a basis for the regional exposure assessment a generic regional model based on fugacity described by Mackay *et al* (1992) has been used. ECETOC (1993) indicated the usefulness of this model by some initial sensitivity analyses and by a preliminary validation comparing calculated data with data measured in the environment. It was recognized that this exercise was limited and needed to be elaborated. In this section a critical review of the parameters used and more extensive sensitivity analyses are described with the goal of defining an acceptable regional model scenario for the European situation.

In Table 1 the parameters used in the regional model according to Mackay *et al* (1992) are summarised. Their suitability for the European situation was also reviewed by comparison with data retrieved from the literature.

Table 1 List of Parameters Used in the Regional Model with Units and Fixed Values

Part A. Substance-Specific Data

Parameter	Unit	input data / calculated[1]
molecular mass	g/mol	input data
melting point	°C	input data
vapour pressure	Pascal	input data
water solubility	mg/l	input data
log (octanol/water) part. coeff.	-	input data
part. coeff. soil/water	l/kg	input data/calculated
part. coeff. sediment/water	l/kg	input data/calculated
part. coeff. susp.sed/water	l/kg	input data/calculated
part. coeff. fish/water	l/kg	input data/calculated
part. coeff. prim. sludge WWTP	l/kg	input data/calculated
part. coeff. sec. sludge WWTP	l/kg	input data/calculated
half life in air	hours	input data
half life in water	hours	input data
half life in soil	hours	input data
half life in sediment	hours	input data
backgr. level in air	µg/m^3	input data
backgr. level in water	mg/l	input data

[1] 'calculated' means: the parameter can be calculated by the program.

4.2.1 Substance-specific Data

The substance-specific data used in the regional model are summarised in Table 1, Part A. It is obvious that these data are variable and will influence the calculated PECs considerably. The effect of uncertainties in their values was already discussed by ECETOC (1993) and will not be repeated here.

A pragmatic approach to handle inaccuracy or uncertainty of substance-specific data in a risk assessment process is to assume that the generated data are correct. Depending on the results of

Table 1, Part B. Environmental and Geographical Data (Fixed per Scenario)

Parameter	Unit	Value	Source
total surface area	km^2	100,000	Mackay *et al* (1992)
water surface fraction	-	0.02	ECETOC[1]
land fraction	-	0.98	1 - (water fraction)
height of air compartment	m	1,000	Mackay *et al* (1992)
depth of water compartment	m	3	USES (1992)
depth of soil compartment	m	0.2	Mackay *et al* (1992)
depth of sediment compartment	m	0.05	Mackay *et al* (1992)
conc. of susp. sed. in water	mg/l	12.5	ECETOC[1]
fraction org. carbon soil	-	0.02	Mackay *et al* (1992)
fraction org. carbon sediment	-	0.04	Mackay *et al* (1992)
fraction org. carbon susp. sed.	-	0.2	Mackay *et al* (1992)
advection residence time air	h	100	Mackay *et al* (1992)
advection residence time water	h	1,000	Mackay *et al* (1992)
advection residence time sediment	h		[2]
burial rate of sediment	mm/y		[2]
temperature of the system	°C	25	

1 discussed in this report.
2 fixed by the assumed sedimentation rate and resuspension rate.

the risk assessment the uncertainty levels of measurements may subsequently be used in sensitivity analyses to determine whether the inaccuracies in these data are significant and need to be diminished.

4.2.2 Generic Regional Environments

The geographical characteristics that are used in the regional model calculations are summarised in Table 1, Part B.

In the HAZCHEM model (ECETOC, 1994b) the soil-water runoff rate (U_{sw}) of Mackay *et al* (1992) was adapted by using the fraction of rain excess multiplied with the rain rate. For most of the European countries the actual rain excess was close to 50% of the total amount of rain. A fixed

Table 1, Part C. Intermedia Transport Parameters, Mass Transfer Coefficients (Fixed)

Parameter	Unit	Value	Symbol
air side air-water MTC	m/h	5	k_a
water side air-water MTC	m/h	0.05	k_w
rain rate	m/h	0.0001	U_r
aerosol deposition	m/h	$6 \cdot 10^{-10}$	U_t
soil-air phase diffusion	m/h	0.02	K_{sa}
soil water phase transport	m/h	0.00001	K_{sw}
soil air boundary layer	m/h	5	K_s
sediment-water diffusion	m/h	0.0001	K_t
sediment deposition velocity	m/h	$5 \cdot 10^{-7}$	U_d
resuspension of sediment layer	m/h	$2.0 \cdot 10^{-7}$	U_{re}
soil water runoff rate	m/h	0.00005	U_{sw}[3]
soil solids runoff rate	m/h	$1 \cdot 10^{-8}$	U_{ss}

[3] fraction runoff (rain excess) multiplied by the rain rate.

fraction of 0.5 for rain runoff according to Mackay *et al* (1992) was therefore used for the sensitivity analyses instead of the actual data on rain excess.

Considering the surface area in percent of water, France and The Netherlands represent the extremes for dry and wet countries, respectively (Table 2). The amount of rain and the rain excess characterise Ireland as a wet country, followed by The Netherlands and the UK. Greece, Spain and France represent the driest European countries.

It should be noted that only the total terrestrial and the aquatic surface area were considered in the sensitivity analyses, which means that the soil surface area was 100% of the total surface minus the aquatic surface area. Although coastal marine zones are known to be relevant in the distribution of land-released substances, they are not included in the model. This aspect should be addressed in future models.

The average water depth of 20 m described by Mackay *et al* (1992) is considered not to be representative for Europe where a value of 3 m is assumed to be more accurate. This figure was also used for The Netherlands (RIVM, VROM, WVC, 1994).

Table 2 **Geographical Data Relevant for the Regional Generic Scenario Modelling for European Countries**

Country	number inhab.	square km	water %	agric. %	pasture %	forest %	other %	rain mm/y	rain excess mm/y
Reference	2	2	1	1	1	1	1	2	3
Belgium & Luxembourg	10,400,000	33,100	0.8	27.1	24.3	21.2	26.6	774	350
Denmark	5,200,000	43,070	1.6	61.9	7.4	11.0	18.1	800	300
France	56,900,000	551,500	0.3	33.9	24.9	26.5	14.4	794	300
Germany	80,400,000	356,910	1.9	34.9	18.1	28.6	16.6	673	350
Greece	10,100,000	131,990	0.9	29.5	39.8	19.8	10.1	414	225
Ireland	3,600,000	70,280	2.0	18.3	62.6	3.9	13.3	1030	500
Italy	58,000,000	301,270	2.4	40.6	17.4	20.7	18.9	773	400
Netherlands	15,200,000	36,850	8.2	22.6	34.4	8.2	26.5	825	350
Portugal	9,800,000	92,390	0.5	31.7	5.7	39.4	22.7	920	250
Spain	39,100,000	504,780	1.0	41.6	22.4	28.9	6.2	520	200
UK	57,700,000	244,880	1.3	29.3	47.1	8.1	14.3	824	300
EC total	346,400,000	2,367,020							
EC average*			1.3	35.5	25.7	23.5	14.0	709	300

References:
1) FAO, 1990;
2) Hunter, 1992;
3) Corine, 1991.

* weighed average

The environmental data such as 'bulk compartment dimensions', 'volume fractions' and 'densities' for the generic scenario were taken from Mackay *et al* (1992) and were not further examined. These figures are hardly controversial or scientifically disputable. Other environmental data are included in Table 1, Part B. Most of these data are also according to Mackay *et al* (1992) and were adopted as valid and representative without further checking.

The concentration of suspended matter and its organic carbon fraction are essential in the regional model because they determine adsorption. Relevant literature data were therefore evaluated.

The organic carbon fraction of the European soils was given by Fraters and Bouwman (1993). The value of 2 %, as was also assumed by Mackay *et al* (1992), appeared to be an acceptable average value for a European generic scenario.

In the model scenario described by Mackay *et al* (1992) the concentration of suspended matter was assumed to be 7.5 mg/l with an organic carbon fraction of 0.2. Some literature data were compiled to illustrate that these assumptions were representative. The particulate organic carbon concentrations (POC) in surface waters is of course very variable in different types of surface waters such as rivers, lakes and wetlands (e.g. swamps). In lakes generally the largest part of organic carbon is present as dissolved organic carbon (DOC), with POC being only 10 % or less of the DOC (Thurman, 1985). Eutrophic lakes for instance have an average DOC content of 10 mg/l. If 10 % was particulate this would give a POC concentration of 1 mg/l. Wetlands mostly have higher DOC and POC concentrations with much larger ranges depending on the type of wetland. Ranges of 3 to 400 mg/l DOC were found, with an average of 30 mg/l (Thurman, 1985).

Rivers have an intermediate position between wetlands and lakes with regard to the organic carbon load. Since large rivers also represent an important part of the surface waters, also with respect to the transport of xenobiotic substances, the suspended matter concentrations of these aquatic ecosystems were taken as representative for the generic scenario. A median POC concentration of the major rivers of the world is 2-6 mg/l, with a mean of 2.5 mg/l. The concentration of POC is 1-30 mg/l for 99% of all rivers in the world. In Table 3 the literature data for some large European rivers are summarised (Thurman, 1985). The range for these rivers is 1-3 mg/l, with 3 mg/l for the river Rhine. Considering the data for the European rivers (Table 3) and the range and mean for the world rivers, a POC concentration of 2.5 mg/l is considered to be an acceptable average to be used for the generic scenario. Assuming that the organic carbon content is 20% of the suspended matter concentration, this results in a suspended matter concentration of 12.5 mg/l assumed for the generic scenario.

Table 3 Particulate Organic Carbon (POC) Concentrations in Rivers (Thurman, 1985)

Rivers	mg/l
Rhone	1.0
Garonne	2.5
Loire	2.0
Rhine	3.0

The mass transfer coefficients (MTC) are summarised in Table 1, Part C. Sensitivity analyses (see Section 4.4.2 below) revealed that the MTC values as given by Mackay *et al* (1992) are suitable for screening purposes with a European model scenario.

4.2.3 Sensitivity Analyses

Sensitivity analyses for geographical parameters were carried out using a selection of relevant geographical data of European countries which are summarised in Table 2. The data from France, The Netherlands, United Kingdom, Ireland and Italy were used in the analysis because these countries exhibit a wide variation of the water surface in combination with the rain rate. These five 'country scenarios' using above mentioned parameters were analysed for the concentrations of 1,2,3-trichlorobenzene (TCB), p-cresol, benzene and hexachlorobenzene (HCB) in air, water, soil and sediment. The release of the substances was assumed to be in air (60%), water (30%) and soil (10%) (Mackay *et al*, 1992). The model settings used were according to Mackay *et al* (1992), except for the (average) depth of the water compartment.

Sensitivity Analysis on Geographical Parameters

For the calculations the following conditions were assumed: biodegradation of the substances according to Mackay *et al* (1992), water % and rain rate country-specific, all other values default. The results are presented in Table 4.

The differences in predicted concentrations for the different countries were largest for the water and sediment compartments but negligible for air and soil. The results demonstrated that varying the two parameters mentioned above will have consequences for the concentrations in water and sediment as could be expected. The highest concentration was about 27 times the lowest concentration. The lowest concentrations in these compartments were always found for the Netherlands and the highest for France. The rain rate and rain excess (calculated as 0.5 times rain rate) are of minor importance in these calculations where a fixed residence time was used. The volume of the water compartment in relation to the residence time determined the concentrations in water and sediment.

Subsequently the data on total water volume and residence time were further analysed. Because household substances enter the (regional) environment via wastewater discharges it is also important for a regional scenario to obtain a realistic (mean) dilution factor for the wastewater discharged. For this purpose the following assumptions for the aquatic compartment were made:

- the amount of wastewater discharged was calculated for each country by assuming a discharge of 200 l per day per inhabitant;

- firstly the dilution factor was calculated as (volume/residence time) / (wastewater flow);

Table 4. Results of the Sensitivity Analysis for Different Geographical Scenarios: Predicted Environmental Concentrations (in g/m^3) for Five Countries with Different Environmental Parameters

	p-Cresol				Benzene			
Country	Water	Air	Soil	Sediment	Water	Air	Soil	Sediment
F	8.01e-03	3.97e-08	4.31e-04	3.07e-03	1.59e-02	1.81e-07	3.40e-04	2.27e-02
NL	2.96e-04	3.95e-08	4.70e-04	1.13e-04	5.82e-04	1.81e-07	3.69e-04	8.33e-04
UK	1.85e-03	3.96e-08	4.41e-04	7.10e-04	3.67e-03	1.81e-07	3.43e-04	5.25e-03
Ir	1.21e-03	3.94e-08	4.51e-04	4.63e-04	2.39e-03	1.81e-07	3.45e-04	3.41e-03
I	1.00e-03	3.96e-08	4.43e-04	3.85e-04	1.99e-03	1.81e-07	3.47e-04	2.84e-03
AVG	2.47e-03	3.96e-08	4.47e-04	9.48e-04	4.90e-03	1.81e-07	3.49e-04	7.02e-03
MIN	2.96e-04	3.94e-08	4.31e-04	1.13e-04	5.82e-04	1.81e-07	3.40e-04	8.33e-04
MAX	8.01e-03	3.97e-08	4.70e-04	3.07e-03	1.59e-02	1.81e-07	3.69e-04	2.27e-02
MAX/MIN	27.1	1.0	1.1	27.1	27.3	1.0	1.1	27.3
MAX-MIN	0.00771	0.00000	0.00004	0.00296	0.01531	0.00000	0.00003	0.02191
	HCB				1,2,3-TCB			
Country	Water	Air	Soil	Sediment	Water	Air	Soil	Sediment
F	2.11e-02	7.96e-07	3.56e-01	1.28e+02	2.02e-02	8.07e-07	2.47e-02	3.48e+00
NL	7.85e-04	7.95e-07	3.86e-01	4.75e+00	7.46e-04	8.07e-07	2.68e-02	1.29e-01
UK	4.88e-03	7.96e-07	3.60e-01	2.95e+01	4.66e-03	8.08e-07	2.49e-02	8.04e-01
Ir	3.18e-03	7.96e-07	3.62e-01	1.92e+01	3.04e-03	8.08e-07	2.50e-02	5.23e-01
I	2.65e-03	7.96e-07	3.64e-01	1.60e+01	2.53e-03	8.07e-07	2.52e-02	4.36e-01
AVG	6.51e-03	7.96e-07	3.66e-01	3.94e+01	6.23e-03	8.07e-07	2.53e-02	1.07e+00
MIN	7.85e-04	7.95e-07	3.56e-01	4.75e+00	7.46e-04	8.07e-07	2.47e-02	1.29e-01
MAX	2.11e-02	7.96e-07	3.86e-01	1.28e+02	2.02e-02	8.08e-07	2.68e-02	3.48e+00
MAX/MIN	26.9	1.0	1.1	26.9	27.1	1.0	1.1	27.1
MAX-MIN	0.02029	0.00000	0.02962	122.79	0.01943	0.00000	0.00205	3.34845

AVG	average,
MAX/MIN	ratio of maximum and minimum values,
MAX-MIN	difference between maximum and minimum values.

- secondly a dilution factor was calculated using a residence time derived from the rain excess for each country as (flow rate from rain) / (wastewater flow). The flow rate from rain was calculated as (rain excess) · (surface area).

The results of these calculations are presented in Table 5 together with the geographic mean values. The assumption of a residence time of 1,000 hours (41.7 days) as in Mackay *et al* (1992) resulted in an mean dilution factor of 32.4. In their original scenario the dilution factor would be 1,378.4 calculated with the average number of inhabitants per km^2 for the European situation (147 inh/km^2). This much higher dilution factor is caused partly by the differences in water depth (20 m) and water surface area (10%) and consequently much larger water volume of the scenario of Mackay. Furthermore it could be shown that the assumed residence time of 41.7 days is not in accordance with the assumed rain characteristics. These would give a residence time of 1,666.7 days assuming that both waterflow and residence time of the water compartment are entirely dependent on rain rate and runoff fraction.

Flow rates and residence times were calculated for the European countries, according to:

rain excess · surface area = country specific flow (in m^3/d);
(then the country-specific residence time is volume / flow).

For most countries this is expected to be a realistic approach with the exception of The Netherlands having a relatively large inflow from rivers in reality. Calculation as above results in a dilution factor of 11.6 which is much lower than the actual dilution factors known (mean 32).

For the European situation an average dilution factor based on the rain excess of 28.1 was found, corresponding to a residence time of 47.5 days. The corresponding geometric mean dilution factor would be 30. Based on the sensitivity analyses and additional calculations as presented in Table 5, recommendations to adapt several parameters are made in Section 5.3.

Sensitivity Analysis on Mass Transfer Coefficients

To be able to determine the relative effect of the values assumed for these parameters, sensitivity analyses were carried out which are described below.

For every substance three different scenarios were used in the calculations, where the input of the substances was assumed to be in air (60%), water (30%) and soil (10%) as in Mackay *et al* (1992).

Table 5 **Water Residence Times and Dilution Factors Calculated from Geographical and Hydrological Characteristics of European Countries**

Country	Water %	Water volume (m^3)	Dilution factor*	Fraction runoff	Flow rate from rain (m^3/d)	Residence time (d)	Dilution factor**
Belgium & Luxembourg	0.8	$7.9 \cdot 10^8$	9.2	0.5	$3.2 \cdot 10^7$	25.0	15.3
Denmark	1.6	$2.1 \cdot 10^9$	47.7	0.4	$3.5 \cdot 10^7$	58.4	34.0
France	0.3	$5.0 \cdot 10^9$	10.5	0.4	$4.5 \cdot 10^8$	11.0	39.8
Germany	1.9	$2.0 \cdot 10^{10}$	30.4	0.5	$3.4 \cdot 10^8$	59.4	21.3
Greece	0.9	$3.6 \cdot 10^9$	42.3	0.5	$8.1 \cdot 10^7$	43.8	40.3
Ireland	2.0	$4.2 \cdot 10^9$	140.6	0.5	$9.6 \cdot 10^7$	43.8	133.7
Italy	2.4	$2.2 \cdot 10^{10}$	44.9	0.5	$3.3 \cdot 10^8$	65.7	28.5
Netherlands	8.2	$9.1 \cdot 10^9$	71.6	0.4	$3.5 \cdot 10^7$	256.5	11.6
Portugal	0.5	$1.4 \cdot 10^9$	17.0	0.3	$6.3 \cdot 10^7$	21.9	32.3
Spain	1.0	$1.5 \cdot 10^{10}$	46.5	0.4	$2.8 \cdot 10^8$	54.7	35.4
UK	1.3	$9.6 \cdot 10^9$	19.9	0.4	$2.0 \cdot 10^8$	47.5	17.4
EC-mean	1.3	$8.4 \cdot 10^9$	32.4	0.4	$1.2 \cdot 10^8$	45.5	29.7

* calculated with a residence time of 41.7 d as assumed in Mackay *et al* (1992).

** calculated on the basis of rain excess.

References:
1) FAO (1990),
2) Hunter (1992),
3) Corine (1991).

In Scenario 1 all data as given by Mackay *et al* (1992) were used. Scenario 2 differs from Scenario 1 by assuming 'no biodegradation' in the various compartments. Additionally, an unrealistic Scenario 3 was set up which differed from Scenario 2 by assuming no advection for air, water and sediment.

The results of the sensitivity analyses shown in Appendix C represent data calculated for seven parameters, i.e. K_a, K_w, U_t, K_{sa}, K_{sw}, K_t and U_{ss} expressed in g/m^3. For explanation of these abbreviations and units see Table 1, Part C. For each parameter five different values were assumed. The third value for each parameter in the table is always identical to that used by Mackay *et al* (1992) (e.g. 5 for K_a). Additionally each parameter was evaluated for two orders of magnitude smaller and two orders of magnitude larger (for K_a from 0.05 - 500). Thus the total range of input values tested for sensitivity was from 1 to 10,000 times the lowest value.

In Appendix C the evaluation of the results for each parameter is given below the calculated concentrations. At first the average value (AVG) and minimum (MIN) and maximum (MAX) values are given for each compartment followed by the range of the output which is expressed as the ratio of the maximum and the minimum value (MAX/MIN). Then the ratio of the output range

(= MAX/MIN) and the input range (= 10,000) is given for each compartment and evaluated as follows:

Ratio	Effect (%) *)	Result
< 0.001	< 0.1	-
≥ 0.001 - < 0.01	< 1	+
≥ 0.01 - < 0.1	1 - < 10	++
≥ 0.1	≥ 10	+++

* e.g. if an output ratio < 10 is compared to the input ratio of 10,000, then the effect is < 0.1 %.

The results are summarised in Table 6. Appendix C shows the data for water, air, soil and sediment for the given parameters in g/m^3 as in Mackay *et al* (1992).

Table 6 Summary of the Results of the Sensitivity Analyses of MTC Values

p-Cresol					**Benzene**				
	Water	Air	Soil	Sediment		Water	Air	Soil	Sediment
Scenario 1					Scenario 1			K_{sa}^{++}	
Scenario 2					Scenario 2	K_w^{+}		K_{sa}^{+++}	
Scenario 3		K_a^{++}	K_a^{++}		Scenario 3				K_w^{+}

HCB					**1,2,3- TCB**				
	Water	Air	Soil	Sediment		Water	Air	Soil	Sediment
Scenario 1	U_t^{+}	U_t^{+}	K_{sa}^{++}		Scenario 1	K_w^{+}		K_{sa}^{+}	
Scenario 2				U_t^{+}	Scenario 2	K_w^{+}		K_{sa}^{++}	K_w^{+}
Scenario 3					Scenario 3				K_w^{+}

In most cases the effect of varying mass transfer coefficients (MTCs) on the results for the tested substances, covering a representative large range of chemical characteristics, was relatively small, often less than 1%. An effect of > 10% was only observed in the case of K_{sa} for benzene in soil in Scenario 2 where no biodegradation was assumed. An effect between 1 and 10% was found in five cases. It should be noticed that an emission scenario with simultaneous input into three compartments was calculated. An input of the total emission into only one compartment will give larger differences in certain cases.

From these results it was concluded that the MTC values as given by Mackay *et al* (1992) are suitable for screening purposes with a European model scenario. The only exception was the soil mass transfer coefficient for soil pores (K_{sa}) for volatile substances for which a further validation is recommended.

4.2.4 Regional Model Requirements

It was concluded that the model described by Mackay *et al* (1992) can be used as a basis for environmental risk assessments on a regional scale. This means that the model is suitable to determine compartments of concern and also to indicate background concentrations (Section 7.3; see also ECETOC, 1994a) although this was checked to a limited extent only. An additional advantage is that the model was published in the open literature and is assumed to represent the state-of-the-art for environmental risk assessment on a regional scale.

The model parameters were critically reviewed for two purposes:

- to check the reality of the parameters where possible;
- to adapt the model to an average European situation.

The review was carried out by evaluating literature and performing sensitivity analyses for some parameters. The following remarks and recommendations can be made concerning the parameters to be used in an environmental risk assessment model based on fugacity for a generic regional scenario representative for Europe employing the model described by Mackay *et al* (1992) as a basis.

- The fraction rain runoff and the rain rate used by Mackay *et al* (1992) are close to the European average, but the rain excess is not in balance with the assumed residence time of the water. For a representative European situation which is in equilibrium these parameters should be calculated from the residence time resulting by the flow calculated from the rain excess. Furthermore, a water depth of 3 m is considered to be more realistic than the 20 m assumed by Mackay *et al* (1992). The soil-water run-off parameter U_{sw} should be formulated as the rain-runoff multiplied with the rain rate.

- On the basis of the geometric mean values of 12 European countries, the following scenario is proposed for a generic European region with a surface area of 100,000 km^2:

  - water surface area: 1.3 %;
  - water depth: 3 m;
  - water volume: $3.9 \cdot 10^9$ m^3;
  - rainfall: 709 mm/y;
  - rain excess: 311 mm/y (resulting in a run-off fraction of 0.4).

  This scenario is consistent with the dilution factor of 30 and the residence time of 46 d as given in Table 5 as the mean values for Europe.

- The average organic carbon fraction of soil for the European situation is 2% according to Fraters and Bouwman (1993), which is similar to the figure used by Mackay *et al* (1992).

- The average organic carbon suspended matter concentration for European rivers taken as an average and representative aquatic ecosystem parameter was 2.5 mg/l (Thurman, 1985). With a representative organic carbon content of 20% this gives a recommended suspended matter concentration of 12.5 mg/l.

4.3 GENERIC LOCAL MODELS

4.3.1 Introduction

The local air, water or soil models are designed to complement regional models in order to refine the prediction of actual substance concentrations for the compartment of concern/interest near or at the source of emission. The level of detail and sophistication of the model formulation will vary depending on the intended purpose, and has been described in detail in by ECETOC (1992).

The usefulness of the proposed environmental exposure scheme to obtain release estimations and predicted environmental concentrations for water, air and soil both at the regional and local level has been illustrated by ECETOC (1993).

Local models can be used to estimate initial (maximum) exposure levels ($PEC_{initial}$) in target compartments. Moreover they are able to quantify temporal and spatial variations in concentrations at some distance from the emission, taking into account fate processes such as (bio)degradation, volatilisation and sorption (PEC_{local}). These local generic models have to be linked to the use

categories: whereas, for example, for chemical intermediates a default river-flow of 60 m^3/s is recommended (see Section 7.1), the release of household chemicals should be treated as outlined below.

4.3.2 Local Model for the Water Compartment

For the aquatic environment, the discharge of substances either directly or via sewage treatment plants, into surface water is the most relevant local scenario. The $PEC_{initial}$ can be simply calculated by dividing the effluent concentration by the actual or a fixed dilution factor. A PEC_{local} should be calculated including biodegradation, volatilisation and sorption.

The RIVMODEL (ten Berge, 1992; see also: ECETOC, 1994b) was developed to predict the fate and concentration profiles (time and space) of the substance after discharge into a river or channel as the receiving water compartment by using modules:

- for advection, settling, resuspension and burial of sediment and degradation according to the QWASI-model of Mackay *et al* (1983);
- for the volatilization of the substance according to Southworth (1979);
- for the quantification of the dispersion and dilution of the waste water according to de Greef and de Nijs (1990).

To allow a standardised assessment a local generic scenario ("unit river") needs to be defined. Due to the wide range in dilution factors and expected variability in flow rates, a rationale had to be developed to propose acceptable default settings. De Greef and de Nijs (1990) determined the distribution of dilution factors for all 466 wastewater treatment plants in The Netherlands which discharge in flowing freshwater systems. This dilution database has been linked to another government database (National Institute of Inland Water and Wastewater Management, RIZA) which lists the type of wastewater treatment applied, the number of inhabitants and the industrial equivalents served by each wastewater treatment plant. This latter database is referred to as the Generic Dutch Model (Versteeg *et al*, 1992). Based on these sources it can be postulated that low dilutions are mostly related to low flow or stream velocities. The data show that for dilution factors of less than 10 the stream velocity is usually less than 1 km/day.

In addition, the Central Bureau of Statistics (CBS, 1990) has listed per capita wastewater flow rates Q, calculated from treatment plant flow rates and population-served data for The Netherlands. The listed median Q ranges from 252 to 347 l/(capita·day), depending on the size of the treatment plant. Larger treatment plants have lower per capita wastewater flow rates than smaller plants. For the discharge of municipal waste, a flow of 200 l/(capita·day) can be adopted as a generic dry weather low flow.

Consequently the following generic scenario for a "UNIT LOWLAND RIVER" receiving the discharge from a small sewage treatment plant could be as follows:

Dilution Factor = 10 or
Wastewater flow = 1,000 m^3/day (i.e. 5,000 eq at 200 l/(capita· day))
River flow = 10,000 m^3/day (i.e. 2m deep, 5m wide at 1 km/day)

Assuming this setting in the RIVMODEL will result in complete mixing within the first kilometre below the discharge (i.e. 160 m) and predicts that biodegradable and/or sorptive compounds are removed to a significant extent within a reasonable distance. The distance for 50% elimination of a compound with a $t_{½}$ of 48 hours and sorption coefficient K_d of 1,000 l/kg is 1,820 m. If no sorption and settling would occur (i.e. K_d = 1 l/kg) the length for 50% elimination increases to more than 5 km. Similarly, if no or very little biodegradation occurs it will take more than 1,000 km to reach 50% elimination of the substance (Table 7).

Table 7 Output for a Generic Lowland Scenario for a Non-Volatile Substance [1]

Substance Properties (biodegradation/adsorption)	Sorption Coefficient k_d (l/kg)	Biodegradation $t_{1/2}$ (hours)	Vapour Pressure (Pa)	50% Elimination Distance (km)
Ready/non-sorptive	100	48	10^{-8}	2.15
Ready/moderately sorptive	1,000	48	10^{-8}	1.82
Ready/highly sorptive	10,000	48	10^{-8}	0.87
No biodeg./non-sorptive	100	10^7	10^{-8}	$8.1 \cdot 10^4$
No biodeg./moderately sorptive	1,000	10^7	10^{-8}	$1.0 \cdot 10^4$
No biodeg./highly sorptive	10,000	10^7	10^{-8}	$1.4 \cdot 10^3$

[1] The following settings were used: River suspended matter concentration 40 mg/l with O.C.content 10% (w/w), depth of sediment layer 3 cm with O.C.content 4% (w/w), burial rate 0.1 mm/year.

Applying this scenario in "RIVMODEL" shows that biodegradation has a substantial influence on the elimination of the substance and that the effect of removal due to sorption is less pronounced, as would be expected for the situation modelled.

However, this scenario will not be realistic for situations with higher flow rates which are more typical of mountainous areas. In that case another generic scenario should envisaged. Such a "UNIT HIGHLAND RIVER" scenario receiving the emission of substances through municipal wastewater treatment plants could be defined as follows:

Dilution Factor = 10;
Wastewater flow = 100,000 m^3/day (i.e. 500,000 eq. at 200 l/(capita·d));
River flow = 1,000,000 m^3/day (i.e. 2m deep, 4m wide at 100 km/d).

Even for biodegradable compounds the 50% elimination distance is relatively long, which can be explained by the high flow rate (factor of 100 higher than the "UNIT LOWLAND RIVER"). With these settings RIVMODEL predicts that volatilization is a more relevant elimination process, as can be expected for such rivers (Table 8).

Table 8 Output for a Generic Highland Scenario for a Biodegradable Substance[1]

Substance Properties (biodegradation/adsorption)	Sorption Coefficient (l/kg)	Biodegradation t/2 (hours)	Vapour Pressure (Pa)	50% Elimination Distance (km)
Non-volatile/non-sorptive	100	48	10^{-8}	201
Non-volatile/moderately sorptive	1,000	48	10^{-8}	120
Non-volatile/highly sorptive	10,000	48	10^{-8}	31
Volatile/non-sorptive	100	48	10^{4}	11
Volatile/moderately sorptive	1,000	48	10^{4}	11
Volatile/highly sorptive	10,000	48	10^{4}	10

[1] The following settings were used: River suspended matter concentration 40 mg/l with O.C.content 10% (w/w), depth of sediment layer 3 cm with O.C.content 4% (w/w), burial rate 0.1 mm/year.

4.3.3 Local Model for the Air Compartment

In the air compartment mixing, advection and degradation are the most important processes that will determine fate and distribution of substances. Even for substances with a vapour pressure much below 1 Pa it is suggested that transport via air is the main mechanism for world-wide distribution. In the Netherlands under normal weather conditions, with an average wind speed of 3 m/s, airborne substances are transported over distances of more than 250 km/day. Mixing within the lower 500 m layer, the mixing layer, is very rapid (Van Jaarsveld, 1990).

Photochemical transformation or degradation processes in air are frequently very rapid. When considering only reaction with OH radicals the half-life for most hydrocarbons is less than 1 day; in general half-lives for other gaseous substances will be less then 10 days. With respect to the mass of substances that are released into the environment, degradation in air is a very important process.

For the purpose of an environmental risk assessment for the air compartment based on a PEC/PNEC comparison there is presently no need for a PEC calculation since the PNEC in air can (as yet) not be assessed. Nevertheless the definition and calculation of $PEC_{initial}$ and PEC_{local} is given below for the reason of completeness and potential use in the future and for the use in the indirect exposure assessment.

$PEC_{initial}$ in air could represent the concentration close to the source taking into account dilution only, similarly to the approach proposed for calculating the $PEC_{initial}$ in water. Because of the difference in the emission and dilution processes it was decided not to differentiate between $PEC_{initial}$ and PEC_{local}.

To calculate the PEC_{local} in air, an aerial distribution model OPS (Van Jaarsveld, 1990) is used. This model is applied both to industrial sources and the emissions from WWTPs. The basic assumptions are a stack height of 10 meters and a wind speed of 3 m/s. Based on these assumptions the calculations show that a plume will reach the surface in the prevailing wind direction at a distance of some 100 meters from the source, for which reason the PEC_{local} is defined at 100 meters from the source(s). However, to include the variability of the wind direction as well as estimating the average concentration in an area around the industrial source or the WWTP, it is proposed to calculate a PEC_{local} which can be used for the indirect exposure of man and exposure of cattle, based on the assumption that exposure is taking place in an area which is between a 100 - 2,000 meters from the source. Taking the concentration only at a distance of 100 meters in the prevailing wind direction as it is done in USES is overconservative. For the direct and indirect exposure either the $PEC_{regional}$ or the PEC_{local} as described above calculating the average concentration should be taken into account (Table 9).

4.3.4 Local Model for the Soil Compartment

Deposition from the air is the most common general route for the exposure of soil. For arable soil direct application via fertilisers, pesticides, sewage sludge and irrigation water may play an important role as well. Therefore soil models are mostly integrated as a module into more complex models, which also contain modules for air and water exposure in order to simulate more realistic

Table 9 Calculation of the PEC_{local}

Parameter	Value	Unit
Wind speed	3	m/s
Emission height	10	m
Radius of the area affected	100 -2000	m
Source strength	1	g/s
PEC_{local}	1	µg/m^3

environmental situations. This is especially appropriate in case of deposition of airborne substances where both the emission (air module) and the fate (soil module) have to be taken into account.

A $PEC_{initial}$ for soil is only useful for substances directly applied to soil or applied via sewage sludge. In that case the $PEC_{initial}$ can be calculated simply by assuming the amount of substance being completely mixed with the soil, assuming a certain mixing depth. Since many relevant processes are not included in this procedure, it should be realized that such a PEC only represents a very unrealistic worst-case.

For a more realistic estimation of the concentration in soil a module was developed, which estimates the steady state concentration after many years of exposure via aerial deposition and sludge application, balanced by elimination processes. This results in a more realistic PEC_{local}, calculated for a point source. The following assumptions were made:

- the possible exposure routes of the arable soil compartment consist of:
    - application of activated sludge from the sewage treatment plant (RIVM, VROM, WVC, 1994);
    - application of pesticides and fertilisers (or via irrigation water);
    - deposition from the air (RIVM, VROM, WVC, 1994);
- the yearly average concentration in air at a distance between 100 and 2,000 meters from the source is estimated, assumed to originate from the sum of emissions of a local industrial plant and a sewage treatment plant;
- a natural soil compartment is included to determine the effect of deposition from the air as the only input (RIVM, VROM, WVC, 1994);

- the removal processes included are:
    - biodegradation;
    - leaching;
    - volatilisation (evaporation).

The details of the module and the equations used are described in detail in Appendix F.

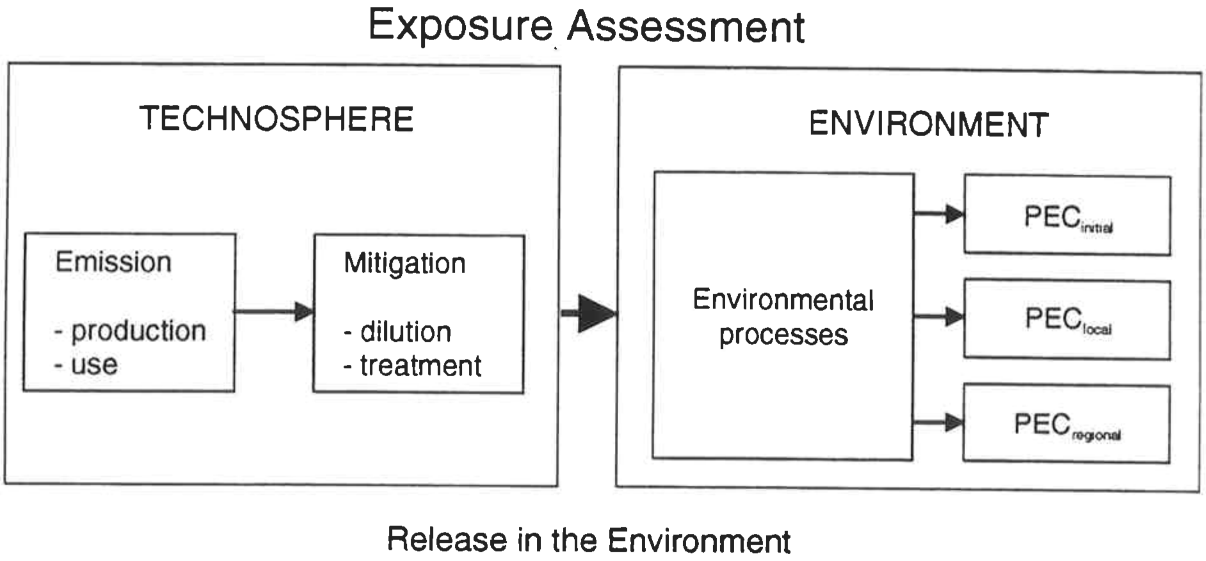
SECTION 5. RELEASE ESTIMATION

5.1 GENERAL ASPECTS

The release of substances can be continuous (e.g. production in a refinery or use of household detergents) or discontinuous (e.g. production of dyestuffs or use of fertilizers).

Release and emission estimations are the first steps in exposure assessment and realistic data are essential for the calculation of Predicted Environmental Concentrations (PECs) (ECETOC, 1993). Release can be defined as the mass flow of a chemical from a process that results in emissions from the technosphere (including production, use and treatment facilities) into the environment. Figure 1 shows release and emission which results in PECs around the emission source, i.e. $PEC_{initial}$, in the local environment of the emission source, i.e. PEC_{local} and in the region, i.e. $PEC_{regional}$. Details are described below.

Figure 2 Relationship of Release and Exposure Assessment



In the screening phase generalised assumptions of the releases, dilutions and eliminations are used based on commonly agreed realistic worst case estimations. To avoid time-consuming single case studies, substances are classified according to their use into different 'use categories' (HEDSET, 1993). In the confirmatory phase physico-chemical properties and specific dilution and elimination steps of the chemical should be taken into account in a still theoretical release estimation model, whereas in the investigative phase monitoring data or test data for pilot or normal scale operations should be used.

Release estimations can refer to both a regional or a local situation. In regional release estimations the releases during the whole life cycle of the chemical to the environmental compartments (air, soil and water) in a region have to be considered. They are basic input data for regional environmental fate models which calculate a predicted regional environmental concentration ($PEC_{regional}$). Local release estimations deal with the releases of the chemicals during particular life stages (e.g. production, use or disposal) at a specific site. A local release estimation is the basis for the calculation of a predicted environmental concentration near the emission site ($PEC_{initial}$) and - after application of a local environmental fate model - a predicted local environmental concentration (PEC_{local}). If more than one use of a substance is known resulting in different releases, it may be sufficient for a local exposure assessment to focus on the most important release, especially where other releases are contributing insignificantly to the PEC.

According to Figure 2, generic release scenarios consist of several of the following components:

- **emission** of the chemical during a specific step of the life cycle;
- **mitigation** before reaching the receiving environmental compartment;
- **release** to the environment.

Releases can occur during the whole life cycle of a substance (production, formulation, use and disposal) into different environmental compartments (air, water and soil). These releases, given as mass of substance per unit time, can vary by several orders of magnitude depending on the use pattern (ECETOC, 1993).

Elimination is defined as a waste processing step which results in decrease of the release. Filters, incinerators and scrubbers may be necessary for reduction of releases into the air and should be included in the evaluation on a case-by-case basis. For releases into surface water, however, the presence of effluent treatment plants is assumed as the default in the exposure assessment.

Dilution can be considered either by applying dilution factors ($PEC_{initial}$) or including them in the environmental fate models through the definition of the receiving environmental compartments

(PEC_{local} or $PEC_{regional}$). It is very important for the calculation of $PEC_{initial}$ values to cover all relevant dilution processes. For releases into surface water, the following dilution processes may occur:

- during processing;
- with other effluents of the processing site;
- in sewage treatment plants;
- in the receiving surface water.

By not taking into account "on site" (internal) and "off site" (external) dilution steps $PEC_{initial}$ will be grossly exaggerated.

5.2 RELEASE INTO AIR, WATER AND SOIL

5.2.1 Release into Air

When a substance is released into the air, the dilution will depend on the relative frequency of various meteorological conditions (e.g. wind speed and direction, temperature profiles). Because of rapid mixing and transport the resulting concentrations in the air may be below any effect concentration. Compounds which are stable under atmospheric conditions may have an effect through indirect exposure, contamination of water or soil via wet and dry deposition or specific mechanisms leading to global warming or ozone depletion. Compounds which are rapidly degradable by airborne oxidants may contribute to smog formation.

5.2.2 Release into Soil

Direct releases into soil are normally restricted to specific classes of compounds like pesticides and fertilizers and are discontinuous. Therefore case-by-case studies are the appropriate approach.

Indirect releases can occur via sewage sludge application, wet and dry deposition or irrigation water.

5.2.3 Release into Surface Water

For many substances the point source releases into the aquatic compartment during production and use are very important. Therefore the volume or flow rate of the receiving surface waters should be taken into account for the calculation of PEC_{local}. For substances that are released in a diffuse manner, the calculation of a $PEC_{regional}$ based on regional generic situations is more appropriate.

5.3 RELEASE ESTIMATION FOR SURFACE WATER

5.3.1 Screening Phase

Local Release Estimation

For the quantification of the release estimation all elements of the use process have to be described. For each of these elements substance-specific data should be taken or - where not available - default values could be used which reflect average or realistic worst case situations. When using worst case assumptions for each element this can easily lead to unrealistically high release estimations.

Scheme 1 indicates the elements used in the release scenario for 'textile dyeing' and the calculation algorithm for the release.

Scheme 1 Release Scenario "Textile Dyeing"

Mass of dyed goods per day	W1	[kg substrate/d]
Mass of dye used per mass of goods	W2	[kg dye/kg substrate]
Degree of fixation of dye onto goods	F	[%]
Release of unfixed dye	$W = \frac{W1 \cdot W2 \cdot (100-F)}{100}$	

If the use process cannot be described in simple terms, a statistical approach may be appropriate. An example is the release estimation of intermediates during their production. Because there are many different production processes for intermediates (batch, continuous etc.) the relevant elements for release are hard to identify. Therefore release data from well examined intermediates were collected and the 90-percentile of the release fractions based on the production volume were calculated (see Appendix A). Scheme 2 shows the release scenario "production of intermediates".

The release of a substance is determined in most cases by the process involved (including treatment) and not by the physico-chemical properties of the substance. For example, the releases of intermediates into surface waters cannot be correlated to their water solubilities as was demonstrated in Figure 3. Another example are reactive dyes. Although highly water-soluble, their release is determined by the fixation process which is chemical binding of the dye to the fibre.

Scheme 2 Release Scenario "Production of Intermediates"

Production volume per day	W1	[kg/d]
90 Percentile of release fraction based on production volume	R	[%]
Release during production	$W = \frac{W1 \cdot R}{100}$ [kg/d]	

Regional release estimation

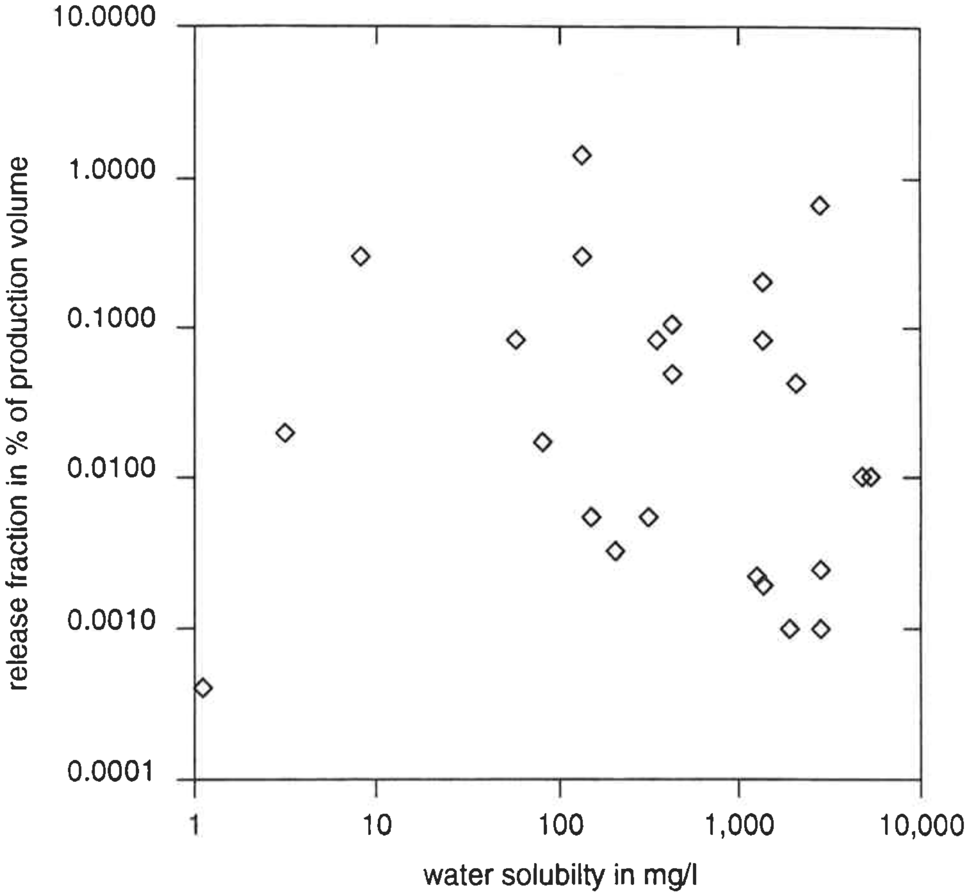
In regional release estimation all releases during the whole life cycle of the substance, i.e. production, formulation, use and disposal, have to be considered. Depending on the substance this can be a very complex and time-consuming task. To overcome this problem substances can be classified in different 'main categories' (HEDSET, 1993) for which release fractions based on production volume can be assigned (Table 10). Similar data for special use patterns are not yet available. The overall releases given by the default values have to be separated into emissions into air, water and soil for use as input data in regional models.

Table 10 Default Release Fractions Related to "Main Categories"

Main Category	Release Fraction of Production Volume	Examples
Closed system	0.01	Chemical intermediates
Enclosed in a matrix	0.1	Plastic additives
Non dispersive use	0.2	Photochemicals
Wide dispersive use	1.0	Solvents, detergents

These values should only be used if more specific data are not available.

Figure 3 Release Fractions (during use) of 25 Intermediates in % of Production Volume*



* Data from BUA reports, see Appendix A, Table A.1.

5.3.2 Confirmatory and Investigative Phases

In order to obtain more realistic release estimates in the confirmatory phase, more substance-specific data should be used instead of considering average generic situations and using default values. For example substance-specific fixation rates of a particular dyestuff may be used instead of an average value.

In the investigative phase, the release estimations as used in the models need to be validated by comparison with measured release data or appropriate monitoring data taking into account the variability of the concentrations with time.

SECTION 6. DEGRADATION KINETICS

6.1 INTRODUCTION

The PEC may be significantly reduced by biological and/or physico-chemical processes and as a consequence may result in a reduction of the PEC/PNEC ratio. For most of the relevant substances for which an exposure assessment has to be executed, the biological degradation processes are most important. In this section background information is given on biodegradability tests and the translation of the results of these tests into kinetic rate constants for several environmental compartments and wastewater treatment plants (WWTP).

Mathematical models currently in use to predict environmental concentrations of substances also require knowledge of the kinetics of biodegradation. Because the environmental exposure assessment is normally based on the parent substance, biodegradation (kinetics) should be related to primary biodegradation. The measurement of primary biodegradation requires specific analytical methods which are sensitive enough to determine concentrations relevant to the environmental compartment of concern. Such methods could well be difficult to develop within a reasonable period of time and it is therefore often necessary to assess primary degradation based on tests using non-specific methods.

The problem therefore is to recommend suitable methods which would allow the necessary data to be obtained for a wide range of substances without the requirement for specific chemical analysis. Given the basic requirements it would seem appropriate as a first step to examine the existing test categories and to consider their potential for providing the necessary information.

6.2 BIODEGRADABILITY TESTS

6.2.1 Ready Biodegradability Tests

The methods for assessing ready biodegradability usually provide the only biodegradation data available at the base set level. However, the use of the present OECD Ready Biodegradability Tests 301 A-F (OECD, 1983) as a basis for exposure assessment raises a number of questions. The mathematical models require information on the kinetics of primary biodegradation. This information cannot be derived from measurements of the extent of ultimate biodegradation for the following reasons:

- A ready biodegradation test determines the rate of ultimate biodegradation of the substance, whereas for the calculation of the PEC rate constants required are related to primary degradation. It should be noted that a substance with a low rate of ultimate biodegradation does not necessarily have a low rate of primary degradation as well.

- In the ready biodegradation test the substance is used as the sole carbon source at a much higher concentration than would normally be expected to occur in the environment. High concentrations of the substance may give rise to problems such as exceeding the water solubility or to toxic effects on the degrading organisms. These conditions will normally not occur in surface waters.

- Low concentrations of the substance in surface waters in the presence of many different carbon sources is likely to result in the degradation by co-metabolic processes rather than the catabolic processes which take place in the ready biodegradation test.

Any one of these factors could lead to an underestimate of the degradation rate resulting in an overestimation of the PEC. A further limitation of the ready biodegradation test is that it will generally not allow the estimation of the percent of ultimate degradation.

6.2.2 Inherent tests

For the purpose of this report, a substance which cannot be classified as "readily" biodegradable but can be shown to be susceptible to microbial attack by inocula from environmental sources is defined as "inherently" biodegradable.

Testing for inherent biodegradability could be performed by means of one of the three OECD Guideline methods, i.e. SCAS, Zahn/Wellens, MITI II. The first two tests measure removal (including biodegradation but also adsorption). Tests in this category have been designed to have very high biodegradation potential. For substances which do not degrade under conditions of inherent tests it is assumed that under environmental conditions biodegradation may be insignificant.

Inherent tests will tend to over-estimate biodegradation in environmental compartments and even in waste water treatment plants especially if long incubation periods are used. These tests should be used with care for predictions of biodegradation kinetics for environmental compartments. They can be used to prove that inherently biodegradable substances disappear through biodegradation under environmental conditions with a low rate (e.g. in the soil compartment).

The Zahn-Wellens test was and currently is used in Germany to make predictions on the elimination of substances in sewage treatment plants. For this purpose the biodegradation results obtained after 7 days are used preferentially.

Finally, it is essential that a distinction be made between biodegradation and adsorption. For soluble substances with low adsorption measured after 3 hours biodegradation can be calculated as described in Directive 88/302/EEC. In other cases this distinction can usually be made by using the bacteria from the inherent test to inoculate a "ready" test based on CO_2 production or oxygen uptake or by directly measuring CO_2 production during the inherent test.

6.2.3 Simulation Tests

Suitable laboratory techniques exist for simulating activated sludge sewage treatment which can provide accurate predictions of the behaviour of substances in this process. In addition, the kinetics of biodegradation can be studied directly and the effects of variation in operating conditions can be assessed. Such tests only provide information on biodegradation if the concentration of the substance in both plant effluent and in the waste activated sludge is determined. In such cases a precise assessment of the initial levels in sludge amended soils is also obtained. These tests are recommended for the confirmatory phase. However, although the test protocol is highly appropriate for sewage treatment, the necessity for specific analysis may severely limits its use, particularly for complex mixtures.

6.3 MODELLING OF WASTEWATER TREATMENT PLANTS (WWTP)

Volatile substances are removed from the aqueous phase to a certain extent by gas stripping and volatilisation depending on the aeration and mixing techniques used in different plants. Some substances are further removed by adsorption processes depending on their molecular structure and on the condition of the sludge flocs. This will lead to the transport of substances from WWTPs to soil with disposed surplus raw sludge used as fertiliser or, more typically, after treatment in anaerobic digesters frequently used in sludge reduction processes.

This section is primarily concerned with estimating the biodegradation of substances during sewage treatment. The ultimate fate of any of the substances which is removed by treatment processes and subsequently transferred unchanged to other environmental compartments is considered in later sections.

As described in Section 4, mathematical models are used to predict levels of the substance in the effluent, the waste sludge and the air emission from the aeration basin. In order to calculate the fraction of the substance removed by biodegradation, rate constants for the biodegradation process are required. Recommendations on how these rate constants should be derived for the Screening, Confirmatory and Investigative phases are outlined below.

6.3.1 Screening Phase

Readily Biodegradable Substances

Readily biodegradable substances are assumed to biodegrade in aerobic surface waters. Experience has shown that readily biodegradable compounds reaching the aeration stage of the sewage treatment process undergo mineralisation greater than 90%. Assuming the 90% as a conservative value the hydraulic retention time in the aeration basin is calculated to be 3 hours. The default value for the rate constant in the WWTP model SIMPLETREAT (Struijs *et al*, 1991) is 3 $hour^{-1}$.

Using a similar approach the corresponding default values for use in the WWTREAT model (Cowan *et al*, 1993) are calculated as 3 and 0.07 $hour^{-1}$ for the dissolved and adsorbed phases respectively.

Inherently Biodegradable Substances

Procedures alternative to the OECD methods for inherent biodegradability (302 A-C) (OECD, 1983) can demonstrate more reliably whether a substance is inherently biodegradable, e.g. by using the tests of ready biodegradability with pre-acclimatised organisms as an inoculum.

In the case of continuous exposure, pre-exposure of the organisms to a substance is essential if results predictive of sewage treatment processes are to be obtained since acclimatisation of the biomass is fundamental to biological treatment of sewage. It should be noted that such processes are also operative in the simulation studies and therefore there is no reason why they should be excluded from preliminary tests designed to provide similar information. In order to provide unequivocal evidence of biodegradation it is preferable if the ready test used is based on measurement of CO_2 production or oxygen uptake.

The introduction of slow growing organisms can occur with the simple batch pre-exposure techniques although these organisms could not easily be sustained in conventional activated sludge plants. Some approaches based on batch tests are described below but for this reason the data should be treated with caution. The use of the SCAS test procedure for acclimatisation is probably unacceptable since sludge retention times are usually too high, often being in the order of about 50 days unless controlled at a more realistic value. Consequently the use of some type of dynamic procedure which facilitates proper control over the growth kinetics of the biomass as it develops under normal WWTP conditions is preferred.

At present the only obvious solution is to run a simulation test under controlled conditions (i.e. defined sludge and hydraulic retention times) to produce an acclimatised inoculum for simple screening tests. Options which would limit the required effort could be:

- a miniaturised version of the porous pot. No analysis is required at this stage and either a synthetic waste water or the supernatant of settled domestic sewage could be used. The use of this type of pre-adaptation should ensure that only micro-organisms that are capable of sustaining a viable population in conventional sewage treatment processes could develop;

- a standard simulation test where a number of test substances are dosed simultaneously.

Samples of sludge or the plant effluent can then be used to inoculate a ready biodegradation test with preference of a protocol where CO_2 evolution or O_2 consumption is measured. Those materials reaching the required pass levels run with the preadapted inoculum are given a biodegradation rate constant of 3 hours^{-1}.

In Germany, the Zahn-Wellens test with an incubation period not longer than 28 days traditionally has been used as a protocol to adapt microorganisms to a given substance. Further critical evaluation of existing data and additional comparative tests will be needed to verify whether such an approach using a simple batch technique can be used as an alternative to the dynamic porous pot approach described in this report.

6.3.2 Confirmatory Phase

At this stage it is necessary to predict the PEC with greater accuracy within the constraints of a laboratory test procedure. It is therefore proposed that in the confirmatory phase rather than using a default value based on a simple test of ultimate biodegradability the rate constant be determined directly and that it should be derived from measurement of primary biodegradation.

In cases where Monod kinetics are considered appropriate, the method described by Cech *et al* (1984) using the acclimated sludge produced as described in 6.3.1 could be applied. This method requires the use of sophisticated respirometers in which the oxygen utilisation rate is measured at several different substrate concentrations in order to determine K_s and μ_{max}, where :

- K_s [mol/l] is defined as the constant analogous to the Michaelis-Menten constant of enzyme kinetics, being numerically equal to the substrate concentration supporting a growth rate equal to $1/2 \cdot \mu_{max}$, and

- μ_{max} [h^{-1}] is defined as the growth rate at saturating concentrations of the nutrients (Stanier *et al*, 1981).

The principal advantage of this method is that the kinetic constants are determined on sludge produced under the operating conditions (realistic hydraulic and sludge retention times) being applied during the acclimatisation period and should be applicable to all processes run in a similar manner.

The values obtained are used in the Monod kinetics option in the HAZCHEM risk assessment model (ECETOC, 1994b) to predict the fate of the substance during sewage treatment.

In those cases where MONOD kinetics are not applicable, the batch activated sludge (BAS) system is currently used to derive biodegradation rate constants. The procedure consists of incubating a low initial substance concentration (0.1 to 2 mg/l) with sludge (2,500 mg/l solids) similar to the approach described by Games *et al* (1982). The primary biodegradation rate constant can be determined, if specific analytical methodology is available. Where this is not the case, the mineralisation rate constant k [day^{-1}] can be calculated from the CO_2-production data using non-linear regression and the exponential model of Equation 3:

$$y = a \cdot (1 - e^{-k(x-c)}) \qquad (3)$$

Where:-

y = CO_2-production in % of theoretical
x = time [d]
a = upper asymptote in % of theoretical
c = lag time [d].

The following limitations of the method should be considered: the low substrate concentration implies the use of radioactive material for the proper detection of the CO_2 evolution thus severely restricting the applicability of the method due to high cost. As pointed out in Section 6.1, CO_2 production is a parameter for *ultimate* biodegradation which does not directly relate to *primary* degradation as needed for the purpose of exposure assessment.

6.3.3 Investigative Phase

In the Investigative Phase the accepted procedures involve laboratory scale simulation tests or, in the case of existing substances, monitoring full-scale sewage treatment plants.

A suitable laboratory technique is the Activated Sludge Simulation Test, which can provide accurate predictions of the WWTP elimination behaviour of a substance under concern. For risk assessment purposes the best solution is to express primary biodegradability directly using specific analytical methods. In addition kinetic data on the biodegradation process can be studied and the effects of variation in operating conditions can be assessed.

For substances which tend to adsorb on sludge, such tests only provide information on biodegradation if the concentration of the substance in both plant effluent and in the waste activated sludge is determined. For these substances the levels in sludge amended soils should also be obtained for the environmental exposure assessment.

Table 11 provides an overview on a recommended sequence of tests to be performed, where necessary, in the Screening, Confirmatory and Investigative phases.

6.4 DEGRADATION IN ENVIRONMENTAL COMPARTMENTS

6.4.1 Background

Specific studies for degradation in soil and other environmental compartments are elaborate and usually involve the synthesis of radiolabelled test material or a specific method capable of detecting the substance at levels relevant to the environmental compartment. In view of the large number of substances to be investigated, such studies cannot be envisaged at the base set level and simpler tests need to be used to provide the data. A new biodegradation study with pre-adapted microorganisms should be developed as proposed in Section 6.3.1. Such a test may also be a useful indicator of the behaviour of substances in the environment. The approach used in this

Table 11 Prediction of Removal in Waste Water Treatment Plants Based on Biodegradation Kinetics

Phase	Test / Result	Model	Default value		
Screening	RB: pass	WWTP	3	$[h^{-1}]$	(liquid phases)
			0.07	$[h^{-1}]$	(solid phases)
	RB: fail	WWTP	0	$[h^{-1}]$	
	IB: pass and preadapted RB: pass	WWTP	3	$[h^{-1}]$	(liquid phases)
			0.07	$[h^{-1}]$	(solid phases)
	IB: pass and preadapted RB: fail	WWTP	0	$[h^{-1}]$	
Confirmatory	Monod	WWTP	K_s	[mol/l]	measured
			μ_{max}	$[h^{-1}]$	measured
	Batch Activated Sludge[1]	WWTP	k	$[d^{-1}]$	measured
Investigative	Simulation tests[2]	-	Measured PEC		
	Monitoring WWTP[2]	-	Measured PEC		

RB Ready Biodegradability
IB Inherent Biodegradability
1 Derived from respirometric test with preadapted inoculum
2 With mass balance

section examines how predictions of primary degradation rates in environmental compartments can be made from the results of the existing screening tests for ready and inherent biodegradability.

6.4.2 Prediction of Environmental Degradation Rates from Screening Data

Various approaches have been made to solve the problem of estimating the biodegradation rates of substances in the environment on the basis of their behaviour in screening level biodegradation tests (eg. Larson, 1983; Howard and Banerjee, 1984; Boethling and Sabljić, 1989; Gledhill *et al*, 1991). One such approach, forming part of the Dutch USES simulation model (RIVM, VROM, WVC, 1994), proposes the use of default values for environmental degradation rate constants which are assigned on the basis of the results of OECD Ready and Inherent biodegradability tests. Whilst this approach has some merit, conceptually, the relationship between the test results and half-lives which have been used to propose rate constants have not been displayed clearly.

The approach used in this section to examine the relationship between the biodegradation rates of substances in screening tests and those in the various environmental compartments was to analyse relevant information from an existing database. The BIODEG database (Howard *et al*, 1987) was found to be suitable for this purpose as it contains such data for a wide range of substances. A summary level search of BIODEG provided data for all those substances in the database with results from screening, soil and surface water biodegradation tests. The relationships between the results of the screening tests for biodegradability and the biodegradation rate constants in the environmental compartments were then assessed on the basis of the following procedure:

- all data sets sufficiently complete to allow an interpretation were included;
- the results of biodegradation studies in freshwater were used in preference to those in marine water;
- where "complete degradation" was indicated in a given period of time, this was taken as being equal to four half-lives;
- the screening level biodegradability classification of each substance was assigned;
- the half-lives for biodegradation were calculated assuming first order kinetics;
- any lag-phase was subtracted from the overall degradation timescale.

Data for a total of 36 substances could be retrieved from the BIODEG database. They represent a wide selection of substances with different physico-chemical properties (e.g. water solubility, partition coefficient). A comparison of half-lives in surface water and soil could be made for 31 substances and is presented in Table 12; full information on CAS-Number, name and available data is given in Appendix B.

The intention was to classify the substances according to the USES classifications of biodegradability. Based on the data it was decided to assign only two classes to the biodegradability:

- "biodegradable" to substances which achieved at least 20% biodegradation in static laboratory batch tests with any inoculum;
- "non-biodegradable" to substances for which there was no evidence of at least "inherent biodegradation".

Table 12 **Comparison of degradation in Surface Water and Soil (substances retrieved from the biodegradation database Howard *et al*, 1987)** (See Appendix B for full data set)

CAS Number	Half-life* in surface water (days)	Half-life in soil (days)
Biodegradable		
57-11-4	1.9	7.6
62-53-3	5	135m
64-17-5	0.13	0.14
79-06-1	3	5
90-15-3	590m	0.07-5.1
108-95-2	2.2	3.4
114-26-1	7	10
124-40-3	0.24	7.1
131-11-3	3	1
139-13-9	2.6	2.8
1836-77-7	10	18
5234-68-4	5	5
84-74-2	3.5	15
87-86-5	25	15
88-06-2	5.4	19
90-30-2	115m	41m
95-57-8	13	1.4
95-95-4	46	78
106-47-8	4	3.4
106-47-9	220	6.3
117-81-7	56	9.7
118-96-7	no degn in 42d	120m
120-83-2	10	10
208-96-8	2	40
593-45-3	14	76
621-64-7	100	45
1886-81-3	25	77m
Non-biodegradable		
55-18-5	No deg in 108d	23m-35
56-55-3	300	90
91-94-1	72	4350m
95-77-2	800m	52.3

m mineralisation rate
* Based on primary biodegradation unless otherwise indicated

The analysis showed that all 30 substances classified as "biodegradable" in a laboratory batch test were also degradable in the corresponding laboratory or field studies for the surface water/sediment compartments. For the 6 substances classified as "non-degradable" in such tests, biodegradation in water/sediment and soil compartments was still observed, although the half-life times (where available) tended to be longer. Test methods used and results varied widely (even for different studies on the same compound). The data showed that for "biodegradable" substances half-life times for primary biodegradation in soil and water/sediment were below 100 days (with the exception of CAS-No. 106-47-9 (4-chlorophenol) which may be due to microbicidal properties of the substance at higher concentrations), including substances which are highly absorbed (e.g. phthalates).

USES also provides default biodegradation rate constants for the sediment compartment of the ecosystem. It was found to be impossible to extract meaningful kinetic data for this compartment from either the BIODEG database or from the general scientific literature. It is extremely difficult to separate the contributions of sediment and water phases to the overall biodegradation of a substance in a water/sediment system. The issue of biodegradation rates in sediment is further complicated by the fact that aerobic degradation is likely to take place only in the top few millimetres of sediment and that degradation at depth will probably occur by anaerobic mechanisms which are not taken into account by any current test system.

6.4.3 Comparison of degradation in water/sediment systems and soil for selected plant protection chemicals

Although the special case of plant protection chemicals will not be addressed in detail in this report - these substances are subject to specific regulations before they can be placed on the market - they are one of the few classes of substances for which behaviour in soil and water/sediment systems (metabolism, rate of degradation under different climatic conditions and evaluation of their potential to contaminate ground water) is well investigated. Therefore some (company in-house) degradation data for soil and water/sediment systems were related to information available from ready and inherent biodegradability studies.

Because plant protection chemicals are normally tested in more sophisticated studies with radiolabelled material or at least compound-specific analysis, only relatively few ready or inherent biodegradability test results were available for evaluation and those studies that were available (e.g. modified Sturm tests) showed that most of the compounds did not reach the pass level for ready or inherent biodegradability although they do undergo biodegradation in soil and in surface water/sediment systems.

Results of degradation in water/sediment and soil were compared for 20 plant protection chemicals from different companies. Since the studies represent confidential company data, the results are given in coded form. All studies were carried out with radiolabelled active substances. In the case of the aquatic degradation studies, the tests were conducted with river water and/or pond water with 1 % (v/v) of sediment. Different German standard soils were normally used to test soil degradation.

classification for biodegradation was used as described in Section 6.4.2. The results are listed in Table 13.

Table 13 Comparison of Degradation in Water/sediment Systems and in Soil

Substance Code	Water/sediment systems			Soil		
	CO_2 at the end of study (%)	Duration (d)	Average half-life (d)	CO_2 at the end of study (%)	Duration (d)	Average half-life (d)
"Biodegradable"						
1003	80.00	90	0.7	80.00		1
2014	65.00	50	10	50.00	140	11
1004	55.00	90	4.7	20.00		20
1015	30.00	90	0.7	60.00		1
1001	20.00	90	2.25	50.00		5
1011	20.00	90	70.45	-		42
2010	20.00	259	56	55.00	365	5
"Non-biodegradable"						
1002	15.00	90	5.2	50.00		1
2008	12.00	73	38.5	34.00	168	55
1010	10.00	90	5.7	10.00		10
2001	9.00	77	100	0.70	120	57.5
1016	5.00	90	91.6	-		7.5
1012	3.00	90	9.5	-		16
2012	2.50	84	20	40.00	365	25
2004	1.75	90	405	60.00	365	20
2002	1.20	70	210			75
2007	1.20	77	58.5	60	270	58.5
1018	1.00	90	334.65	-		160
2006	1.00	122	500	1.70	225	88
2009	0.50	73	38.5	1.00	365	40

Based on the CO_2 evolution criterion of 20%, 7 out of the 20 substances examined are expected to be "biodegradable". The measured half-life times observed for "biodegradable" substances are below 50 and 75 days for soil and water/sediment systems, respectively. For those substances classified as "non-biodegradable", the half-life times show a much wider variation, where about 50% of the substances are still below 50 and 75 days for soil and water/sediment systems, respectively.

below 50 and 75 days for soil and water/sediment systems, respectively. For those substances classified as "non-biodegradable", the half-life times show a much wider variation, where about 50% of the substances are still below 50 and 75 days for soil and water/sediment systems, respectively.

From the table it can be shown that most of the substances classified as "non-biodegradable" are degraded in the water/sediment and soil compartments with half-lives shorter than one year. Hence the default half-life time of 580 days for soil and surface water in case of inherently biodegradable compounds (20-70% biodegradation) as proposed in the current version of USES will usually lead to an overestimation of PECs.

SECTION 7. ILLUSTRATIONS OF PEC CALCULATIONS

7.1 CALCULATION OF $PEC_{INITIAL}$ FOR THE AQUATIC COMPARTMENT

$PEC_{initial}$ can be calculated by means of generic emission scenarios derived from case studies using realistic worst case assumptions. In the development of such generic emission scenarios it should be kept in mind that several worst case assumptions in one scenario will lead to an unrealistically high $PEC_{initial}$ because, for example, three 90-percentile assumptions end up in a 99.9-percentile assumption.

Extreme local situations have to be regulated specifically by local authorities and cannot be covered by a European risk assessment. For some substances regulations on emissions exist and should be noted when establishing an emission scenario.

Emission scenarios cover release, elimination and dilution processes. Release estimation and elimination in a sewage treatment plant due to biodegradation, sorption and volatilisation is described in previous sections. Other elimination processes e.g. sorption to activated carbon are difficult to be included in generic emission scenarios and will require substance-specific evaluation.

In the following examples emission scenarios are given which use different approaches for the calculation of $PEC_{initial}$.

EXAMPLE 1 Hospital Disinfectant

The use of the disinfectant in a hospital is a realistic worst case assumption; private use would give lower environmental concentrations.

In Table 14 an emission scenario is given which is based on the concentration of the active ingredient in the disinfectant and the various dilutions. Sewage of instrumental and other disinfection is mixed with other hospital sewage and released to a public sewage treatment facility. The disinfectant is assumed to have a 90 % elimination rate in the sewage treatment plant. The sewage portion of the disinfectant solutions in hospital sewage was derived from the literature (Gode and Hachmann, 1992).

Table 14 Emission Scenario "Hospital Disinfectant" Based on Concentration and Dilutions

Concentration of active ingredient C	2,000 mg/l
Sewage portion of the disinfectant solutions in hospital sewage is < 0.2% resulting in dilution D_1	> 500
Dilution during release into the public sewage system network D_2 (assumed value)	10
Elimination in the sewage treatment plant E (%)	90
Dilution during outlet of the sewage plant into a small river D_3	10
Overall dilution factor $D = D_1 \cdot D_2 \cdot D_3$	> 50,000

$$PEC_{initial} = \frac{C}{D} \cdot \left(\frac{100 - E}{100} \right) < 4 \mu g/l$$

In Table 15, a case study for the release of an aldehyde as the active ingredient in a hospital disinfectant is given for the situation in Darmstadt (Germany) which is based on specific use pattern.

Table 15 Case Study Release of an Aldehyde as Active Ingredient in a Hospital Disinfectant for the Situation in Darmstadt

Consumption rate of disinfectant in municipal hospital	2,800 kg/a
Content of aldehyde (worst case)	10 %
Consumption of aldehyde in municipal hospital	280 kg/a = 0.77 kg/d
Number of beds in municipal hospital	1,100
Specific consumption per bed and day	0.77 kg/d·1,100 = 0.7 g/d·bed
Total number of hospital beds in Darmstadt	1,700
Total consumption of aldehyde based on 1,700 beds W	0.7 g/d · 1,700 = 1.2 kg/d
Elimination in waste water treatment E	90 %
Flow of wwt facility Q	42,000 m^3/d
Dilution in surface water D	10

$$PEC_{initial} = \frac{W}{Q \cdot D} \cdot \left(\frac{100 - E}{100} \right) = 0.3 \mu g/l$$

From the consumption of the disinfectant in the municipal hospital of Darmstadt (1,100 beds) and an assumed content of 10% (worst case) of the aldehyde (Nottebrock, 1992) a specific consumption per bed and day is calculated. Because there are other hospitals in Darmstadt the total number of hospital beds is 1,700 which has to be considered for the calculation of the total consumption of the hospital disinfectant in Darmstadt. For the elimination in waste water treatment 90 % is assumed. The flow of the waste water treatment facility is 42,000 m^3/d (Arendt *et al*, 1983) and for the dilution in surface water a factor of 10 was used.

For both cases it must be emphasised that it is assumed that all of the active ingredient remains intact and ends up in wastewater. This is a real worst case assumption leading to a $PEC_{initial}$ which is higher than it would be in the real situation.

EXAMPLE 2 Intermediates

If the dilutions of the substance in the technosphere are small compared to the dilution in the receiving surface water, an emission scenario as described in the following example is appropriate.

General Principles

Release estimation is based on:

- production volume per year;
- an emission factor for production of the intermediate;
- an emission factor for use of the intermediate;
- an elimination factor in biological waste water treatment facilities.

The initial concentration in rivers is calculated from the emission to the receiving surface water (e.g. in g/s) and the river flow (m^3/s):

$$PEC_{Initial} = \frac{W}{Q} \cdot \frac{f_R}{100} \cdot \left(\frac{100-E}{100}\right) \qquad (6)$$

Where:-

W = production volume per time unit (e.g. t/a or kg/s)

f_R = total release fraction $f_R = f_{R,P} + f_{R,U}$ (in %)

$f_{R,P}$ = release fraction for production of the intermediate (in %)

$f_{R,U}$ = release fraction for use of the intermediate (in %)

E = elimination in biological waste water treatment (in %)

Q = river flow (m^3/s)

It is assumed that production and use of the substance occurs 365 days per year.

In the screening phase the approach presented is more feasible than the calculation of effluent concentrations in combination with dilution factors because it is based on readily available data.

Emission factors

There are different parameters influencing emissions during production and use of the intermediate. Physico-chemical properties, wet or dry processes, type of reaction, batch or continuous production and on- or on/off site handling are presumed to play a key role. However, experience in plant operation shows that the major discriminating factor between the above mentioned parameters is the differentiation between wet and dry processes. In this context wet processes are those where water is used either during reaction, work up or vessel cleaning. Dry processes are those where no water at all is used.

Generally the production of very reactive, water sensitive compounds like acid chlorides, isocyanates or acid anhydrides is performed without any water. Also intermediates which are made in gas phase reactions like carbon disulphide or diketene are normally handled without water. In Germany these plants are defined in the plant licensing as not producing any waste water and hence they are not attached to any sewer.

In order to obtain reliable data on release factors for production and use of intermediates, 29 BUA Reports were examined (Appendix A). These release factors were analysed statistically to get 90 percentiles for the release during production and use. From these data release factors are proposed and are given in Table 16.

Table 16 Proposed Release Fractions of Production Volume for Intermediates

Release fraction $f_{R,P}$ (%) for production		Release fraction $f_{R,U}$ (%) for use	
wet	dry	wet	dry
0.3	0	0.7	0

Elimination factors

Elimination through plant integrated physico-chemical treatment

Treatment at the plant (e.g. adsorption to activated carbon, precipitation etc.) is already included in the release factors. For 3,3'-Dichlorobenzidine the difference before and after this treatment is outlined in Table 17.

Table 17 Release Fractions of Production Volume without and with Physico-Chemical Treatment

Name	CAS No.	BUA No.	Release fraction (%) during production	
			before physico-chem.treatment	after physico-chem.treatment
3,3'-Dichloro-benzidine	91-94-1	30	0.06	0.012

Elimination in biological waste water treatment

For readily biodegradable substances or substances which are not biodegradable the elimination can be estimated using the table in Chapter 11, Appendix 4 of EEC (1994) or by using an appropriate waste water treatment model.

For those substances which are not readily but inherently biodegradable estimation methods for the calculation of elimination in the waste water treatment system from laboratory test results were proposed in Section 6.3.1.

River-flows

Plants for intermediates are normally located on larger rivers. To verify this assumption, data on plant locations, plant capacities, rivers and mean river flows were collected (Appendix A, Tables A.3 and A.4). Data on plant locations and plant capacities were taken from

- BUA reports listed in Table A.1;
- Data on Bulk Chemicals (Chem-facts Germany, 1992).

For some substances only total capacities for Germany were available from the BUA reports. Mean river flows for the plant locations were given by the companies or taken from 'Daten zur Umwelt 1990/91' (UBA, 1990/91). For locations at estuaries like the Jadebusen (Wilhelmshaven) mean riverflows are not applicable due to the tides.

In Table A.3 the data were listed in substance order. For the calculation of the 90-percentile of the river-flows the data were presented in river-flow order (Table A.4).

The 'Emscher' listed at the top of Table A.4 is not a real river because it ends up in a sewage treatment facility before discharging into river Rhine. Therefore the data for the 'Emscher' were not used in the calculation.

For the remaining 112 locations the 90 percentile of the riverflows is 60 m^3/s (see Table A.5). This value should be used as a default value for Q in the calculation of $PEC_{initial}$ if no specific data are available.

7.2 CALCULATION OF PEC_{LOCAL} FOR THE AQUATIC COMPARTMENT

For the calculation of PEC_{local} for the aquatic compartment the river model RIVMOD (ten Berge, 1992) can be used.

RIVMOD allows the calculation of the elimination of a substance in a biological waste water treatment facility, e.g. according to Cowan *et al* (1993), and the subsequent fate and distribution in a river. The distribution in the surface water as well as in sediment is given as a concentration profile along and across the river. Elimination in the river is also calculated and given as the downstream distance where 50% is eliminated.

As an example the detergent LAS was chosen. LAS was monitored in the river Isar near Munich (Schöberl *et al*, 1994) and for the calculation of PEC_{local} the data on release of LAS, size and operating parameters of the waste water treatment facility Munich II and the river parameters and background concentration of LAS in the river Isar at that site were used (see Appendix E). The calculated elimination in the waste water treatment facility as well as the concentration in the river 1,400 meters downstream where LAS was measured are in good agreement (Table 18).

Table 18 PEC$_{local}$ Calculation for LAS at WWTP Munich II

Discharged LAS	63 kg/h	
Water flow in WWT Munich II	216,000 m^3/d	
Resulting influent concentration in WWT	7 mg/l	
	Calculated	Measured
Removal in WWT	98.7%	98.8%
Effluent concentration WWT (dissolved + suspended)	90 µg/l	67 ± 32 µg/l
Background conc. of LAS upstream		9 µg/l
PEC$_{local}$ in river Isar 1400m downstream (dissolved + suspended)	19 µg/l	11 ± 3 µg/l

7.3 CALCULATION OF PEC$_{REGIONAL}$

For the calculation of PEC$_{regional}$ the modelling program HAZCHEM Version 2.0 was used (ECETOC, 1994b). In HAZCHEM elimination in a biological waste water treatment facility is modelled according Namkung and Rittmann (1987). Fate and distribution in the different environmental compartments are calculated by a fugacity model which is based on Mackay level III (Mackay *et al*, 1992).

As an example the plasticiser Di-2-ethylhexylphthalate (DEHP) was selected (see also ECETOC, 1994a). The PEC$_{regional}$ for the different compartments are calculated for the region of the European Union, release data were provided by the European Council for plasticisers and intermediates (ECPI, 1993).

In Table 19 the PEC$_{regional}$ values for the different compartments which were calculated with HAZCHEM are listed and compared to measured data (details see Appendix D; see also ECETOC, 1994a). Measured and calculated values for air, water and sediment are in good agreement.

Table 19 Comparison of Measured Environmental Levels for DEHP with Calculated Levels for Different Compartments

MEDIUM	MEASURED	REFERENCE	CALCULATED (HAZCHEM)
Air (mg/m^3)	$0.4\text{-}2.9 \cdot 10^{-6}$ $\leq 5 \cdot 10^{-6}$ (remote areas)	1 2,3	$0.6 \cdot 10^{-6}$
Water (mg/l)	$0.05\text{-}30 \cdot 10^{-3}$ $< 0.1\text{-}4.0 \cdot 10^{-3}$ (rivers, lakes) up to 0.3 (rivers, lakes) $0.05\text{-}1.4 \cdot 10^{-3}$ (ground water at waste water infiltration sites)	1 2 3 3	$1.2 \cdot 10^{-3}$ (surface water) $0.13 \cdot 10^{-6}$ (ground water)
Sediment (mg/kg)	1-70 (river sediment) (up to 1,500 sediment near discharge points) 1.8-18.3 (Rhine) 0.1-8.9 (Weser)	2 2 4 4	0.7
Soil (mg/kg)			$0.1 \cdot 10^{-3}$ (arable) $0.22 \cdot 10^{-3}$ (natural)

1	IARC (1982)
2	IPCS (1992)
3	UK-MAFF (1987)
4	Furtmann (1993)

SECTION 8. CONCLUSIONS AND RECOMMENDATIONS

Regional Generic Model

Sensitivity analyses and a critical review of parameters have shown that fugacity models of the "Mackay level III" type as described in this report are in principle suitable for risk assessment on a regional scale.

Basically these models can be used to indicate environmental compartments of concern in the longer term, i.e. in a qualitative manner.

For chemicals mainly released via diffuse sources, these models may also be used quantitatively, provided that the amounts emitted into the environment can be estimated with a sufficient degree of accuracy. The model published by Mackay *et al* (1992) was used as a basis and was adapted to represent a generic European scenario.

Major adaptations were considered necessary for geographic parameters, such as the water depth and the water residence time, which should be related to the rain excess. The parameters proposed to represent a realistic European generic scenario based on the geometrical means are summarised in Section 4.2.4.

Local Generic Models for Air, Water and Soil

To calculate environmental concentrations in local scenarios, approaches for the water, soil and air compartments are proposed. For the water compartment a model is proposed that simulates a discharge (direct or via a WWTP) into a river. This can be adequately modelled with RIVMODEL (ten Berge, 1992). Based on literature data from The Netherlands, it can be concluded that generally low waste water discharges are coupled to low flows and low dilution situations. High waste water discharges are usually released into surface waters with higher flow rates and higher dilutions, as could be expected. Accordingly two scenarios have been proposed, a lowland river scenario with low flow rate and a mountain area river scenario with higher flow rate.

An environmental risk assessment for air and soil in these compartments is presently only possible to a limited extent. However, concentrations are also needed to calculate indirect exposure of man.

A scenario for local air and soil modelling is presented in this report which includes the most relevant exposure routes. A minimum resource area is not yet well established, but an acceptable approach representing the present state-of-the-art is described in this report. Further details on indirect human exposure are given in ECETOC (1994a).

Release and Emission Estimation

Reliable data on release and emission of a substance are the key elements for the calculation of realistic Predicted Environmental Concentrations for the different environmental compartments.

In the majority of cases release of a substance is determined by the process involved including dedicated treatment and not by the physico-chemical data of the substance. For example, high water solubility of a reactive dye does not necessarily lead to a high release because this is determined by the fixation process, i.e. chemical binding of the dye to the fibre. This shows that for the different use categories process-oriented release scenarios are necessary.

Emission estimation requires scenarios which cover release, elimination and dilution processes. It is important to use process-oriented release data, to consider all dilution processes (internal and external) and to use reliable elimination data e.g. in a biological waste water treatment plant. For emission scenarios default values for process data, elimination and dilution should be given which cover an average (generic) situation and which can be overwritten when substance-specific data are available. Using only worst case data would lead to unrealistically high PECs.

Up till now only few of the release and emission scenarios available fulfil the requirements mentioned above. There is an urgent need therefore to establish additional scenarios and to improve a number of others. Otherwise for many substances no realistic release and emission estimation is possible.

Biodegradation Kinetics

For the calculation of predicted environmental concentrations (PECs) information on the kinetics of primary biodegradation (degradation of the parent compound) is needed. It is difficult or almost impossible to derive kinetic biodegradation data directly from simple screening tests on ready biodegradation as they are normally available at base set level of the notification of new chemicals. Since ready biodegradation tests are based on the measurement of ultimate biodegradation, no direct correlation between the results from these tests and primary biodegradation exists. Therefore

- as a first step - default half-life times/rate constants have to be assigned to substances according to the results obtained in screening tests.

For the prediction of biodegradation rates in the waste water treatment plant a tiered approach including three steps is proposed, whereby steps 2 and 3 are required only if the PEC needs to be refined because of an unfavourable PEC/PNEC ratio. At the screening phase a default rate constant of 3 h^{-1} can be assigned to ready biodegradable compounds and to those which reached the corresponding pass level after acclimatisation. Acclimatisation - a process of key importance in waste water treatment - must be performed under strictly controlled conditions similar to those occurring in sewage works. At the confirmatory phase rate constants should be directly determined from measurement of primary biodegradation or based on respirometric methods whereas at the investigative phase comparative measurements of influent and effluent concentrations replace the use of default values or calculated rate constants.

An attempt was made to derive biodegradation half-life times for surface waters and soil by evaluating a biodegradation database and industry biodegradation data on plant protection chemicals. Data on soil and surface water half-life times were compared with results on ultimate biodegradability. Due to the limitations of the available data no recommendations on scientifically based default values to be used at screening level could be given although the data suggest that the default values used within existing risk assessment schemes may be overly conservative. At the confirmatory phase of the environmental exposure assessment the biodegradation rates in soil and surface waters will have to be derived from primary biodegradation testing requiring specific analytical methods or radiolabelled materials. For soil, standard simulation tests are available.

APPENDIX A. RELEASE OF INTERMEDIATES TO THE AQUEOUS ENVIRONMENT

This Appendix provides the data used for the development of a release scenario for intermediates. Table A.1 contains release data for a number of well examined substances. In Tables A.2 and A.3 the frequencies of the release of intermediates during production and use are given. Tables A.4 and A.5 provide locations and capacities of German production sites together with the local river flows. The 90 percentile of the river flows can be taken from Table A.5.

Table A.1 Release of Intermediates to Water before Waste Water Treatment

Name	CAS No.	BUA Report No.	Water Solub. (mg/l)[1]	Production volume (t/a)[2]	Production year	Release via synthesis (%)[3]	process type	Release via use (%)[2]	process type	Total release (%)[2]
Vinyl chloride	75-01-4	35		1,500,000	1979	0.0007	wet	0.0021	wet	0.0028
Carbon disulphide	75-15-0	83		52,700	1990	0	dry	-[4]		-[4]
Vinylidene chloride	75-35-4	33	2,500 (21)	20,000	1985	0.004	wet	0.0025	wet	0.0065
1,2,3,4,5,5-Hexachloro-1,3-cyclopentadien	77-47-4	25	1,1 (22)	5,000	?	0.006	wet	0.0004	wet	0.0064
3-Chloro-o-toluidine	87-60-5	55	4,500 (20)	500	1989	0.002	wet	< 0.01	wet	< 0.012
o-Nitrotoluene	88-72-2	41	437 (20)	45,000	1988	0.001	wet	0.05	wet	0.051
o-Nitroaniline	88-74-4	28		6,000	1987	0.3	wet	?	?	-
o-Nitrophenol	88-75-5	75	1,260 (20)	500	1988/89	0.024	wet	0.1	wet	0.12
2,5-Dichloronitrobenzene	89-61-0	65	80 (20)	2,400	1990	0.02	wet	0.017	wet	0.037
o-Nitroanisole	91-23-6	09	1,690 (30)	4,000	1987	1.0	wet	< 0.001	no release	1.0
N,N-Diethylaniline	91-66-7	40	130 (20)	1,200	1987/88	0.06	wet	1.4	wet	1.46
3,3'-Dichlorobenzidine	91-94-1	30	3 (25)	2,500	1987	0.012	wet	0.02	wet	0.032
o-Dichlorobenzene	95-50-1	53	140 (20)	12,000	1989	0.002	wet	0.3	wet	0.3
3-Chloro-p-toluidine	95-74-9	55	2,500 (25)	4,500	1989	0.002	wet	< 0.001	wet	0.002
5-Chloro-o-toluidine	95-79-4	55	1,200 (25)	200	1989	0.002	wet	0.02	wet	0.022
1-Chloro-2,4-dinitrobenzene and other isomers	97-00-7	42	350 (20)	4,500	1988/89	0.3	wet	0.04	wet	0.34
3-Trifluoromethylaniline	98-16-8	44	5,000 (20)	1,000	1988/89	< 0.02	wet	< 0.01	wet	< 0.03
Nitrobenzene	98-95-3	59	1,900 (20)	200,000	1989	0.001	wet	0.042	wet	0.043
m-Nitrotoluene	99-08-1	41	419 (20)	2,500	1988	0.001	wet	0.11	wet	0.11
1,2-Dichloro-4-nitrobenzene	99-54-7	52	151 (20)	14,000	1988/89	0.048	wet	< 0.005	wet	0.05
p-Nitrotoluene	99-99-0	41	345 (20)	25,000	1988	0.005	wet	0.1	wet	0.11

Name	CAS No.	BUA Report No.	Water Solub. (mg/l)[1]	Production volume (t/a)[2]	Production year	Release via synthesis (%)[3]	process type	Release via use (%)[2]	process type	Total release (%)[2]
p-Nitrophenol	100-02-7	75	12,400 (20)	2,000	1988/89	0.018	wet	0.003	wet	0.021
Tributylamine	102-82-9	23		600	1987	< 0.024	wet	?	?	-
N-Ethylaniline	103-69-5	51	2,670 (20)	1,800	1989	0.7	wet	0.7	wet	1.4
Acetic anhydride	108-24-7	70		170,000	1990	0	dry	0	dry	0
o-Chloroaniline/ m-Chloroaniline	108-42-9/ 95-51-2	57		5,000	1987	0.3	wet	1.1	wet	1.4
3,3'-Dimethoxybenzidene	119-90-4	27	60 (25)	500	1986	< 0.01	wet	< 0.1	wet	< 0.11
o-Tolidine	119-93-7	26	1,300 (25)	500	1987	< 0.01	wet	0.2	wet	< 0.21
2-Chloro-4-nitroaniline	121-87-9	43	300 (25)	1,500	1988	0.0075	wet	0.005	wet	0.0125
Adipic acid	124-04-9	68	15,000 (20)	230,000	1991	0.009	wet	0	polymeris.	0.009
2,4-Dinitrochloro-1-nitrobenzene	611-06-3	64	188 (20)	1,500	1990	0.01	wet	0.003	wet	0.013

[1] (temperature in °C)
[2] in Germany
[3] % of production volume
[4] special use in viscose production

Table A.2 Calculation of Frequency for the Release of Intermediates during Production - Part 1

No. of substances	Cumulative count.	%	Cumulative %	Release %
1	1	3.4	3.4	0.0007
3	4	10.3	13.8	0.001
4	8	13.8	27.6	0.002
1	9	3.4	31.0	0.004
1	10	3.4	34.5	0.005
1	11	3.4	37.9	0.006
1	12	3.4	41.4	0.008
1	13	3.4	44.8	0.009
3	16	10.3	55.2	0.010
1	17	3.4	58.6	0.012
1	18	3.4	62.1	0.018
2	20	6.9	69.0	0.020
2	22	6.9	75.9	0.024
1	23	3.4	79.3	0.048
1	24	3.4	82.8	0.060
3	**27**	**10.3**	**93.1**	**0.300***
1	28	3.4	96.6	0.700
1	29	3.4	100.0	1.000

* 90 percentile is < 0.3 %

Table A.3 Calculation of Frequency for the Release of Intermediates during Use - Part 2

No. of substances	Cumulative count	%	Cumulative %	Release %
1	1	3.7	3.7	0
1	2	3.7	7.4	0.0004
2	4	7.4	14.8	0.001
1	5	3.7	18.5	0.002
1	6	3.7	22.2	0.003
2	8	7.4	29.6	0.003
2	10	7.4	37.0	0.005
2	12	7.4	44.4	0.010
1	13	3.7	48.1	0.017
2	15	7.4	55.6	0.020
1	16	3.7	59.3	0.040
1	17	3.7	63.0	0.042
1	18	3.7	66.7	0.050
3	21	11.1	77.8	0.100
1	22	3.7	81.5	0.110
1	23	3.7	85.2	0.200
1	24	3.7	88.9	0.300
1	**25**	**3.7**	**92.6**	**0.700***
1	26	3.7	96.3	1.100
1	27	3.7	100.0	1.400

* 90 percentile is < 0.7%

Table A.4 Location, Capacity and River Flows of Production Sites for Bulk Intermediates in Germany

CAS-Nr.	*Substance*	*Company*	*Plant Location*	*Capacity [mT/a]*	*River*	*Mean flow [m^3/sec]*
75-01-4	Vinyl chloride	BASF	Ludwigshafen	100,000	Rhein	1260
		Hoechst	Gendorf	160,000	Alz	5
		Hoechst	Knapsack	100,000	Rhein	2270
		Hüls	Marl	350,000	Lippe	31
		Solvay	Rheinberg	200,000	Rhein	2270
		Wacker Chemie	Burghausen	225,000	Alzkanal	60
		Wacker Chemie	Köln	225,000	Rhein	2270
		ICI	Wilhelmshaven	225,000	Jadebusen	
		Total		**1,135,000**		
75-15-0	Carbon disulphide	Carbosulf	Köln-Weidenpesch	85,000	Rhein	2270
75-35-4	Vinylidene chloride	BASF AG	Ludwigshafen	20,000	Rhein	1260
87-60-5	3-Chloro-o-toluidine	Hoechst AG	Ff.-Griesheim	500	Main	188
88-72-2	o-Nitrotoluene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**45,000**		
88-74-4	o-Nitroaniline	Bayer AG	Leverkusen	3,500	Rhein	2270
		Hoechst AG	Ff.-Griesheim	2,500	Main	188
		Total		**6,000**		
88-75-5	o-Nitrophenol	Hoechst AG	Ff.-Griesheim	500	Main	188
89-61-2	2,5-Dichloronitrobenzene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**2,400**		
91-23-6	o-Nitroanisole	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**4,000**		
91-66-7	N,N-diethylaniline	Bayer AG	Leverkusen	1,000	Rhein	2270
91-94-1	3,3'-dichlorobenzidine	Hoechst AG	Ff.-Griesheim	2,500	Main	188
95-50-1	o-Dichlorobenzene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**12,000**		
95-74-9	3-Chloro-p-toluidene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**4,500**		

CAS-Nr.	***Substance***	***Company***	***Plant Location***	***Capacity [mT/a]***	***River***	***Mean flow [m³/sec]***
95-79-4	5-Chloro-o-toluidene	Hoechst AG	Ff.-Griesheim	200	Main	188
97-00-7	1-Chloro-2,4-dinitrobenzene	Hoechst AG	Frankfurt	2,400	Main	188
		Bayer AG	Leverk. /Dormagen	1,100	Rhein	2270
97-00-7	1-Chloro-2,4-dinitrobenzene/ 1-Chloro-2,6-dinitrobenzene	Hoechst AG	Frankfurt	1,000	Main	188
		Total		**4,500**		
98-16-8	3-Trifluoromethylaniline	Hoechst AG	Frankfurt	1,000	Main	188
98-95-3	Nitrobenzene	Bayer AG	Uerdingen	200,000	Rhein	2270
		Hoechst AG	Ff.-Griesheim	< 4,000	Main	188
		Total		**204,000**		
99-08-1	m-Nitrotoluene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**2,500**		
99-54-7	1,2-Dichloro-4-nitrobenzene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**14,000**		
99-99-0	p-Nitrotoluene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**25,000**		
100-02-7	p-Nitrophenol	Bayer AG	Dormagen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**2,000**		
102-82-9	Tributylamine	BASF AG	Ludwigshafen		Rhein	1260
		Ruhrchemie	Oberhausen		Emscher	18
		Total		**600**		
103-69-5	N-Ethylaniline	Bayer AG	Krefeld-Uerdingen	1,300	Rhein	2270
		BASF AG	Ludwigshafen	500	Rhein	1260
		Total		**1,800**		
108-24-7	Acetic anhydride	Hoechst AG	Knapsack	80,000	Rhein	2270
		Rhone Poulenc	Freiburg	40,000	Rhein	1260
		Wacker	Burghausen	10,000	Alzkanal	60
		Total		**130,000**		

CAS-Nr.	***Substance***	***Company***	***Plant Location***	***Capacity [m T/a]***	***River***	***Mean flow [m^3/sec]***
108-42-9	m-Chloroaniline	Bayer AG	Leverkusen	2,000	Rhein	2270
95-51-2/	o-Chloroaniline/	Bayer AG	Leverkusen		Rhein	2270
108-42-9	m-Chloroaniline	Hoechst AG	Hoechst	4,000	Main	188
		Total		**6,000**		
119-90-4	3,3'-Dimethoxybenzidine	Hoechst AG	Ff.-Griesheim	500	Main	188
119-93-7	o-Tolidine	Hoechst AG	Ff.-Griesheim	500	Main	188
121-87-9	o-Chloro-p-nitroaniline	Hoechst AG	Ff.-Griesheim		Main	188
		Bayer AG	Leverkusen		Rhein	2270
		BASF AG	Ludwigshafen		Rhein	1260
		Total		**1,500**		
124-04-9	Adipic acid	BASF AG	Ludwigshafen	180,000	Rhein	1260
		Bayer AG	KR-Uerdingen	42,000	Rhein	2270
		Huels	Marl		Lippe	31
		Total		**222,000**		
611-06-3	2,4-Dichloro-1-nitrobenzene	Bayer AG	Leverkusen		Rhein	2270
		Hoechst AG	Ff.-Griesheim		Main	188
		Total		**1,500**		
75-07-0	Acetaldehyde	Hoechst AG	Frankfurt/ Main	130,000	Main	188
		Hoechst AG	Knapsack	120,000	Rhein	2270
		Huels	Herne	80,000	Emscher	8
		Wacker	Burghausen	60,000	Alzkanal	60
		Total		**390,000**		
64-19-7	Acetic acid	BASF AG	Ludwigshafen	40,000	Rhein	1260
		Chemviron Carbon	Bodenfelde	5,000	Weser	149
		Hoechst AG	Frankfurt/ Main	270,000	Main	188
		Hoechst AG	Knapsack	250,000	Rhein	2270
		Wacker	Burghausen	80,000	Alzkanal	60
		Total		**645,000**		
67-64-1	Acetone	Phenolchemie	Gladbeck	315,000	Emscher	12
		RWE-DEA	Moers-Meerbeck	3,600	Rhein	2270
		Total		**318,600**		
79-10-7	Acrylic acid	BASF AG	Ludwigshafen	36,000	Rhein	1260
		Huels	Marl	60,000	Lippe	31
		Total		**96,000**		

CAS-Nr.	***Substance***	***Company***	***Plant Location***	***Capacity [mT/a]***	***River***	***Mean flow [m^3/sec]***
107-13-1	Acrylonitrile	Erdölchemie	Köln-Worringen	26,000	Rhein	2270
		Hoechst AG	Münchmünster (8071)		Donau	326
		Total		**26,000**		
62-53-3	Aniline	BASF AG	Ludwigshafen	30,000	Rhein	1260
		Bayer AG	KR-Uerdingen	150,000	Rhein	2270
		Total		**180,000**		
105-60-2	Caprolactame	BASF AG	Ludwigshafen	150,000	Rhein	1260
98-82-8	Cumene	Huels	Marl	140,000	Lippe	31
		Ruhr-Oel	GE-Buer	400,000	Emscher	12
		Total		**540,000**		
110-82-7	Cyclohexane	Ruhr-Oel	GE-Buer	100,000	Emscher	12
		Wintershall	Lingen (4450)	130,000	Ems	79
		Total		**230,000**		
120-61-6	Dimethyl terephthalate [DMT]	Hoechst AG	Gerreshofen	140,000	Lech	120
		Hoechst AG	Offenbach	95,000	Main	188
		Huels AG	Luelsdorf	155,000	Rhein	2270
		Huels AG	Steyerberg	190,000	Aue	11
		Total		**580,000**		
106-89-8	Epichlorhydrin	Solvay	Rheinberg	50,000	Rhein	2270
64-17-5	Ethanol	Erdölchemie	Köln-Worringen	60,000	Rhein	2270
		Holtzmann	KA-Maxau	45,000	Rhein	1260
		Huels	Herne		Emscher	8
		Total		**105,000**		
100-41-4	Ethylbenzene	BASF AG	Ludwigshafen	300,000	Rhein	1260
		Huels	Marl	300,000	Lippe	31
		Rhein. Olefin Werke	Wesseling	430,000	Rhein	2270
		DEA Mineralöl	Heide	12,000	Elbemündung	
		Total		**1,042,000**		

CAS-Nr.	***Substance***	***Company***	***Plant Location***	***Capacity [m T/a]***	***River***	***Mean flow [m^3/sec]***
50-00-0	Formaldehyde	Bakelite	Duisburg	50,000	Rhein	2270
		BASF AG	Ludwigshafen	1,200,000	Rhein	1260
		Bayer AG	Leverkusen	55,000	Rhein	2270
		Bayer AG	KR-Uerdingen	50,000	Rhein	2270
		DEGUSSA	Bruchhausen	110,000	Ruhr	19
		DEGUSSA	Mombach	110,000	Rhein	1600
		ELF-Atochem	Perl (6643)	40,000	Mosel	171
		GAF-Huels	Marl	190,000	Lippe	31
		Pfleiderer	Peiting	20,000	Lech	120
		Ticona	Kelsterbach	44,000	Main	188
		Total		**1,869,000**		
108-31-6	Maleic anhydride	BASF AG	Ludwigshafen	6,000	Rhein	1260
		RWE-DEA	Moers-Meerbeck	12,000	Rhein	2270
		Total		**18,000**		
80-62-4	Methyl methacrylate	BASF AG	Ludwigshafen	36,000	Rhein	1260
		DEGUSSA	Wesseling	60,000	Rhein	2270
		Total		**96,000**		
79-11-8	Chloroacetic acid	Hoechst AG	Gerreshofen	35,000	Lech	120
		Hoechst AG	Knapsack	60,000	Rhein	2270
		Total		**95,000**		
108-95-2	Phenol	Phenolchemie	Gladbeck	500,000	Emscher	12
		Rütgerswerke	Castrop-Rauxel	10,000	Emscher	6
		Total		**510,000**		
57-55-6	Propylene glycol	BASF AG	Ludwigshafen	40,000	Rhein	1260
		Erdölchemie	Köln-Worringen	150,000	Rhein	2270
		Huels	Marl	21,000	Lippe	31
		Total		**211,000**		
100-42-5	Styrene	BASF AG	Ludwigshafen	550,000	Rhein	1260
		Huels	Marl	295,000	Lippe	31
		Rhein. Olefin Werke	Wesseling	420,000	Rhein	2270
		Total		**1,265,000**		
108-05-4	Vinyl acetate	Hoechst AG	Frankfurt/ Main	140,000	Main	188
		Wacker AG	Burghausen	80,000	Alzkanal	60
		Total		**220,000**		

Table A.5 **Location, Capacity and River Flows of Production Sites for Bulk Intermediates in Germany**

CAS-Nr.	*Substance*	*Company*	*Plant Location*	*Capacity [mT/a]*	*River*	*Mean flow [m^3/sec]*	*No.*
108-95-2	Phenol	Rütgerswerke	Castrop-Rauxel	10,000	Emscher	6	
64-17-5	Ethanol	Huels	Herne		Emscher	8	
75-07-0	Acetaldehyde	Huels	Herne	80,000	Emscher	8	
108-95-2	Phenol	Phenolchemie	Gladbeck	500,000	Emscher	12	
110-82-7	Cyclohexane	Ruhr-Oel	GE-Buer	100,000	Emscher	12	
67-64-1	Acetone	Phenolchemie	Gladbeck	315,000	Emscher	12	
98-82-8	Cumene	Ruhr-Oel	GE-Buer	400,000	Emscher	12	
102-82-9	Tributylamine	Ruhrchemie	Oberhausen		Emscher	18	
75-01-4	Vinyl chloride	Hoechst	Gendorf	160,000	Alz	5	**1**
120-61-6	Dimethyl terephthalate [DMT]	Huels AG	Steyerberg	190,000	Aue	11	**2**
50-00-0	Formaldehyde	Degussa	Bruchhausen	110,000	Ruhr	19	**3**
100-41-4	Ethylbenzene	Huels	Marl	300,000	Lippe	31	**4**
100-42-5	Styrene	Huels	Marl	295,000	Lippe	31	**5**
124-04-9	Adipic acid	Huels	Marl		Lippe	31	**6**
50-00-0	Formaldehyde	GAF-Huels	Marl	190,000	Lippe	31	**7**
57-55-6	Propylene glycol	Huels	Marl	21,000	Lippe	31	**8**
75-01-4	Vinyl chloride	Huels	Marl	350,000	Lippe	31	**9**
79-10-7	Acrylic acid	Huels	Marl	60,000	Lippe	31	**10**
98-82-8	Cumene	Huels	Marl	140,000	Lippe	31	**11**
108-05-4	Vinyl acetate	Wacker AG	Burghausen	80,000	Alzkanal	60	**12**
108-24-7	Acetic anhydride	Wacker	Burghausen	10,000	Alzkanal	60	**13**
64-19-7	Acetic acid	Wacker	Burghausen	80,000	Alzkanal	60	**14**
75-01-4	Vinyl chloride	Wacker Chemie	Burghausen		Alzkanal	60	**15**
75-07-0	Acetaldehyde	Wacker	Burghausen	60,000	Alzkanal	60	**16**
110-82-7	Cyclohexane	Wintershall	Lingen (4450)	130,000	Ems	79	**17**
120-61-6	Dimethyl terephthalate [DMT]	Hoechst AG	Gersthofen	140,000	Lech	120	**18**

CAS-Nr.	***Substance***	***Company***	***Plant Location***	***Capacity [mT/a]***	***River***	***Mean flow $[m^3/sec]$***	***No.***
50-00-0	Formaldehyde	Pfleiderer	Peiting	20,000	Lech	120	**19**
79-11-8	Chloroacetic acid	Hoechst AG	Gersthofen	35,000	Lech	120	**20**
64-19-7	Acetic acid	Chemviron Carbon	Bodenfelde	5,000	Weser	149	**21**
50-00-0	Formaldehyde	ELF-Atochem	Perl (6643)	40,000	Mosel	171	**22**
100-02-7	o-Nitrophenol	Hoechst AG	Ff.-Griesheim		Main	188	**23**
108-05-4	Vinyl acetate	Hoechst AG	Frankfurt/Main	140,000	Main	188	**24**
119-90-4	3,3'-Dimethoxybenzidine	Hoechst AG	Ff.-Griesheim	500	Main	188	**25**
119-93-7	o-Tolidine	Hoechst AG	Ff.-Griesheim	500	Main	188	**26**
120-61-6	Dimethyl terephthalate [DMT]	Hoechst AG	Offenbach	95,000	Main	188	**27**
121-87-9	2-Chloro-4-nitroaniline	Hoechst AG	Ff.-Griesheim		Main	188	**28**
50-00-0	Formaldehyde	Ticona	Kelsterbach	44,000	Main	188	**29**
611-06-3	2,4-Dichloro-1-nitrobenzene	Hoechst AG	Ff.-Griesheim		Main	188	**30**
64-19-7	Acetic acid	Hoechst AG	Frankfurt/Main	270,000	Main	188	**31**
75-07-0	Acetaldehyde	Hoechst AG	Frankfurt/Main	130,000	Main	188	**32**
87-60-5	3-Chloro-o-toluidine	Hoechst AG	Ff.-Griesheim	500	Main	188	**33**
88-72-2	o-Nitrotoluene	Hoechst AG	Ff.-Griesheim		Main	188	**34**
88-74-4	o-Nitroaniline	Hoechst AG	Ff.-Griesheim	2,500	Main	188	**35**
88-75-5	o-Nitrophenol	Hoechst AG	Ff.-Griesheim	500	Main	188	**36**
89-61-2	2,5-Dichloronitrobenzene	Hoechst AG	Ff.-Griesheim		Main	188	**37**
91-23-6	o-Nitroanisole	Hoechst AG	Ff.-Griesheim		Main	188	**38**
91-94-1	3,3'-Dichlorobenzidine	Hoechst AG	Ff.-Griesheim	2,500	Main	188	**39**
95-50-1	o-Dichlorobenzene	Hoechst AG	Ff.-Griesheim		Main	188	**40**
95-51-2	o-Chloroaniline	Hoechst AG	Hoechst	4,000	Main	188	**41**
95-74-9	3-Chloro-p-toluidine	Hoechst AG	Ff.-Griesheim		Main	188	**42**
95-79-4	5-Chloro-o-toluidine	Hoechst AG	Ff.-Griesheim	200	Main	188	**43**
97-00-7	1-Chloro-2,4-dinitrobenzene	Hoechst AG	Frankfurt	2,400	Main	188	**44**

CAS-Nr.	***Substance***	***Company***	***Plant Location***	***Capacity [m T/a]***	***River***	***Mean flow [m³/sec]***	***No.***
97-00-7	1-Chloro-2,4-dinitrobenzene/ 1-Chloro-2,6-dinitrobenzene	Hoechst AG	Frankfurt	1,000	Main	188	**45**
98-16-8	3-Trifluoromethylaniline	Hoechst AG	Frankfurt	1,000	Main	188	**46**
98-95-3	Nitrobenzene	Hoechst AG	Ff.-Griesheim	< 4,000	Main	188	**47**
99-08-1	m-Nitrotoluene	Hoechst AG	Ff.-Griesheim		Main	188	**48**
99-54-7	1,2-Dichloro-4-nitrobenzene	Hoechst AG	Ff.-Griesheim		Main	188	**49**
99-99-0	p-Nitrotoluene	Hoechst AG	Ff.-Griesheim		Main	188	**50**
107-13-1	Acrylonitrile	Hoechst AG	Münchsmünster (8071)		Donau	326	**51**
100-41-4	Ethylbenzene	BASF AG	Ludwigshafen	300,000	Rhine	1260	**52**
100-42-5	Styrene	BASF AG	Ludwigshafen	550,000	Rhine	1260	**53**
102-82-9	Tributylamine	BASF AG	Ludwigshafen		Rhine	1260	**54**
103-69-5	N-ethylaniline	BASF AG	Ludwigshafen	500	Rhine	1260	**55**
105-60-2	Caprolactam	BASF AG	Ludwigshafen	150,000	Rhine	1260	**56**
108-24-7	Acetic anhydride	Rhone Poulenc	Freiburg	40,000	Rhine	1260	**57**
108-31-6	Maleic anhydride	BASF AG	Ludwigshafen	6,000	Rhine	1260	**58**
121-87-9	2-Chloro-4-nitroaniline	BASF AG	Ludwigshafen		Rhine	1260	**59**
124-04-9	Adipic acid	BASF AG	Ludwigshafen	180,000	Rhine	1260	**60**
50-00-0	Formaldehyde	BASF AG	Ludwigshafen	1,200,000	Rhine	1260	**61**
57-55-6	Propylene glycol	BASF AG	Ludwigshafen	40,000	Rhine	1260	**62**
62-53-3	Aniline	BASF AG	Ludwigshafen	30,000	Rhine	1260	**63**
64-17-5	Ethanol	Holtzmann	KA-Maxau	45,000	Rhine	1260	**64**
64-19-7	Acetic acid	BASF AG	Ludwigshafen	40,000	Rhine	1260	**65**
75-01-4	Vinyl chloride	BASF	Ludwigshafen	100,000	Rhine	1260	**66**
75-35-4	Vinylidene chloride	BASF AG	Ludwigshafen	20,000	Rhine	1260	**67**
79-10-7	Acrylic acid	BASF AG	Ludwigshafen	36,000	Rhine	1260	**68**
80-62-4	Methyl methacrylate	BASF AG	Ludwigshafen	36,000	Rhine	1260	**69**
50-00-0	Formaldehyde	DEGUSSA	Mombach	110,000	Rhine	1600	**70**
50-00-0	Formaldehyde	Bayer AG	Leverkusen	55,000	Rhine	2270	**71**
100-02-7	p-Nitrophenol	Bayer AG	Dormagen		Rhine	2270	**72**

CAS-Nr.	***Substance***	***Company***	***Plant Location***	***Capacity [mT/a]***	***River***	***Mean flow [m³/sec]***	***No.***
100-41-4	Ethylbenzene	Rhein. Olefin Werke	Wesseling	430,000	Rhine	2270	**73**
100-42-5	Styrene	Rhein. Olefin Werke	Wesseling	420,000	Rhine	2270	**74**
103-69-5	N-Ethylaniline	Bayer AG	Krefeld-Uerdingen	1,300	Rhine	2270	**75**
106-89-8	Epichlorhydrin	Solvay	Rheinberg	50,000	Rhine	2270	**76**
107-13-1	Acrylonitrile	Erdölchemie	Köln-Worringen	26,000	Rhine	2270	**77**
108-24-7	Acetic anhydride	Hoechst AG	Knapsack	80,000	Rhine	2270	**78**
108-31-6	Maleic anhydride	RWE-DEA	Moers-Meerbeck	12,000	Rhine	2270	**79**
108-42-9	m-Chloroaniline	Bayer AG	Leverkusen	2,000	Rhine	2270	**80**
120-61-6	Dimethyl terephthalate [DMT]	Huels AG	Luelsdorf	155,000	Rhine	2270	**81**
121-87-9	2-Chloro-4-nitroaniline	Bayer AG	Leverkusen		Rhine	2270	**82**
124-04-9	Adipic acid	Bayer AG	KR-Uerdingen	42,000	Rhine	2270	**83**
50-00-0	Formaldehyde	Bakelite	Duisburg	50,000	Rhine	2270	**84**
50-00-0	Formaldehyde	Bayer AG	KR-Uerdingen	50,000	Rhine	2270	**85**
57-55-6	Propylene glycol	Erdölchemie	Köln-Worringen	150,000	Rhine	2270	**86**
611-06-3	2,4-Dichloro-nitrobenzene	Bayer AG	Leverkusen		Rhine	2270	**87**
62-53-3	Aniline	Bayer AG	KR-Uerdingen	150,000	Rhine	2270	**88**
64-17-5	Ethanol	Erdölchemie	Köln-Worringen	60,000	Rhine	2270	**89**
64-19-7	Acetic Acid	Hoechst AG	Knapsack	250,000	Rhine	2270	**90**
67-64-1	Acetone	RWE-DEA	Moers-Meerbeck	3,600	Rhine	2270	**91**
75-01-4	Vinyl chloride	Hoechst	Knapsack	100,000	Rhine	2270	**92**
75-01-4	Vinyl chloride	Solvay	Rheinberg	200,000	Rhine	2270	**93**
75-01-4	Vinyl chloride	Wacker Chemie	Köln		Rhine	2270	**94**
75-07-0	Acetaldehyde	Hoechst AG	Knapsack	120,000	Rhine	2270	**95**
75-15-0	Carbon disulphide	Carbosulf	Köln-Weidenpesch	85,000	Rhine	2270	**96**
79-11-8	Chloroacetic acid	Hoechst AG	Knapsack	60,000	Rhine	2270	**97**
80-62-4	Methyl methacrylate	DEGUSSA	Wesseling	60,000	Rhine	2270	**98**

CAS-Nr.	*Substance*	*Company*	*Plant Location*	*Capacity [mT/a]*	*River*	*Mean flow [m^3/sec]*	*No.*
88-72-2	o-Nitrotoluene	Bayer AG	Leverkusen		Rhine	2270	**99**
88-74-4	o-Nitroaniline	Bayer AG	Leverkusen	3,500	Rhine	2270	**100**
89-61-2	2,5-Dichloronitrobenzene	Bayer AG	Leverkusen		Rhine	2270	**101**
91-23-6	o-Nitroanisole	Bayer AG	Leverkusen		Rhine	2270	**102**
91-66-7	N,N-Diethylaniline	Bayer AG	Leverkusen	1,000	Rhine	2270	**103**
95-50-1	o-Dichlorobenzene	Bayer AG	Leverkusen		Rhine	2270	**104**
95-51-2	o-Chloroaniline	Bayer AG	Leverkusen		Rhine	2270	**105**
95-74-9	3-Chloro-p-toluidene	Bayer AG	Leverkusen		Rhine	2270	**106**
97-00-7	1-Chloro-2,4-dinitrobenzene	Bayer AG	Leverkusen		Rhine	2270	**107**
97-00-7	1-Chloro-2,4-dinitrobenzene	Bayer AG	Dormagen		Rhine	2270	**108**
98-95-3	Nitrobenzene	Bayer AG	Uerdingen	200,000	Rhine	2270	**109**
99-08-1	m-Nitrotoluene	Bayer AG	Leverkusen		Rhine	2270	**110**
99-54-7	1,2-Dichloro-4-nitrobenzene	Bayer AG	Leverkusen		Rhine	2270	**111**
99-99-0	p-Nitrotoluene	Bayer AG	Leverkusen		Rhine	2270	**112**

Table A.6 presents a summary of the previous Table A.5. It can be seen that more than 90% of the bulk intermediates made in Germany are produced at sites with river-flows of 60 m^3/s or more. Therefore it was suggested to use this river-flow value as a default in the release scenario for intermediates (Section 7.1).

Table A.6 Calculation of the 90 percentile of the River Flows

No. of sites with given flow	Cumulative count.	%	Cumulative %	River flow m^3/s
41	41	36.6	36.6	2,270
1	42	0.9	37.5	1,600
19	61	17.0	54.5	1,260
1	62	0.9	55.4	326
28	90	25.0	80.4	188
1	91	0.9	81.3	171
1	92	0.9	82.1	149
3	95	2.7	84.8	120
1	96	0.9	85.7	79
5	101	4.5	**90.2**	**60**
8	109	7.1	97.3	31
1	110	0.9	98.2	19
1	111	0.9	99.1	11
1	112	0.9	100.0	5

APPENDIX B. SUBSTANCES RETRIEVED FROM THE BIODEGRADATION DATABASE (Howard *et al*, 1987)

Table B.1 "Biodegradable" Substances

CAS Number	Name	Half-life[1] in surface water (days)	Half-life in soil (days)	Comments
57-11-4	Stearic acid	1.9	7.6 (3.4-13)	
62-53-3	Aniline	5 (5-26)	135m (108-161)	Lower water rates at high concentrations
64-17-5	Ethanol	0.13	0.14	
79-06-1	Acrylamide	3 (1-12.5)	5 (3.3-7.5)	
90-15-3	1-Naphthol	590m (490-700)	0.07-5.1	photodeg. may be important
108-95-2	Phenol	2.2 (0.1-9.0)	3.4 (0.11-13)	
114-26-1	Propoxur	7	10 (1-66)	
124-40-3	Dimethylamine	0.24 (0.05-0.6)	7.1 (2.2-14)	
131-11-3	Dimethylphthalate	3	1	
139-13-9	Nitrilotriacetic acid	2.6 (0.5-19)	2.8 (2.0-4.0)	
629-97-0	Docosane	3.2p		poor screening data
1836-77-7	1,3,5-Trichloro-2-(4-nitrophenoxy) benzene	10 (6-14)	18 (6-31)	
5234-68-4	Carboxin	5	5 (3-8)	
84-74-2	Di-n-butylphthalate	3.5 (0.90-7.5)	15 (2.4-32)	
87-86-5	Pentachlorophenol	25 (15-104)	15	Water results variable
88-06-2	2,4,6-Trichlorophenol	5.4 (3.2-7.6)	19 (0.69-38)	

CAS Number	Name	Half-life[1] in surface water (days)	Half-life in soil (days)	Comments
90-12-0	1-Methylnaphthalene	4	-	Soil rates cannot be evaluated
90-30-2	N-Phenyl-1-naphthylamine	115m (11-220)	41m	
95-57-8	o-Chlorophenol	13 (2.2-24)	1.4 (0.38-2.3)	
95-95-4	2,4,5-Trichlorophenol	46 (23-69)	78 (68m-87)	
106-47-8	p-Chloroaniline	4	3.4 (60-800m)	
106-47-9	p-Chlorophenol	220 (20-490)	6.3 (4.5-7.9)	Slow in water at low temp.
110-44-4	Cyclohexane	38 (3.3m-72)	16000m	
117-81-7	Di-(2-ethylhexyl)-phthalate	56 (5-140) (21m-1930m)	9.7 (38m-70m)	
118-96-7	2,4,6-Trinitrotoluene	no degn in 42d	120m	
120-83-2	2,4-Dichlorophenol	10 (3-30)	10 (6-16)	Good database
208-96-8	Acenaphthylene	2 (1-3)	40 (12-121)	Water tests acclimatised
593-45-3	Octadecane	14 (1.4-26)	76 (50-89)	T1/2<3d in Rhine
621-64-7	N-Nitrosodi-propylamine	100 (50-200)	45	
1886-81-3	Dodecylbenzene sulphonate	25	77m (74m-80m)	Degradation in water slower at low temperature

1	Based on primary biodegradation unless otherwise indicated
m	mineralisation rate
p	polluted site

Table B.2 "Non-Biodegradable" Substances

CAS Number	Name	Half-life[1] in surface water (days)	Half-life* in soil (days)	Comments
55-18-5	N-Nitroso-diethylamine	No deg in 108d	23m-35	
56-55-3	Benz(A)-anthracene	300 (60-600)	90 (58-269)	Degrades fast in water after long adaptation phase
91-94-1	3,3'-Dichloro-benzidine	72	4350m	Poor data base for this product
95-77-2	3,4-Dichloro-phenol	800m (511-1146)	52.3	No proper screening data, but probably not degradable
132-64-9	Dibenzofuran			Poor screening data but readily biodeg in soil and GW from polluted sites
709-98-8	Propanil			No useful screening data but rapidly biodeg in soil and water

m mineralisation rate

[1] Based on primary biodegradation unless otherwise indicated

APPENDIX C. SENSITIVITY ANALYSES

The results of the sensitivity analyses for the different mass transfer coefficients (MTCs) are summarised in the following tables.

The evaluation of the results for each parameter is given below for the calculated concentrations. At first the average value (AVG) and minimum (MIN) and maximum (MAX) values are given for each compartment followed by the range of the output which is expressed as the ratio of the maximum and the minimum value (MAX/MIN). Then the ratio of the output range (=MAX/MIN) and the input range (=10,000) is given for each compartment and evaluated as follows:

Ratio	Effect (%)[1]	Result
< 0.001	< 0.1	-
≥ 0.001 - < 0.01	< 1	+
≥ 0.01 - < 0.1	1 - 10	++
≥ 0.1	≥ 10	+++

[1] e.g. if an output ratio < 10 is compared to the input ratio of 10,000, then the effect is < 0.1 %.

Table C.1: Sensitivity Analyses

Sensitivity analysis, Scenario 1: with biodegradation, all variables default					**Sensitivity analysis, Scenario 2:** no biodegradation, other variables default					**Sensitivity analysis, Scenario 3:** no biodeg., no advection in air water soil, other variables default				
Substance: Benzene					Substance: Benzene					Substance: Benzene				
Ka	water	air	soil	sediment	Ka	water	air	soil	sediment	Ka	water	air	soil	sediment
	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00		3.74e-04	3.74e-04	0.00	4.03e-04
0.05	2.72e-04	1.39e-07	5.05e-04	3.90e-04	0.05	1.04e-03	7.61e-07	5.75e-04	2.03e-03	0.05	6.35e+02	1.35e+02	1.02e+03	1.27e+03
0.5	2.21e-04	1.50e-07	3.88e-04	3.17e-04	0.5	5.54e-04	8.54e-07	4.30e-04	1.09e-03	0.5	6.09e+02	1.35e+02	1.01e+03	1.21e+03
5	2.02e-04	1.54e-07	3.76e-04	2.89e-04	5	4.47e-04	8.74e-07	4.16e-04	8.75e-04	5	6.06e+02	1.35e+02	1.01e+03	1.21e+03
50	1.99e-04	1.54e-07	3.74e-04	2.85e-04	50	4.34e-04	8.77e-07	4.15e-04	8.51e-04	50	6.06e+02	1.35e+02	1.01e+03	1.21e+03
500	1.99e-04	1.54e-07	3.74e-04	2.85e-04	500	4.33e-04	8.77e-07	4.14e-04	8.49e-04	500	6.06e+02	1.35e+02	1.01e+03	1.21e+03
AVG	2.19e-04	1.50e-07	4.03e-04	3.13e-04	AVG	5.81e-04	8.49e-07	4.50e-04	1.14e-03	AVG	6.12e+02	1.35e+02	1.01e+03	1.22e+03
MIN	1.99e-04	1.39e-07	3.74e-04	2.85e-04	MIN	4.33e-04	7.61e-07	4.14e-04	8.49e-04	MIN	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MAX	2.72e-04	1.54e-07	5.05e-04	3.90e-04	MAX	1.04e-03	8.77e-07	5.75e-04	2.03e-03	MAX	6.35e+02	1.35e+02	1.02e+03	1.27e+03
MAX/MIN	1.4	1.1	1.3	1.4	MAX/MIN	2.4	1.2	1.4	2.4	MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.37e-04	1.11e-04	1.35e-04	1.37e-04	OUTP/INP	2.39e-04	1.15e-04	1.39e-04	2.39e-04	OUTP/INP	1.05e-04	1.00e-04	1.00e-04	1.05e-04
RESULT	-	-	-	-	RESULT	-	-	-	-	RESULT	-	-	-	-
Kw	water	air	soil	sediment	Kw	water	air	soil	sediment	Kw	water	air	soil	sediment
	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00		3.74e-04	3.74e-04	0.00	4.03e-04
0.0005	2.95e-04	1.35e-07	3.76e-04	4.22e-04	0.0005	1.47e-03	6.78e-07	4.15e-04	2.88e-03	0.0005	1.25e+03	1.33e+02	1.00e+03	2.50e+03
0.005	2.83e-04	1.38e-07	3.76e-04	4.04e-04	0.005	1.21e-03	7.28e-07	4.15e-04	2.36e-03	0.005	6.65e+02	1.35e+02	1.01e+03	1.33e+03
0.05	2.02e-04	1.54e-07	3.76e-04	2.89e-04	0.05	4.47e-04	8.74e-07	4.16e-04	8.75e-04	0.05	6.06e+02	1.35e+02	1.01e+03	1.21e+03
0.5	6.79e-05	1.80e-07	3.76e-04	9.71e-05	0.5	8.62e-05	9.43e-07	4.17e-04	1.69e-04	0.5	6.00e+02	1.35e+02	1.01e+03	1.20e+03
5	3.03e-05	1.88e-07	3.76e-04	4.33e-05	5	3.63e-05	9.53e-07	4.17e-04	7.10e-05	5	6.00e+02	1.35e+02	1.01e+03	1.20e+03
AVG	1.75e-04	1.59e-07	3.76e-04	2.51e-04	AVG	6.49e-04	8.35e-07	4.16e-04	1.27e-03	AVG	7.45e+02	1.34e+02	1.01e+03	1.49e+03
MIN	3.03e-05	1.35e-07	3.76e-04	4.33e-05	MIN	3.63e-05	6.78e-07	4.15e-04	7.10e-05	MIN	6.00e+02	1.33e+02	1.00e+03	1.20e+03
MAX	2.95e-04	1.88e-07	3.76e-04	4.22e-04	MAX	1.47e-03	9.53e-07	4.17e-04	2.88e-03	MAX	1.25e+03	1.35e+02	1.01e+03	2.50e+03
MAX/MIN	9.7	1.4	1.0	9.7	MAX/MIN	40.5	1.4	1.0	40.5	MAX/MIN	2.1	1.0	1.0	2.1
OUTP/INP	9.74e-04	1.39e-04	1.00e-04	9.74e-04	OUTP/INP	4.05e-03	1.41e-04	1.00e-04	4.05e-03	OUTP/INP	2.09e-04	1.01e-04	1.01e-04	2.09e-04
RESULT	-	-	-	-	RESULT	+	-	-	+	RESULT	-	-	-	-

Sensitivity analysis, Scenario 1:					**Sensitivity analysis, Scenario 2:**					**Sensitivity analysis, Scenario 3:**				
with biodegradation, all variables default					no biodegradation, other variables default					no biodeg., no advection in air water soil, other variables default				
Substance: Benzene					Substance: Benzene					Substance: Benzene				
Ut	water	air	soil	sediment	Ut	water	air	soil	sediment	Ut	water	air	soil	sediment
	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00		3.74e-04	3.74e-04	0.00	4.03e-04
6.00e-12	2.02e-04	1.54e-07	3.76e-04	2.89e-04	6.00e-12	4.47e-04	8.74e-07	4.16e-04	8.75e-04	6.00e-12	6.06e+02	1.35e+02	1.01e+03	1.21e+03
6.00e-11	2.02e-04	1.54e-07	3.76e-04	2.89e-04	6.00e-11	4.47e-04	8.74e-07	4.16e-04	8.75e-04	6.00e-11	6.06e+02	1.35e+02	1.01e+03	1.21e+03
6.00e-10	2.02e-04	1.54e-07	3.76e-04	2.89e-04	6.00e-10	4.47e-04	8.74e-07	4.16e-04	8.75e-04	6.00e-10	6.06e+02	1.35e+02	1.01e+03	1.21e+03
6.00e-09	2.02e-04	1.54e-07	3.76e-04	2.89e-04	6.00e-09	4.47e-04	8.74e-07	4.16e-04	8.75e-04	6.00e-09	6.06e+02	1.35e+02	1.01e+03	1.21e+03
6.00e-08	2.02e-04	1.54e-07	3.76e-04	2.89e-04	6.00e-08	4.47e-04	8.74e-07	4.16e-04	8.75e-04	6.00e-08	6.06e+02	1.35e+02	1.01e+03	1.21e+03
AVG	2.02e-04	1.54e-07	3.76e-04	2.89e-04	AVG	4.47e-04	8.74e-07	4.16e-04	8.75e-04	AVG	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MIN	2.02e-04	1.54e-07	3.76e-04	2.89e-04	MIN	4.47e-04	8.74e-07	4.16e-04	8.75e-04	MIN	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MAX	2.02e-04	1.54e-07	3.76e-04	2.89e-04	MAX	4.47e-04	8.74e-07	4.16e-04	8.75e-04	MAX	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MAX/MIN	1.0	1.0	1.0	1.0	MAX/MIN	1.0	1.0	1.0	1.0	MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04	OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04	OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-	RESULT	-	-	-	-	RESULT	-	-	-	-
Ksa	water	air	soil	sediment	Ksa	water	air	soil	sediment	Ksa	water	air	soil	sediment
	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00		3.74e-04	3.74e-04	0.00	4.03e-04
0.0002	2.07e-04	1.39e-07	3.53e-03	2.97e-04	0.0002	5.15e-04	8.61e-07	1.77e-02	1.01e-03	0.0002	6.08e+02	1.35e+02	1.48e+03	1.21e+03
0.002	2.05e-04	1.46e-07	2.00e-03	2.93e-04	0.002	4.59e-04	8.72e-07	3.65e-03	9.00e-04	0.002	6.07e+02	1.35e+02	1.10e+03	1.21e+03
0.02	2.02e-04	1.54e-07	3.76e-04	2.89e-04	0.02	4.47e-04	8.74e-07	4.16e-04	8.75e-04	0.02	6.06e+02	1.35e+02	1.01e+03	1.21e+03
0.2	2.01e-04	1.55e-07	4.36e-05	2.88e-04	0.2	4.45e-04	8.75e-07	4.94e-05	8.72e-04	0.2	6.06e+02	1.35e+02	1.00e+03	1.21e+03
2	2.01e-04	1.55e-07	6.93e-06	2.88e-04	2	4.45e-04	8.75e-07	1.23e-05	8.72e-04	2	6.06e+02	1.35e+02	1.00e+03	1.21e+03
AVG	2.03e-04	1.50e-07	1.19e-03	2.91e-04	AVG	4.62e-04	8.71e-07	4.37e-03	9.05e-04	AVG	6.07e+02	1.35e+02	1.12e+03	1.21e+03
MIN	2.01e-04	1.39e-07	6.93e-06	2.88e-04	MIN	4.45e-04	8.61e-07	1.23e-05	8.72e-04	MIN	6.06e+02	1.35e+02	1.00e+03	1.21e+03
MAX	2.07e-04	1.55e-07	3.53e-03	2.97e-04	MAX	5.15e-04	8.75e-07	1.77e-02	1.01e-03	MAX	6.08e+02	1.35e+02	1.48e+03	1.21e+03
MAX/MIN	1.0	1.1	509.2	1.0	MAX/MIN	1.2	1.0	1440.7	1.2	MAX/MIN	1.0	1.0	1.5	1.0
OUTP/INP	1.03e-04	1.12e-04	5.09e-02	1.03e-04	OUTP/INP	1.16e-04	1.02e-04	1.44e-01	1.16e-04	OUTP/INP	1.00e-04	1.00e-04	1.48e-04	1.00e-04
RESULT	-	-	++	-	RESULT	-	-	+++	-	RESULT	-	-	-	-

Sensitivity analysis, Scenario 1: with biodegradation, all variables default					**Sensitivity analysis, Scenario 2:** no biodegradation, other variables default					**Sensitivity analysis, Scenario 3:** no biodeg., no advection in air water soil, other variables default				
Substance: Benzene					Substance: Benzene					Substance: Benzene				
Uss	water	air	soil	sediment	Uss	water	air	soil	sediment	Uss	water	air	soil	sediment
	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00		3.74e-04	3.74e-04	0.00	4.03e-04
1.00e-10	2.02e-04	1.54e-07	3.76e-04	2.89e-04	1.00e-10	4.47e-04	8.74e-07	4.16e-04	8.75e-04	1.00e-10	6.06e+02	1.35e+02	1.01e+03	1.21e+03
1.00e-09	2.02e-04	1.54e-07	3.76e-04	2.89e-04	1.00e-09	4.47e-04	8.74e-07	4.16e-04	8.75e-04	1.00e-09	6.06e+02	1.35e+02	1.01e+03	1.21e+03
1.00e-08	2.02e-04	1.54e-07	3.76e-04	2.89e-04	1.00e-08	4.47e-04	8.74e-07	4.16e-04	8.75e-04	1.00e-08	6.06e+02	1.35e+02	1.01e+03	1.21e+03
1.00e-07	2.02e-04	1.54e-07	3.76e-04	2.89e-04	1.00e-07	4.47e-04	8.74e-07	4.16e-04	8.75e-04	1.00e-07	6.06e+02	1.35e+02	1.01e+03	1.21e+03
0.000001	2.02e-04	1.54e-07	3.76e-04	2.89e-04	0.000001	4.47e-04	8.74e-07	4.16e-04	8.75e-04	0.000001	6.06e+02	1.35e+02	1.01e+03	1.21e+03
AVG	2.02e-04	1.54e-07	3.76e-04	2.89e-04	AVG	4.47e-04	8.74e-07	4.16e-04	8.75e-04	AVG	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MIN	2.02e-04	1.54e-07	3.76e-04	2.89e-04	MIN	4.47e-04	8.74e-07	4.16e-04	8.75e-04	MIN	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MAX	2.02e-04	1.54e-07	3.76e-04	2.89e-04	MAX	4.47e-04	8.74e-07	4.16e-04	8.75e-04	MAX	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MAX/MIN	1.0	1.0	1.0	1.0	MAX/MIN	1.0	1.0	1.0	1.0	MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04	OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04	OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-	RESULT	-	-	-	-	RESULT	-	-	-	-
Kt	water	air	soil	sediment	Kt	water	air	soil	sediment	Kt	water	air	soil	sediment
	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00		3.74e-04	3.74e-04	0.00	4.03e-04
1e-06	2.02e-04	1.54e-07	3.76e-04	7.62e-05	1e-06	4.47e-04	8.74e-07	4.16e-04	2.36e-03	1e-06	6.06e+02	1.35e+02	1.01e+03	8.82e+03
1e-05	2.02e-04	1.54e-07	3.76e-04	7.62e-05	1e-05	4.47e-04	8.74e-07	4.16e-04	2.36e-03	1e-05	6.06e+02	1.35e+02	1.01e+03	8.82e+03
1e-04	2.02e-04	1.54e-07	3.76e-04	7.62e-05	1e-04	4.47e-04	8.74e-07	4.16e-04	2.36e-03	1e-04	6.06e+02	1.35e+02	1.01e+03	8.82e+03
1e-03	2.02e-04	1.54e-07	3.76e-04	7.62e-05	1e-03	4.47e-04	8.74e-07	4.16e-04	2.36e-03	1e-03	6.06e+02	1.35e+02	1.01e+03	8.82e+03
1e-02	2.02e-04	1.54e-07	3.76e-04	7.62e-05	1e-02	4.47e-04	8.74e-07	4.16e-04	2.36e-03	1e-02	6.06e+02	1.35e+02	1.01e+03	8.82e+03
AVG	2.02e-04	1.54e-07	3.76e-04	7.62e-05	AVG	4.47e-04	8.74e-07	4.16e-04	2.36e-03	AVG	6.06e+02	1.35e+02	1.01e+03	8.82e+03
MIN	2.02e-04	1.54e-07	3.76e-04	7.62e-05	MIN	4.47e-04	8.74e-07	4.16e-04	2.36e-03	MIN	6.06e+02	1.35e+02	1.01e+03	8.82e+03
MAX	2.02e-04	1.54e-07	3.76e-04	7.62e-05	MAX	4.47e-04	8.74e-07	4.16e-04	2.36e-03	MAX	6.06e+02	1.35e+02	1.01e+03	8.82e+03
MAX/MIN	1.0	1.0	1.0	1.0	MAX/MIN	1.0	1.0	1.0	1.0	MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04	OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04	OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-	RESULT	-	-	-	-	RESULT	-	-	-	-

Sensitivity analysis, Scenario 1:
with biodegradation, all variables default

Substance: Benzene

Ksw	water	air	soil	sediment
	0.00	0.00	0.00	0.00
1e-07	2.02e-04	1.54e-07	3.76e-04	2.89e-04
1e-06	2.02e-04	1.54e-07	3.76e-04	2.89e-04
1e-05	2.02e-04	1.54e-07	3.76e-04	2.89e-04
1e-04	2.02e-04	1.54e-07	3.69e-04	2.89e-04
1e-03	2.02e-04	1.54e-07	3.14e-04	2.88e-04
AVG	2.02e-04	1.54e-07	3.62e-04	2.89e-04
MIN	2.02e-04	1.54e-07	3.14e-04	2.88e-04
MAX	2.02e-04	1.54e-07	3.76e-04	2.89e-04
MAX/MIN	1.0	1.0	1.2	1.0
OUTP/INP	1.00e-04	1.00e-04	1.20e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 2:
no biodegradation, other variables default

Substance: Benzene

Ksw	water	air	soil	sediment
	0.00	0.00	0.00	0.00
1e-07	4.47e-04	8.74e-07	4.17e-04	8.75e-04
1e-06	4.47e-04	8.74e-07	4.17e-04	8.75e-04
1e-05	4.47e-04	8.74e-07	4.16e-04	8.75e-04
1e-04	4.47e-04	8.74e-07	4.08e-04	8.75e-04
1e-03	4.46e-04	8.74e-07	3.43e-04	8.74e-04
AVG	4.46e-04	8.74e-07	4.00e-04	8.75e-04
MIN	4.46e-04	8.74e-07	3.43e-04	8.74e-04
MAX	4.47e-04	8.74e-07	4.17e-04	8.75e-04
MAX/MIN	1.0	1.0	1.2	1.0
OUTP/INP	1.00e-04	1.00e-04	1.21e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 3:
no biodeg., no advection in air water soil, other variables default

Substance: Benzene

Ksw	water	air	soil	sediment
	3.74e-04	3.74e-04	0.00	4.03e-04
1e-07	6.06e+02	1.35e+02	1.01e+03	1.21e+03
1e-06	6.06e+02	1.35e+02	1.01e+03	1.21e+03
1e-05	6.06e+02	1.35e+02	1.01e+03	1.21e+03
1e-04	6.06e+02	1.35e+02	1.01e+03	1.21e+03
1e-03	6.06e+02	1.35e+02	1.01e+03	1.21e+03
AVG	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MIN	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MAX	6.06e+02	1.35e+02	1.01e+03	1.21e+03
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 1:

with biodegradation, all variables default

Substance: p-Cresol

Ka	water	air	soil	sediment
	0.00	0.00	0.00	0.00
0.05	3.63e-05	3.95e-08	4.78e-04	1.39e-05
0.5	3.63e-05	3.95e-08	4.79e-04	1.39e-05
5	3.65e-05	3.93e-08	4.80e-04	1.40e-05
50	3.84e-05	3.83e-08	4.79e-04	1.47e-05
500	4.97e-05	3.21e-08	4.71e-04	1.91e-05
AVG	3.94e-05	3.77e-08	4.77e-04	1.51e-05
MIN	3.63e-05	3.21e-08	4.71e-04	1.39e-05
MAX	4.97e-05	3.95e-08	4.80e-04	1.91e-05
MAX/MIN	1.4	1.2	1.0	1.4
OUTP/INP	1.37e-04	1.23e-04	1.02e-04	1.37e-04
RESULT	-	-	-	-

Kw	water	air	soil	sediment
	0.00	0.00	0.00	0.00
0.0005	3.64e-05	3.94e-08	4.80e-04	1.40e-05
0.005	3.65e-05	3.93e-08	4.80e-04	1.40e-05
0.05	3.65e-05	3.93e-08	4.80e-04	1.40e-05
0.5	3.65e-05	3.93e-08	4.80e-04	1.40e-05
5	3.65e-05	3.93e-08	4.80e-04	1.40e-05
AVG	3.65e-05	3.93e-08	4.80e-04	1.40e-05
MIN	3.64e-05	3.93e-08	4.80e-04	1.40e-05
MAX	3.65e-05	3.94e-08	4.80e-04	1.40e-05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 2:

no biodegradation, other variables default

Substance: p-Cresol

Ka	water	air	soil	sediment
	0.00	0.00	0.00	0.00
0.05	2.63e-03	4.55e-07	5.29e-02	3.94e-03
0.5	2.58e-03	4.64e-07	5.00e-02	3.87e-03
5	2.62e-03	4.58e-07	4.76e-02	3.92e-03
50	3.05e-03	3.74e-07	4.24e-02	4.57e-03
500	3.84e-03	2.22e-07	3.35e-02	5.76e-03
AVG	2.95e-03	3.95e-07	4.52e-02	4.41e-03
MIN	2.58e-03	2.22e-07	3.35e-02	3.87e-03
MAX	3.84e-03	4.64e-07	5.29e-02	5.76e-03
MAX/MIN	1.5	2.1	1.6	1.5
OUTP/INP	1.49e-04	2.09e-04	1.58e-04	1.49e-04
RESULT	-	-	-	-

Kw	water	air	soil	sediment
	0.00	0.00	0.00	0.00
0.0005	2.60e-03	4.62e-07	4.78e-02	3.89e-03
0.005	2.61e-03	4.58e-07	4.76e-02	3.91e-03
0.05	2.62e-03	4.58e-07	4.76e-02	3.92e-03
0.5	2.62e-03	4.58e-07	4.76e-02	3.92e-03
5	2.62e-03	4.58e-07	4.76e-02	3.92e-03
AVG	2.61e-03	4.59e-07	4.76e-02	3.91e-03
MIN	2.60e-03	4.58e-07	4.76e-02	3.89e-03
MAX	2.62e-03	4.62e-07	4.78e-02	3.92e-03
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.01e-04	1.01e-04	1.00e-04	1.01e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 3:

no biodeg., no advection in air water soil, other variables default

Substance: p-Cresol

Ka	water	air	soil	sediment
	4.79e-04	4.71e-04	0.00	4.77e-04
0.05	6.78e+04	4.17e-03	2.64e+02	1.03e+05
0.5	6.75e+04	4.26e-02	2.57e+03	1.03e+05
5	6.58e+04	3.63e-01	2.13e+04	1.00e+05
50	6.04e+04	1.36e+00	7.97e+04	9.17e+04
500	5.76e+04	1.88e+00	1.10e+05	8.75e+04
AVG	6.38e+04	7.30e-01	4.27e+04	9.69e+04
MIN	5.76e+04	4.17e-03	2.64e+02	8.75e+04
MAX	6.78e+04	1.88e+00	1.10e+05	1.03e+05
MAX/MIN	1.2	449.3	415.8	1.2
OUTP/INP	1.18e-04	4.49e-02	4.16e-02	1.18e-04
RESULT	-	++	++	-

Kw	water	air	soil	sediment
	4.79e-04	4.71e-04	0.00	4.77e-04
0.0005	6.62e+04	2.84e-01	1.67e+04	1.01e+05
0.005	6.59e+04	3.54e-01	2.08e+04	1.00e+05
0.05	6.58e+04	3.63e-01	2.13e+04	1.00e+05
0.5	6.58e+04	3.64e-01	2.14e+04	1.00e+05
5	6.58e+04	3.64e-01	2.14e+04	1.00e+05
AVG	6.59e+04	3.46e-01	2.03e+04	1.00e+05
MIN	6.58e+04	2.84e-01	1.67e+04	1.00e+05
MAX	6.62e+04	3.64e-01	2.14e+04	1.01e+05
MAX/MIN	1.0	1.3	1.3	1.0
OUTP/INP	1.01e-04	1.28e-04	1.28e-04	1.01e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 1:
with biodegradation, all variables default
Substance: p-Cresol

Ut	water	air	soil	sediment
	0.00	0.00	0.00	0.00
6.00e-12	3.65e-05	3.93e-08	4.80e-04	1.40e-05
6.00e-11	3.65e-05	3.93e-08	4.80e-04	1.40e-05
6.00e-10	3.65e-05	3.93e-08	4.80e-04	1.40e-05
6.00e-09	3.65e-05	3.93e-08	4.80e-04	1.40e-05
6.00e-08	3.65e-05	3.93e-08	4.80e-04	1.40e-05
AVG	3.65e-05	3.93e-08	4.80e-04	1.40e-05
MIN	3.65e-05	3.93e-08	4.80e-04	1.40e-05
MAX	3.65e-05	3.93e-08	4.80e-04	1.40e-05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Ksa	**water**	**air**	**soil**	**sediment**
	0.00	0.00	0.00	0.00
0.0002	3.65e-05	3.93e-08	4.80e-04	1.40e-05
0.002	3.65e-05	3.93e-08	4.80e-04	1.40e-05
0.02	3.65e-05	3.93e-08	4.80e-04	1.40e-05
0.2	3.65e-05	3.93e-08	4.81e-04	1.40e-05
2	3.65e-05	3.92e-08	4.91e-04	1.40e-05
AVG	3.65e-05	3.93e-08	4.82e-04	1.40e-05
MIN	3.65e-05	3.92e-08	4.80e-04	1.40e-05
MAX	3.65e-05	3.93e-08	4.91e-04	1.40e-05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.02e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 2:
no biodegradation, other variables default
Substance: p-Cresol

Ut	water	air	soil	sediment
	0.00	0.00	0.00	0.00
6.00e-12	2.62e-03	4.58e-07	4.76e-02	3.92e-03
6.00e-11	2.62e-03	4.58e-07	4.76e-02	3.92e-03
6.00e-10	2.62e-03	4.58e-07	4.76e-02	3.92e-03
6.00e-09	2.62e-03	4.58e-07	4.76e-02	3.92e-03
6.00e-08	2.62e-03	4.57e-07	4.77e-02	3.92e-03
AVG	2.62e-03	4.58e-07	4.76e-02	3.92e-03
MIN	2.62e-03	4.57e-07	4.76e-02	3.92e-03
MAX	2.62e-03	4.58e-07	4.77e-02	3.92e-03
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Ksa	**water**	**air**	**soil**	**sediment**
	0.00	0.00	0.00	0.00
0.0002	2.62e-03	4.57e-07	4.79e-02	3.93e-03
0.002	2.62e-03	4.57e-07	4.78e-02	3.92e-03
0.02	2.62e-03	4.58e-07	4.76e-02	3.92e-03
0.2	2.57e-03	4.66e-07	4.53e-02	3.86e-03
2	2.39e-03	5.01e-07	3.56e-02	3.58e-03
AVG	2.57e-03	4.68e-07	4.48e-02	3.84e-03
MIN	2.39e-03	4.57e-07	3.56e-02	3.58e-03
MAX	2.62e-03	5.01e-07	4.79e-02	3.93e-03
MAX/MIN	1.1	1.1	1.3	1.1
OUTP/INP	1.10e-04	1.10e-04	1.35e-04	1.10e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 3:
no biodeg., no advection in air water soil, other variables default
Substance: p-Cresol

Ut	water	air	soil	sediment
	4.79e-04	4.71e-04	0.00	4.77e-04
6.00e-12	6.58e+04	3.63e-01	2.13e+04	1.00e+05
6.00e-11	6.58e+04	3.63e-01	2.13e+04	1.00e+05
6.00e-10	6.58e+04	3.63e-01	2.13e+04	1.00e+05
6.00e-09	6.58e+04	3.63e-01	2.13e+04	1.00e+05
6.00e-08	6.58e+04	3.62e-01	2.14e+04	1.00e+05
AVG	6.58e+04	3.63e-01	2.13e+04	1.00e+05
MIN	6.58e+04	3.62e-01	2.13e+04	1.00e+05
MAX	6.58e+04	3.63e-01	2.14e+04	1.00e+05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.01e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Ksa	**water**	**air**	**soil**	**sediment**
	4.79e-04	4.71e-04	0.00	4.77e-04
0.0002	6.58e+04	3.62e-01	2.14e+04	1.00e+05
0.002	6.58e+04	3.62e-01	2.14e+04	1.00e+05
0.02	6.58e+04	3.63e-01	2.13e+04	1.00e+05
0.2	6.58e+04	3.74e-01	2.11e+04	1.00e+05
2	6.59e+04	4.26e-01	2.02e+04	1.00e+05
AVG	6.58e+04	3.78e-01	2.11e+04	1.00e+05
MIN	6.58e+04	3.62e-01	2.02e+04	1.00e+05
MAX	6.59e+04	4.26e-01	2.14e+04	1.00e+05
MAX/MIN	1.0	1.2	1.1	1.0
OUTP/INP	1.00e-04	1.18e-04	1.06e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 1:

with biodegradation, all variables default

Substance: p-Cresol

Uss	water	air	soil	sediment
	0.00	0.00	0.00	0.00
1.00e-10	3.65e-05	3.93e-08	4.80e-04	1.40e-05
1.00e-09	3.65e-05	3.93e-08	4.80e-04	1.40e-05
1.00e-08	3.65e-05	3.93e-08	4.80e-04	1.40e-05
1.00e-07	3.65e-05	3.93e-08	4.80e-04	1.40e-05
0.000001	3.65e-05	3.93e-08	4.80e-04	1.40e-05
AVG	3.65e-05	3.93e-08	4.80e-04	1.40e-05
MIN	3.65e-05	3.93e-08	4.80e-04	1.40e-05
MAX	3.65e-05	3.93e-08	4.80e-04	1.40e-05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Kt	water	air	soil	sediment
	0.00	0.00	0.00	0.00
1e-06	3.65e-05	3.93e-08	4.80e-04	9.09e-07
1e-05	3.65e-05	3.93e-08	4.80e-04	9.09e-07
1e-04	3.65e-05	3.93e-08	4.80e-04	9.09e-07
1e-03	3.65e-05	3.93e-08	4.80e-04	9.09e-07
1e-02	3.65e-05	3.93e-08	4.80e-04	9.10e-07
AVG	3.65e-05	3.93e-08	4.80e-04	9.09e-07
MIN	3.65e-05	3.93e-08	4.80e-04	9.09e-07
MAX	3.65e-05	3.93e-08	4.80e-04	9.10e-07
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 2:

no biodegradation, other variables default

Substance: p-Cresol

Uss	water	air	soil	sediment
	0.00	0.00	0.00	0.00
1.00e-10	2.62e-03	4.58e-07	4.76e-02	3.92e-03
1.00e-09	2.62e-03	4.58e-07	4.76e-02	3.92e-03
1.00e-08	2.62e-03	4.58e-07	4.76e-02	3.92e-03
1.00e-07	2.62e-03	4.58e-07	4.76e-02	3.92e-03
0.000001	2.62e-03	4.58e-07	4.76e-02	3.92e-03
AVG	2.62e-03	4.58e-07	4.76e-02	3.92e-03
MIN	2.62e-03	4.58e-07	4.76e-02	3.92e-03
MAX	2.62e-03	4.58e-07	4.76e-02	3.92e-03
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Kt	water	air	soil	sediment
	0.00	0.00	0.00	0.00
1e-06	2.62e-03	4.58e-07	4.76e-02	9.23e-03
1e-05	2.62e-03	4.58e-07	4.76e-02	9.23e-03
1e-04	2.62e-03	4.58e-07	4.76e-02	9.23e-03
1e-03	2.62e-03	4.58e-07	4.76e-02	9.23e-03
1e-02	2.62e-03	4.58e-07	4.76e-02	9.23e-03
AVG	2.62e-03	4.58e-07	4.76e-02	9.23e-03
MIN	2.62e-03	4.58e-07	4.76e-02	9.23e-03
MAX	2.62e-03	4.58e-07	4.76e-02	9.23e-03
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 3:

no biodeg., no advection in air water soil, other variables default

Substance: p-Cresol

Uss	water	air	soil	sediment
	4.79e-04	4.71e-04	0.00	4.77e-04
1.00e-10	6.58e+04	3.63e-01	2.13e+04	1.00e+05
1.00e-09	6.58e+04	3.63e-01	2.13e+04	1.00e+05
1.00e-08	6.58e+04	3.63e-01	2.13e+04	1.00e+05
1.00e-07	6.58e+04	3.63e-01	2.13e+04	1.00e+05
0.000001	6.58e+04	3.63e-01	2.13e+04	1.00e+05
AVG	6.58e+04	3.63e-01	2.13e+04	1.00e+05
MIN	6.58e+04	3.63e-01	2.13e+04	1.00e+05
MAX	6.58e+04	3.63e-01	2.13e+04	1.00e+05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Kt	water	air	soil	sediment
	4.79e-04	4.71e-04	0.00	4.77e-04
1e-06	6.43e+04	3.55e-01	2.08e+04	7.31e+05
1e-05	6.43e+04	3.55e-01	2.08e+04	7.31e+05
1e-04	6.43e+04	3.55e-01	2.08e+04	7.31e+05
1e-03	6.43e+04	3.55e-01	2.08e+04	7.31e+05
1e-02	6.43e+04	3.55e-01	2.08e+04	7.30e+05
AVG	6.43e+04	3.55e-01	2.08e+04	7.31e+05
MIN	6.43e+04	3.55e-01	2.08e+04	7.30e+05
MAX	6.43e+04	3.55e-01	2.08e+04	7.31e+05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis, Scenario 1:					**Sensitivity analysis, Scenario 2:**					**Sensitivity analysis, Scenario 3:**				
with biodegradation, all variables default					no biodegradation, other variables default					no biodeg., no advection in air water soil, other variables default				
Substance: p-Cresol					Substance: p-Cresol					Substance: p-Cresol				
Ksw	water	air	soil	sediment	Ksw	water	air	soil	sediment	Ksw	water	air	soil	sediment
	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00		4.79e-04	4.71e-04	0.00	4.77e-04
1e-07	3.65e-05	3.94e-08	4.77e-04	1.40e-05	1e-07	2.71e-03	4.41e-07	5.25e-02	4.05e-03	1e-07	6.58e+04	3.42e-01	2.17e+04	9.99e+04
1e-06	3.65e-05	3.94e-08	4.78e-04	1.40e-05	1e-06	2.70e-03	4.43e-07	5.19e-02	4.04e-03	1e-06	6.58e+04	3.44e-01	2.17e+04	9.99e+04
1e-05	3.65e-05	3.93e-08	4.80e-04	1.40e-05	1e-05	2.62e-03	4.58e-07	4.76e-02	3.92e-03	1e-05	6.58e+04	3.63e-01	2.13e+04	1.00e+05
1e-04	3.65e-05	3.91e-08	4.94e-04	1.40e-05	1e-04	2.37e-03	5.06e-07	3.42e-02	3.55e-03	1e-04	6.59e+04	4.34e-01	2.00e+04	1.00e+05
1e-03	3.65e-05	3.88e-08	5.14e-04	1.40e-05	1e-03	2.24e-03	5.30e-07	2.75e-02	3.36e-03	1e-03	6.59e+04	4.78e-01	1.92e+04	1.00e+05
AVG	3.65e-05	3.92e-08	4.89e-04	1.40e-05	AVG	2.53e-03	4.75e-07	4.27e-02	3.78e-03	AVG	6.58e+04	3.92e-01	2.08e+04	1.00e+05
MIN	3.65e-05	3.88e-08	4.77e-04	1.40e-05	MIN	2.24e-03	4.41e-07	2.75e-02	3.36e-03	MIN	6.58e+04	3.42e-01	1.92e+04	9.99e+04
MAX	3.65e-05	3.94e-08	5.14e-04	1.40e-05	MAX	2.71e-03	5.30e-07	5.25e-02	4.05e-03	MAX	6.59e+04	4.78e-01	2.17e+04	1.00e+05
MAX/MIN	1.0	1.0	1.1	1.0	MAX/MIN	1.2	1.2	1.9	1.2	MAX/MIN	1.0	1.4	1.1	1.0
OUTP/INP	1.00e-04	1.01e-04	1.08e-04	1.00e-04	OUTP/INP	1.21e-04	1.20e-04	1.91e-04	1.21e-04	OUTP/INP	1.00e-04	1.40e-04	1.13e-04	1.00e-04
RESULT	-	-	-	-	RESULT	-	-	-	-	RESULT	-	-	-	-

Sensitivity analysis (with biodeg)

Other variables default

Substance: 1,2,3-TCB

Ka	water	air	soil	sediment
	4.15e-04	4.14e-04	0.00	4.50e-04
0.05	9.11e-04	5.74e-07	3.04e-02	1.57e-01
0.5	5.70e-04	6.63e-07	2.76e-02	9.82e-02
5	4.13e-04	7.02e-07	2.72e-02	7.12e-02
50	3.92e-04	7.07e-07	2.72e-02	6.75e-02
500	3.90e-04	7.08e-07	2.72e-02	6.71e-02
AVG	5.35e-04	6.71e-07	2.79e-02	9.22e-02
MIN	3.90e-04	5.74e-07	2.72e-02	6.71e-02
MAX	9.11e-04	7.08e-07	3.04e-02	1.57e-01
MAX/MIN	2.3	1.2	1.1	2.3
OUTP/INP	2.34e-04	1.23e-04	1.12e-04	2.34e-04
RESULT	-	-	-	-

Kw	water	air	soil	sediment
	4.15e-04	4.14e-04	0.00	4.50e-04
0.0005	1.03e-03	5.50e-07	2.71e-02	1.78e-01
0.005	8.98e-04	5.83e-07	2.72e-02	1.55e-01
0.05	4.13e-04	7.02e-07	2.72e-02	7.12e-02
0.5	1.17e-04	7.75e-07	2.73e-02	2.02e-02
5	7.17e-05	7.86e-07	2.73e-02	1.24e-02
AVG	5.06e-04	6.79e-07	2.72e-02	8.73e-02
MIN	7.17e-05	5.50e-07	2.71e-02	1.24e-02
MAX	1.03e-03	7.86e-07	2.73e-02	1.78e-01
MAX/MIN	14.4	1.4	1.0	14.4
OUTP/INP	1.44e-03	1.43e-04	1.00e-04	1.44e-03
RESULT	+	-	-	+

Sensitivity analysis (no biodeg)

Other variables default

Substance: 1,2,3-TCB

Ka	water	air	soil	sediment
	1.21e+03	1.21e+03	0.00	1.22e+03
0.05	1.23e-03	7.20e-07	9.60e-02	3.57e-01
0.5	6.81e-04	8.27e-07	7.23e-02	1.97e-01
5	4.70e-04	8.69e-07	6.99e-02	1.36e-01
50	4.43e-04	8.74e-07	6.97e-02	1.28e-01
500	4.40e-04	8.74e-07	6.96e-02	1.27e-01
AVG	6.53e-04	8.33e-07	7.55e-02	1.89e-01
MIN	4.40e-04	7.20e-07	6.96e-02	1.27e-01
MAX	1.23e-03	8.74e-07	9.60e-02	3.57e-01
MAX/MIN	2.8	1.2	1.4	2.8
OUTP/INP	2.80e-04	1.21e-04	1.38e-04	2.80e-04
RESULT	-	-	-	-

Kw	water	air	soil	sediment
	1.21e+03	1.21e+03	0.00	1.22e+03
0.0005	1.46e-03	6.76e-07	6.97e-02	4.22e-01
0.005	1.20e-03	7.26e-07	6.97e-02	3.49e-01
0.05	4.70e-04	8.69e-07	6.99e-02	1.36e-01
0.5	1.23e-04	9.36e-07	7.00e-02	3.57e-02
5	7.50e-05	9.45e-07	7.00e-02	2.17e-02
AVG	6.66e-04	8.30e-07	6.99e-02	1.93e-01
MIN	7.50e-05	6.76e-07	6.97e-02	2.17e-02
MAX	1.46e-03	9.45e-07	7.00e-02	4.22e-01
MAX/MIN	19.4	1.4	1.0	19.4
OUTP/INP	1.94e-03	1.40e-04	1.01e-04	1.94e-03
RESULT	+	-	-	+

Sensitivity analysis (with biodeg)

No advection in air water sediment, other variables default

Substance: 1,2,3-TCB

Ka	water	air	soil	sediment
	2.72e-02	2.72e-02	0.00	2.79e-02
0.05	1.25e+03	1.07e+02	1.41e+05	5.45e+05
0.5	1.14e+03	1.07e+02	1.41e+05	4.95e+05
5	1.13e+03	1.08e+02	1.41e+05	4.90e+05
50	1.12e+03	1.08e+02	1.41e+05	4.89e+05
500	1.12e+03	1.08e+02	1.41e+05	4.89e+05
AVG	1.15e+03	1.07e+02	1.41e+05	5.02e+05
MIN	1.12e+03	1.07e+02	1.41e+05	4.89e+05
MAX	1.25e+03	1.08e+02	1.41e+05	5.45e+05
MAX/MIN	1.1	1.0	1.0	1.1
OUTP/INP	1.11e-04	1.01e-04	1.00e-04	1.11e-04
RESULT	-	-	-	-

Kw	water	air	soil	sediment
	2.72e-02	2.72e-02	0.00	2.79e-02
0.0005	2.33e+03	1.03e+02	1.35e+05	1.02e+06
0.005	1.24e+03	1.07e+02	1.40e+05	5.39e+05
0.05	1.13e+03	1.08e+02	1.41e+05	4.90e+05
0.5	1.11e+03	1.08e+02	1.41e+05	4.85e+05
5	1.11e+03	1.08e+02	1.41e+05	4.84e+05
AVG	1.39e+03	1.07e+02	1.39e+05	6.03e+05
MIN	1.11e+03	1.03e+02	1.35e+05	4.84e+05
MAX	2.33e+03	1.08e+02	1.41e+05	1.02e+06
MAX/MIN	2.1	1.0	1.0	2.1
OUTP/INP	2.10e-04	1.04e-04	1.04e-04	2.10e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg) Other variables default				
Substance: 1,2,3-TCB				
Ut	water	air	soil	sediment
	4.15e-04	4.14e-04	0.00	4.50e-04
6.00e-12	4.13e-04	7.02e-07	2.72e-02	7.12e-02
6.00e-11	4.13e-04	7.02e-07	2.72e-02	7.12e-02
6.00e-10	4.13e-04	7.02e-07	2.72e-02	7.12e-02
6.00e-09	4.13e-04	7.02e-07	2.72e-02	7.12e-02
6.00e-08	4.13e-04	7.02e-07	2.73e-02	7.12e-02
AVG	4.13e-04	7.02e-07	2.72e-02	7.12e-02
MIN	4.13e-04	7.02e-07	2.72e-02	7.12e-02
MAX	4.13e-04	7.02e-07	2.73e-02	7.12e-02
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Ksa	water	air	soil	sediment
	4.15e-04	4.14e-04	0.00	4.50e-04
0.0002	4.14e-04	6.71e-07	4.30e-02	7.13e-02
0.002	4.14e-04	6.76e-07	4.08e-02	7.13e-02
0.02	4.13e-04	7.02e-07	2.72e-02	7.12e-02
0.2	4.12e-04	7.41e-07	7.09e-03	7.11e-02
2	4.12e-04	7.52e-07	1.90e-03	7.10e-02
AVG	4.13e-04	7.08e-07	2.40e-02	7.12e-02
MIN	4.12e-04	6.71e-07	1.90e-03	7.10e-02
MAX	4.14e-04	7.52e-07	4.30e-02	7.13e-02
MAX/MIN	1.0	1.1	22.6	1.0
OUTP/INP	1.00e-04	1.12e-04	2.26e-03	1.00e-04
RESULT	-	-	+	-

Sensitivity analysis (no biodeg) Other variables default				
Substance: 1,2,3-TCB				
Ut	water	air	soil	sediment
	1.21e+03	1.21e+03	0.00	1.22e+03
6.00e-12	4.70e-04	8.69e-07	6.99e-02	1.36e-01
6.00e-11	4.70e-04	8.69e-07	6.99e-02	1.36e-01
6.00e-10	4.70e-04	8.69e-07	6.99e-02	1.36e-01
6.00e-09	4.70e-04	8.69e-07	6.99e-02	1.36e-01
6.00e-08	4.70e-04	8.68e-07	7.03e-02	1.36e-01
AVG	4.70e-04	8.69e-07	7.00e-02	1.36e-01
MIN	4.70e-04	8.68e-07	6.99e-02	1.36e-01
MAX	4.70e-04	8.69e-07	7.03e-02	1.36e-01
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.01e-04	1.00e-04
RESULT	-	-	-	-
Ksa	water	air	soil	sediment
	1.21e+03	1.21e+03	0.00	1.22e+03
0.0002	5.64e-04	8.50e-07	1.68e+00	1.63e-01
0.002	4.97e-04	8.63e-07	5.37e-01	1.44e-01
0.02	4.70e-04	8.69e-07	6.99e-02	1.36e-01
0.2	4.66e-04	8.69e-07	8.44e-03	1.35e-01
2	4.66e-04	8.69e-07	2.10e-03	1.35e-01
AVG	4.93e-04	8.64e-07	4.60e-01	1.43e-01
MIN	4.66e-04	8.50e-07	2.10e-03	1.35e-01
MAX	5.64e-04	8.69e-07	1.68e+00	1.63e-01
MAX/MIN	1.2	1.0	803.8	1.2
OUTP/INP	1.21e-04	1.02e-04	8.04e-02	1.21e-04
RESULT	-	-	++	-

Sensitivity analysis (with biodeg) No advection in air water sediment, other variables default				
Substance: 1,2,3-TCB				
Ut	water	air	soil	sediment
	2.72e-02	2.72e-02	0.00	2.79e-02
6.00e-12	1.13e+03	1.08e+02	1.40e+05	4.90e+05
6.00e-11	1.13e+03	1.08e+02	1.40e+05	4.90e+05
6.00e-10	1.13e+03	1.08e+02	1.41e+05	4.90e+05
6.00e-09	1.12e+03	1.07e+02	1.44e+05	4.88e+05
6.00e-08	1.08e+03	1.02e+02	1.75e+05	4.72e+05
AVG	1.12e+03	1.06e+02	1.48e+05	4.86e+05
MIN	1.08e+03	1.02e+02	1.40e+05	4.72e+05
MAX	1.13e+03	1.08e+02	1.75e+05	4.90e+05
MAX/MIN	1.0	1.1	1.3	1.0
OUTP/INP	1.04e-04	1.06e-04	1.25e-04	1.04e-04
RESULT	-	-	-	-
Ksa	water	air	soil	sediment
	2.72e-02	2.72e-02	0.00	2.79e-02
0.0002	1.02e+03	9.70e+01	2.05e+05	4.45e+05
0.002	1.09e+03	1.04e+02	1.61e+05	4.76e+05
0.02	1.13e+03	1.08e+02	1.41e+05	4.90e+05
0.2	1.13e+03	1.08e+02	1.38e+05	4.92e+05
2	1.13e+03	1.08e+02	1.38e+05	4.92e+05
AVG	1.10e+03	1.05e+02	1.56e+05	4.79e+05
MIN	1.02e+03	9.70e+01	1.38e+05	4.45e+05
MAX	1.13e+03	1.08e+02	2.05e+05	4.92e+05
MAX/MIN	1.1	1.1	1.5	1.1
OUTP/INP	1.11e-04	1.11e-04	1.49e-04	1.11e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)				
Other variables default				
Substance: 1,2,3-TCB				
Uss	water	air	soil	sediment
	4.15e-04	4.14e-04	0.00	4.50e-04
1.00e-10	4.13e-04	7.02e-07	2.72e-02	7.12e-02
1.00e-09	4.13e-04	7.02e-07	2.72e-02	7.12e-02
1.00e-08	4.13e-04	7.02e-07	2.72e-02	7.12e-02
1.00e-07	4.13e-04	7.02e-07	2.72e-02	7.12e-02
0.000001	4.13e-04	7.02e-07	2.72e-02	7.12e-02
AVG	4.13e-04	7.02e-07	2.72e-02	7.12e-02
MIN	4.13e-04	7.02e-07	2.72e-02	7.12e-02
MAX	4.13e-04	7.02e-07	2.72e-02	7.12e-02
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Kt	water	air	soil	sediment
	4.15e-04	4.14e-04	0.00	4.50e-04
1e-06	4.13e-04	7.02e-07	2.72e-02	7.87e-02
1e-05	4.13e-04	7.02e-07	2.72e-02	7.87e-02
1e-04	4.13e-04	7.02e-07	2.72e-02	7.87e-02
1e-03	4.13e-04	7.02e-07	2.72e-02	7.87e-02
1e-02	4.13e-04	7.02e-07	2.72e-02	7.87e-02
AVG	4.13e-04	7.02e-07	2.72e-02	7.87e-02
MIN	4.13e-04	7.02e-07	2.72e-02	7.87e-02
MAX	4.13e-04	7.02e-07	2.72e-02	7.87e-02
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (no biodeg)				
Other variables default				
Substance: 1,2,3-TCB				
Uss	water	air	soil	sediment
	1.21e+03	1.21e+03	0.00	1.22e+03
1.00e-10	4.70e-04	8.69e-07	7.00e-02	1.36e-01
1.00e-09	4.70e-04	8.69e-07	7.00e-02	1.36e-01
1.00e-08	4.70e-04	8.69e-07	7.00e-02	1.36e-01
1.00e-07	4.70e-04	8.69e-07	7.00e-02	1.36e-01
0.000001	4.70e-04	8.69e-07	7.00e-02	1.36e-01
AVG	4.70e-04	8.69e-07	7.00e-02	1.36e-01
MIN	4.70e-04	8.69e-07	7.00e-02	1.36e-01
MAX	4.70e-04	8.69e-07	7.00e-02	1.36e-01
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Kt	water	air	soil	sediment
	1.21e+03	1.21e+03	0.00	1.22e+03
1e-06	4.69e-04	8.68e-07	6.99e-02	1.81e-01
1e-05	4.69e-04	8.68e-07	6.99e-02	1.81e-01
1e-04	4.69e-04	8.68e-07	6.99e-02	1.81e-01
1e-03	4.69e-04	8.68e-07	6.99e-02	1.81e-01
1e-02	4.69e-04	8.68e-07	6.99e-02	1.81e-01
AVG	4.69e-04	8.68e-07	6.99e-02	1.81e-01
MIN	4.69e-04	8.68e-07	6.99e-02	1.81e-01
MAX	4.69e-04	8.68e-07	6.99e-02	1.81e-01
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)				
No advection in air water sediment, other variables default				
Substance: 1,2,3-TCB				
Uss	water	air	soil	sediment
	2.72e-02	2.72e-02	0.00	2.79e-02
1.00e-10	1.12e+03	1.08e+02	1.41e+05	4.90e+05
1.00e-09	1.12e+03	1.08e+02	1.41e+05	4.90e+05
1.00e-08	1.12e+03	1.08e+02	1.41e+05	4.90e+05
1.00e-07	1.12e+03	1.08e+02	1.41e+05	4.90e+05
0.000001	1.12e+03	1.08e+02	1.41e+05	4.90e+05
AVG	1.12e+03	1.08e+02	1.41e+05	4.90e+05
MIN	1.12e+03	1.08e+02	1.41e+05	4.90e+05
MAX	1.12e+03	1.08e+02	1.41e+05	4.90e+05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Kt	water	air	soil	sediment
	2.72e-02	2.72e-02	0.00	2.79e-02
1e-06	1.11e+03	1.06e+02	1.39e+05	8.60e+05
1e-05	1.11e+03	1.06e+02	1.39e+05	8.60e+05
1e-04	1.11e+03	1.06e+02	1.39e+05	8.60e+05
1e-03	1.11e+03	1.06e+02	1.39e+05	8.60e+05
1e-02	1.11e+03	1.06e+02	1.39e+05	8.60e+05
AVG	1.11e+03	1.06e+02	1.39e+05	8.60e+05
MIN	1.11e+03	1.06e+02	1.39e+05	8.60e+05
MAX	1.11e+03	1.06e+02	1.39e+05	8.60e+05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg) Other variables default				
Substance: 1,2,3-TCB				
Ksw	water	air	soil	sediment
	4.15e-04	4.14e-04	0.00	4.50e-04
1e-07	4.13e-04	7.02e-07	2.73e-02	7.12e-02
1e-06	4.13e-04	7.02e-07	2.73e-02	7.12e-02
1e-05	4.13e-04	7.02e-07	2.72e-02	7.12e-02
1e-04	4.13e-04	7.03e-07	2.68e-02	7.12e-02
1e-03	4.13e-04	7.10e-07	2.30e-02	7.12e-02
AVG	4.13e-04	7.04e-07	2.63e-02	7.12e-02
MIN	4.13e-04	7.02e-07	2.30e-02	7.12e-02
MAX	4.13e-04	7.10e-07	2.73e-02	7.12e-02
MAX/MIN	1.0	1.0	1.2	1.0
OUTP/INP	1.00e-04	1.01e-04	1.19e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (no biodeg) Other variables default				
Substance: 1,2,3-TCB				
Ksw	water	air	soil	sediment
	1.21e+03	1.21e+03	0.00	1.22e+03
1e-07	4.70e-04	8.69e-07	7.02e-02	1.36e-01
1e-06	4.70e-04	8.69e-07	7.02e-02	1.36e-01
1e-05	4.70e-04	8.69e-07	6.99e-02	1.36e-01
1e-04	4.70e-04	8.69e-07	6.70e-02	1.36e-01
1e-03	4.69e-04	8.69e-07	4.73e-02	1.36e-01
AVG	4.70e-04	8.69e-07	6.49e-02	1.36e-01
MIN	4.69e-04	8.69e-07	4.73e-02	1.36e-01
MAX	4.70e-04	8.69e-07	7.02e-02	1.36e-01
MAX/MIN	1.0	1.0	1.5	1.0
OUTP/INP	1.00e-04	1.00e-04	1.48e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg) No advection in air water sediment, other variables default				
Substance: 1,2,3-TCB				
Ksw	water	air	soil	sediment
	2.72e-02	2.72e-02	0.00	2.79e-02
1e-07	1.13e+03	1.08e+02	1.41e+05	4.90e+05
1e-06	1.13e+03	1.08e+02	1.41e+05	4.90e+05
1e-05	1.13e+03	1.08e+02	1.41e+05	4.90e+05
1e-04	1.13e+03	1.08e+02	1.40e+05	4.90e+05
1e-03	1.13e+03	1.08e+02	1.40e+05	4.91e+05
AVG	1.13e+03	1.08e+02	1.40e+05	4.90e+05
MIN	1.13e+03	1.08e+02	1.40e+05	4.90e+05
MAX	1.13e+03	1.08e+02	1.41e+05	4.91e+05
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.01e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)
Other variables default
Substance: HCB

Ka	water	air	soil	sediment
	4.24e-02	3.35e-02	0.00	4.52e-02
0.05	9.38e-04	5.79e-07	4.03e-01	5.67e+00
0.5	6.84e-04	6.51e-07	3.93e-01	4.14e+00
5	4.74e-04	7.10e-07	3.92e-01	2.87e+00
50	4.36e-04	7.20e-07	3.92e-01	2.64e+00
500	4.32e-04	7.21e-07	3.92e-01	2.61e+00
AVG	5.93e-04	6.76e-07	3.95e-01	3.59e+00
MIN	4.32e-04	5.79e-07	3.92e-01	2.61e+00
MAX	9.38e-04	7.21e-07	4.03e-01	5.67e+00
MAX/MIN	2.2	1.2	1.0	2.2
OUTP/INP	2.17e-04	1.25e-04	1.03e-04	2.17e-04
RESULT	-	-	-	-
Kw	**water**	**air**	**soil**	**sediment**
	4.24e-02	3.35e-02	0.00	4.52e-02
0.0005	9.88e-04	5.67e-07	3.91e-01	5.98e+00
0.005	8.84e-04	5.96e-07	3.91e-01	5.35e+00
0.05	4.74e-04	7.10e-07	3.92e-01	2.87e+00
0.5	1.89e-04	7.89e-07	3.93e-01	1.14e+00
5	1.43e-04	8.02e-07	3.94e-01	8.65e-01
AVG	5.35e-04	6.93e-07	3.92e-01	3.24e+00
MIN	1.43e-04	5.67e-07	3.91e-01	8.65e-01
MAX	9.88e-04	8.02e-07	3.94e-01	5.98e+00
MAX/MIN	6.9	1.4	1.0	6.9
OUTP/INP	6.91e-04	1.41e-04	1.01e-04	6.91e-04
RESULT	-	-	-	-

Sensitivity analysis (no biodeg)
Other variables default
Substance: HCB

Ka	water	air	soil	sediment
	9.17e+04	8.75e+04	0.00	9.69e+04
0.05	1.05e-03	6.80e-07	4.04e+00	8.29e+00
0.5	7.41e-04	7.61e-07	3.11e+00	5.87e+00
5	5.05e-04	8.25e-07	3.02e+00	4.00e+00
50	4.64e-04	8.36e-07	3.01e+00	3.68e+00
500	4.60e-04	8.37e-07	3.01e+00	3.64e+00
AVG	6.43e-04	7.88e-07	3.24e+00	5.10e+00
MIN	4.60e-04	6.80e-07	3.01e+00	3.64e+00
MAX	1.05e-03	8.37e-07	4.04e+00	8.29e+00
MAX/MIN	2.3	1.2	1.3	2.3
OUTP/INP	2.28e-04	1.23e-04	1.34e-04	2.28e-04
RESULT	-	-	-	-
Kw	**water**	**air**	**soil**	**sediment**
	9.17e+04	8.75e+04	0.00	9.69e+04
0.0005	1.09e-03	6.67e-07	3.01e+00	8.67e+00
0.005	9.72e-04	7.00e-07	3.01e+00	7.70e+00
0.05	5.05e-04	8.25e-07	3.02e+00	4.00e+00
0.5	1.99e-04	9.07e-07	3.03e+00	1.58e+00
5	1.50e-04	9.20e-07	3.03e+00	1.19e+00
AVG	5.84e-04	8.04e-07	3.02e+00	4.63e+00
MIN	1.50e-04	6.67e-07	3.01e+00	1.19e+00
MAX	1.09e-03	9.20e-07	3.03e+00	8.67e+00
MAX/MIN	7.3	1.4	1.0	7.3
OUTP/INP	7.28e-04	1.38e-04	1.01e-04	7.28e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)
No advection in air water sediment, other variables default
Substance: HCB

Ka	water	air	soil	sediment
	3.92e-01	3.92e-01	0.00	3.95e-01
0.05	2.78e+02	5.77e+00	6.37e+05	4.32e+06
0.5	1.81e+02	6.87e+00	6.76e+05	2.81e+06
5	1.70e+02	7.01e+00	6.80e+05	2.64e+06
50	1.69e+02	7.02e+00	6.81e+05	2.63e+06
500	1.69e+02	7.02e+00	6.81e+05	2.63e+06
AVG	1.93e+02	6.74e+00	6.71e+05	3.01e+06
MIN	1.69e+02	5.77e+00	6.37e+05	2.63e+06
MAX	2.78e+02	7.02e+00	6.81e+05	4.32e+06
MAX/MIN	1.6	1.2	1.1	1.6
OUTP/INP	1.65e-04	1.22e-04	1.07e-04	1.65e-04
RESULT	-	-	-	-
Kw	**water**	**air**	**soil**	**sediment**
	3.92e-01	3.92e-01	0.00	3.95e-01
0.0005	6.64e+02	4.76e+00	4.62e+05	1.03e+07
0.005	2.33e+02	6.72e+00	6.52e+05	3.63e+06
0.05	1.70e+02	7.01e+00	6.80e+05	2.64e+06
0.5	1.63e+02	7.04e+00	6.83e+05	2.54e+06
5	1.63e+02	7.04e+00	6.84e+05	2.53e+06
AVG	2.79e+02	6.51e+00	6.32e+05	4.33e+06
MIN	1.63e+02	4.76e+00	4.62e+05	2.53e+06
MAX	6.64e+02	7.04e+00	6.84e+05	1.03e+07
MAX/MIN	4.1	1.5	1.5	4.1
OUTP/INP	4.08e-04	1.48e-04	1.48e-04	4.08e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)
Other variables default

Substance: HCB				
Ut	water	air	soil	sediment
	4.24e-02	3.35e-02	0.00	4.52e-02
6.00e-12	4.73e-04	7.11e-07	3.89e-01	2.86e+00
6.00e-11	4.73e-04	7.11e-07	3.89e-01	2.86e+00
6.00e-10	4.74e-04	7.10e-07	3.92e-01	2.87e+00
6.00e-09	4.75e-04	7.03e-07	4.24e-01	2.87e+00
6.00e-08	4.89e-04	6.39e-07	7.12e-01	2.96e+00
AVG	4.77e-04	6.95e-07	4.61e-01	2.89e+00
MIN	4.73e-04	6.39e-07	3.89e-01	2.86e+00
MAX	4.89e-04	7.11e-07	7.12e-01	2.96e+00
MAX/MIN	1.0	1.1	1.8	1.0
OUTP/INP	1.03e-04	1.11e-04	1.83e-04	1.03e-04
RESULT	-	-	-	-
Ksa	water	air	soil	sediment
	4.24e-02	3.35e-02	0.00	4.52e-02
0.0002	4.74e-04	7.00e-07	4.38e-01	2.87e+00
0.002	4.74e-04	7.01e-07	4.33e-01	2.87e+00
0.02	4.74e-04	7.10e-07	3.92e-01	2.87e+00
0.2	4.73e-04	7.47e-07	2.18e-01	2.86e+00
2	4.73e-04	7.75e-07	8.32e-02	2.86e+00
AVG	4.73e-04	7.27e-07	3.13e-01	2.86e+00
MIN	4.73e-04	7.00e-07	8.32e-02	2.86e+00
MAX	4.74e-04	7.75e-07	4.38e-01	2.87e+00
MAX/MIN	1.0	1.1	5.3	1.0
OUTP/INP	1.00e-04	1.11e-04	5.27e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (no biodeg)
Other variables default

Substance: HCB				
Ut	water	air	soil	sediment
	9.17e+04	8.75e+04	0.00	9.69e+04
6.00e-12	5.05e-04	8.25e-07	2.99e+00	4.00e+00
6.00e-11	5.05e-04	8.25e-07	2.99e+00	4.00e+00
6.00e-10	5.05e-04	8.25e-07	3.02e+00	4.00e+00
6.00e-09	5.08e-04	8.24e-07	3.31e+00	4.03e+00
6.00e-08	5.40e-04	8.15e-07	6.16e+00	4.28e+00
AVG	5.13e-04	8.23e-07	3.70e+00	4.06e+00
MIN	5.05e-04	8.15e-07	2.99e+00	4.00e+00
MAX	5.40e-04	8.25e-07	6.16e+00	4.28e+00
MAX/MIN	1.1	1.0	2.1	1.1
OUTP/INP	1.07e-04	1.01e-04	2.06e-04	1.07e-04
RESULT	-	-	-	-
Ksa	water	air	soil	sediment
	9.17e+04	8.75e+04	0.00	9.69e+04
0.0002	6.26e-04	7.92e-07	2.63e+01	4.96e+00
0.002	5.69e-04	8.08e-07	1.54e+01	4.51e+00
0.02	5.05e-04	8.25e-07	3.02e+00	4.00e+00
0.2	4.92e-04	8.28e-07	3.89e-01	3.89e+00
2	4.90e-04	8.29e-07	9.50e-02	3.88e+00
AVG	5.36e-04	8.16e-07	9.05e+00	4.25e+00
MIN	4.90e-04	7.92e-07	9.50e-02	3.88e+00
MAX	6.26e-04	8.29e-07	2.63e+01	4.96e+00
MAX/MIN	1.3	1.0	277.3	1.3
OUTP/INP	1.28e-04	1.05e-04	2.77e-02	1.28e-04
RESULT	-	-	++	-

Sensitivity analysis (with biodeg)
No advection in air water sediment, other variables default

Substance: HCB				
Ut	water	air	soil	sediment
	3.92e-01	3.92e-01	0.00	3.95e-01
6.00e-12	2.49e+02	1.06e+01	6.22e+05	3.88e+06
6.00e-11	2.39e+02	1.01e+01	6.30e+05	3.71e+06
6.00e-10	1.70e+02	7.01e+00	6.80e+05	2.64e+06
6.00e-09	5.37e+01	1.71e+00	7.66e+05	8.35e+05
6.00e-08	2.05e+01	2.00e-01	7.91e+05	3.18e+05
AVG	1.46e+02	5.93e+00	6.98e+05	2.28e+06
MIN	2.05e+01	2.00e-01	6.22e+05	3.18e+05
MAX	2.49e+02	1.06e+01	7.91e+05	3.88e+06
MAX/MIN	12.2	53.0	1.3	12.2
OUTP/INP	1.22e-03	5.30e-03	1.27e-04	1.22e-03
RESULT	+	+	-	+
Ksa	water	air	soil	sediment
	3.92e-01	3.92e-01	0.00	3.95e-01
0.0002	5.22e+01	1.93e+00	7.66e+05	8.11e+05
0.002	7.53e+01	2.92e+00	7.49e+05	1.17e+06
0.02	1.70e+02	7.01e+00	6.80e+05	2.64e+06
0.2	2.39e+02	9.97e+00	6.31e+05	3.72e+06
2	2.50e+02	1.05e+01	6.22e+05	3.89e+06
AVG	1.57e+02	6.46e+00	6.90e+05	2.45e+06
MIN	5.22e+01	1.93e+00	6.22e+05	8.11e+05
MAX	2.50e+02	1.05e+01	7.66e+05	3.89e+06
MAX/MIN	4.8	5.4	1.2	4.8
OUTP/INP	4.80e-04	5.43e-04	1.23e-04	4.80e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)				
Other variables default				
Substance: HCB				
Uss	water	air	soil	sediment
	4.24e-02	3.35e-02	0.00	4.52e-02
1.00e-10	4.72e-04	7.10e-07	3.95e-01	2.86e+00
1.00e-09	4.72e-04	7.10e-07	3.95e-01	2.86e+00
1.00e-08	4.72e-04	7.10e-07	3.95e-01	2.86e+00
1.00e-07	4.72e-04	7.10e-07	3.95e-01	2.86e+00
0.000001	4.72e-04	7.10e-07	3.95e-01	2.86e+00
AVG	4.72e-04	7.10e-07	3.95e-01	2.86e+00
MIN	4.72e-04	7.10e-07	3.95e-01	2.86e+00
MAX	4.72e-04	7.10e-07	3.95e-01	2.86e+00
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Kt	water	air	soil	sediment
	4.24e-02	3.35e-02	0.00	4.52e-02
1e-06	4.73e-04	7.10e-07	3.92e-01	2.89e+00
1e-05	4.73e-04	7.10e-07	3.92e-01	2.89e+00
1e-04	4.73e-04	7.10e-07	3.92e-01	2.89e+00
1e-03	4.73e-04	7.10e-07	3.92e-01	2.89e+00
1e-02	4.73e-04	7.10e-07	3.92e-01	2.89e+00
AVG	4.73e-04	7.10e-07	3.92e-01	2.89e+00
MIN	4.73e-04	7.10e-07	3.92e-01	2.89e+00
MAX	4.73e-04	7.10e-07	3.92e-01	2.89e+00
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (no biodeg)				
Other variables default				
Substance: HCB				
Uss	water	air	soil	sediment
	9.17e+04	8.75e+04	0.00	9.69e+04
1.00e-10	4.97e-04	8.27e-07	3.19e+00	3.94e+00
1.00e-09	4.97e-04	8.27e-07	3.19e+00	3.94e+00
1.00e-08	4.97e-04	8.27e-07	3.19e+00	3.94e+00
1.00e-07	4.97e-04	8.27e-07	3.19e+00	3.94e+00
0.000001	4.97e-04	8.27e-07	3.19e+00	3.94e+00
AVG	4.97e-04	8.27e-07	3.19e+00	3.94e+00
MIN	4.97e-04	8.27e-07	3.19e+00	3.94e+00
MAX	4.97e-04	8.27e-07	3.19e+00	3.94e+00
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Kt	water	air	soil	sediment
	9.17e+04	8.75e+04	0.00	9.69e+04
1e-06	5.04e-04	8.24e-07	3.02e+00	4.05e+00
1e-05	5.04e-04	8.24e-07	3.02e+00	4.05e+00
1e-04	5.04e-04	8.24e-07	3.02e+00	4.05e+00
1e-03	5.04e-04	8.24e-07	3.02e+00	4.05e+00
1e-02	5.04e-04	8.24e-07	3.02e+00	4.05e+00
AVG	5.04e-04	8.24e-07	3.02e+00	4.05e+00
MIN	5.04e-04	8.24e-07	3.02e+00	4.05e+00
MAX	5.04e-04	8.24e-07	3.02e+00	4.05e+00
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)				
No advection in air water sediment, other variables default				
Substance: HCB				
Uss	water	air	soil	sediment
	3.92e-01	3.92e-01	0.00	3.95e-01
1.00e-10	1.59e+02	6.70e+00	6.87e+05	2.48e+06
1.00e-09	1.59e+02	6.70e+00	6.87e+05	2.48e+06
1.00e-08	1.59e+02	6.70e+00	6.87e+05	2.48e+06
1.00e-07	1.59e+02	6.70e+00	6.87e+05	2.48e+06
0.000001	1.59e+02	6.70e+00	6.87e+05	2.48e+06
AVG	1.59e+02	6.70e+00	6.87e+05	2.48e+06
MIN	1.59e+02	6.70e+00	6.87e+05	2.48e+06
MAX	1.59e+02	6.70e+00	6.87e+05	2.48e+06
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-
Kt	water	air	soil	sediment
	3.92e-01	3.92e-01	0.00	3.95e-01
1e-06	1.69e+02	6.98e+00	6.78e+05	2.73e+06
1e-05	1.69e+02	6.98e+00	6.78e+05	2.73e+06
1e-04	1.69e+02	6.98e+00	6.78e+05	2.73e+06
1e-03	1.69e+02	6.98e+00	6.78e+05	2.73e+06
1e-02	1.69e+02	6.98e+00	6.78e+05	2.73e+06
AVG	1.69e+02	6.98e+00	6.78e+05	2.73e+06
MIN	1.69e+02	6.98e+00	6.78e+05	2.73e+06
MAX	1.69e+02	6.98e+00	6.78e+05	2.73e+06
MAX/MIN	1.0	1.0	1.0	1.0
OUTP/INP	1.00e-04	1.00e-04	1.00e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)
Other variables default

Substance: HCB				
Ksw	water	air	soil	sediment
	4.24e-02	3.35e-02	0.00	4.52e-02
1e-07	4.74e-04	7.10e-07	3.93e-01	2.87e+00
1e-06	4.74e-04	7.10e-07	3.93e-01	2.87e+00
1e-05	4.74e-04	7.10e-07	3.92e-01	2.87e+00
1e-04	4.74e-04	7.11e-07	3.89e-01	2.87e+00
1e-03	4.73e-04	7.17e-07	3.58e-01	2.87e+00
AVG	4.74e-04	7.11e-07	3.85e-01	2.87e+00
MIN	4.73e-04	7.10e-07	3.58e-01	2.87e+00
MAX	4.74e-04	7.17e-07	3.93e-01	2.87e+00
MAX/MIN	1.0	1.0	1.1	1.0
OUTP/INP	1.00e-04	1.01e-04	1.10e-04	1.00e-04
RESULT	-	-	-	-

Sensitivity analysis (no biodeg)
Other variables default

Substance: HCB				
Ksw	water	air	soil	sediment
	9.17e+04	8.75e+04	0.00	9.69e+04
1e-07	5.05e-04	8.25e-07	3.05e+00	4.00e+00
1e-06	5.05e-04	8.25e-07	3.05e+00	4.00e+00
1e-05	5.05e-04	8.25e-07	3.02e+00	4.00e+00
1e-04	5.04e-04	8.25e-07	2.81e+00	3.99e+00
1e-03	4.98e-04	8.27e-07	1.67e+00	3.95e+00
AVG	5.04e-04	8.25e-07	2.72e+00	3.99e+00
MIN	4.98e-04	8.25e-07	1.67e+00	3.95e+00
MAX	5.05e-04	8.27e-07	3.05e+00	4.00e+00
MAX/MIN	1.0	1.0	1.8	1.0
OUTP/INP	1.01e-04	1.00e-04	1.82e-04	1.01e-04
RESULT	-	-	-	-

Sensitivity analysis (with biodeg)
No advection in air water sediment, other variables default

Substance: HCB				
Ksw	water	air	soil	sediment
	3.92e-01	3.92e-01	0.00	3.95e-01
1e-07	1.70e+02	6.99e+00	6.81e+05	2.64e+06
1e-06	1.70e+02	6.99e+00	6.81e+05	2.64e+06
1e-05	1.70e+02	7.01e+00	6.80e+05	2.64e+06
1e-04	1.74e+02	7.18e+00	6.78e+05	2.71e+06
1e-03	1.99e+02	8.27e+00	6.59e+05	3.10e+06
AVG	1.77e+02	7.28e+00	6.76e+05	2.74e+06
MIN	1.70e+02	6.99e+00	6.59e+05	2.64e+06
MAX	1.99e+02	8.27e+00	6.81e+05	3.10e+06
MAX/MIN	1.2	1.2	1.0	1.2
OUTP/INP	1.18e-04	1.18e-04	1.03e-04	1.18e-04
RESULT	-	-	-	-

APPENDIX D. ENVIRONMENTAL LEVELS OF DEHP AS CALCULATED BY HAZCHEM

Environmentally relevant input data on compound

name of substance		DEHP	Reference
CAS number		117-82-7	
vapour pressure	(Pascal)	.000022	Quackenbos, 1954
boiling point	°C	370	
water solubility	(mg/l)	.041	BUA Report No. 4
log(octanol/water) part. coeff.		4.88	BUA Report No. 4
molecular weight		390	
melting point	°C	-46	
environmental temperature	°C	20	
degradation half life air	(hours)	24	ECETOC, 1993
degradation half life water	(hours)	720	ECETOC, 1993
degradation half life soil	(hours)	1025	ECETOC, 1993
degradation half life sedim.	(hours)	4500	estimated from IPCS, 1992
part. coeff. prim. sludge WWTP	(l/kg)	9330	calculated
part. coeff. sec. sludge WWTP	(l/kg)	11500	calculated
part. coeff. susp. part./w	(l/kg)	3110	calculated
part. coeff. sediment/water	(l/kg)	1560	calculated
part. coeff. soil/water	(l/kg)	1560	calculated
part. coeff. fish/water	(l/kg)	3790	calculated
part. coeff. earthworm/water	(l/kg)	1670	calculated

Environmental release pattern of DEHP

Production volume kg/hr	50000	ECPI, 1993

		type of main	
	fraction	use	prod
Chemicals used in polymers	1	5	2

Release to air	62.1	ECPI, 1993
Release to waste water	28.5	ECPI, 1993
Release to surface water	348	ECPI, 1993
Release to soil	2.28	ECPI, 1993
Total release	440	

input data on waste water treatment plant

discharged compound is DEHP

number of inhabitant equivalents	3.5E+08
waste water/inhabitant/day (l/day)	200
concentration of primary sludge (g/l)	.22
O.C.-content of primary sludge (w/w)	.3
hydraulic retention time (hours)	7
sludge retention time (hours)	216
sludge conc. aeration tank (g/l)	2.5
O.C.-content of secondary sludge (w/w)	.37
sludge conc. effluent (mg/l)	40
discharge of compound in kg/hour	28.5
biodegradation rate (l/h)	3
µmax Monod-kinetiek (l/hr)	1.5
Michaelis-Menten constant (mg/l)	.5
biodegr. in adsorbed state (y/n)	n

Fate of compound DEHP in WWTP (Namkung & Rittmann, 1987)

```
total influent concentration (mg/l)         9.77E-03

effluent concentration (dissolved mg/l)     2.47E-04
effluent concentration (suspended mg/l)     1.14E-04

amount biodegraded per hour (kg)            14.0
amount volatilized per hour (kg)            3.15E-04
removed via primary sludge per hour (kg)    12.8
removed via second. sludge per hour (kg)    .672
removed via effl./hour (dissolved kg)       .721
removed via effl./hour (suspended kg)       .332

primary sludge production per hour (kg)     428000
second. sludge production per hour (kg)     236000

comp. conc. in primary sludge (mg/kg)       29.9
comp. conc. in second. sludge (mg/kg)       2.84

percentage removal by primary sludge        44.8
percentage removal by biodegradation        49.1
percentage total removal                    96.3
```

Emission rates to regional environmental compartments of DEHP

```
Advective residence time air (h)         85.5
Advective residence time water (h)       1100

Direct emission to air (kg/h)            62.1
Direct emission to water (kg/h)          348
Direct emiss. to arable soil (kg/hr)     2.28

WWTP emission to air (kg/h)              3.15E-04
WWTP emission to water (kg/h)            1.05
WWTP emission to arable soil (kg/hr)     13.4
```

Mackay level 3 calculation on DEHP

```
Steady state mass in area   (kg)         1004000
Mass % in air                            .136
Mass % in water dissolved                10.5
Mass % in water suspended                .490
Mass % in arable soil                    5.45
Mass % in natural soil                   1.92
Mass % in sediment                       81.5

Overall residence time   h               2280
Degradation residence time  h            3120
Advection residence time h               8490

Air conc µg/m3                           5.76E-04
Dissolved water conc mg/liter            1.14E-03
Suspended water conc mg/liter            5.33E-05
Arable soil conc ppm                     1.26E-04
Natural soil conc ppm                    2.90E-04
Sediment conc ppm                        .692
Susp.solids conc ppm                     3.55
```

APPENDIX E. CALCULATION FOR LAS AT WWTP MUNICH II AND THE RIVER ISAR

Name of Substance		LAS	COMMENTS
CAS number		2615-29-2	
Vapour pressure	(Pascal)	1,00E-10	ECETOC, 1993
Water solubility	(mg/l)	350	ECETOC, 1993
Log(octanol/water) part. coeff.		2,5	ECETOC, 1993
Molecular weight		347	ECETOC, 1993
Half life in water	(hours)	24	
Half life in sediment	(hours)	24	
Part. coeff. prim. sludge WWTP		3000	
Part. coeff. sec. sludge WWTP		3000	
Part. coeff. susp. matter river		1000	
Part. coeff. sediment		1000	

Input data on waste water treatment plant

Discharged compound is LAS

Number of inhabitant equivalents		1,000,000	Schöberl *et al*, 1994
Waste water/inhabitant/day	(l/day)	216,0	Schöberl *et al*, 1994
Concentration of primary sludge	(g/l)	0,14	Schöberl *et al*, 1994
O.C.-content of primary sludge	(w/w)	30%	Struijs *et al*, 1991
Hydraulic retention time	(hours)	3,6	Schöberl *et al*, 1994
Sludge retention time	(hours)	475,2	Schöberl *et al*, 1994
Sludge conc. aeration tank	(g/l)	3	Schöberl *et al*, 1994
O.C.-content of secondary sludge	(w/w)	53%	Namkung & Rittmann, 1987
Sludge conc. effluent	(mg/l)	1,3	Schöberl *et al*, 1994
Discharge of compound in kg/hour		63,0	
Biodegradation rate	(1/h)	3	
Biodegr. in adsorbed state	(y/n)	n	

Input data on receiving water

River water flow	(m^3/sec)	17,36	Schöberl *et al*, 1994
Concentration in river	(µg/l)	9,00	Schöberl *et al*, 1994
Concentration susp. matter	(mg/l)	0,50	
O.C.-content susp. matter	(w/w)	20%	Mackay *et al*, 1992
Depth of sediment layer	(meter)	0,01	
O.C.-content of sediment	(w/w)	4%	Mackay *et al*, 1992
Burial rate of sediment	(mm/year)	0,10	
Wind velocity at 10m heigth	(m/sec)	3,00	
River width	(meter)	40,00	Schöberl *et al*, 1994
River depth	(meter)	0,50	Schöberl *et al*, 1994
Y-distance from river bank	(meter)	20,00	
Mixing diameter in river	(meter)	40,00	Schöberl *et al*, 1994
1st X-distance downstream	(meter)	200,00	
2nd X-distance downstream	(meter)	5,000,00	
X-distance step	(meter)	200,00	

Fate of compound LAS in WWTP (Cowan *et al*, 1993)			**LAS monitoring results** (Schöberl *et al*, 1994)
Total influent concentration	(mg/l)	7	
Effluent concentration	(dissolved mg/l)	0,0902	0,067 +/- 0,032
Effluent concentration	(suspended mg/l)	0,0004	
Amount biodegraded per hour	(kg)	49,71	
Amount volatilised per hour	(kg)	2,89E-13	
Removed via primary sludge per hour	(kg)	12,42	
Removed via second. sludge per hour	(kg)	5,50E-02	
Removed via effl./hour	(dissolved kg)	0,812	
Removed via effl./hour	(suspended kg)	3,17E-03	
Primary sludge production per hour	(kg)	840	
Second. sludge production per hour	(kg)	203	
Comp. conc. in primary sludge	(mg/kg)	14788,7	
Comp. conc. in second. sludge	(mg/kg)	270,5	
Percentage removal by primary sludge		19,7%	14,0%
Percentage removal by biodegradation		78,9%	
Percentage total removal		98,7%	98,8%

Emission rates to environmental compartments of LAS

WWTP emission to air	(kg/h)	2,89E-13
WWTP emission to water	(kg/h)	0,81
Volume of effluent	(m^3/sec)	2,50
WWTP emission to arable soil	(kg/h)	12,48

Fraction of elimination contributed by

(Bio)degradation		98,8%
Volatilisation		0,0%
Sedimentation		1,2%
Total elimination per second		8,12E-06
Length for complete mixing	(meter)	36,300,0
Length for 50% elimination	(meter)	84,800,0

Table E.1 Calculated Concentration of LAS in the Water Compartment

Distance Downstream	Dissolved µg/l	Suspended µg/l
200	19.20	0.00961
400	19.20	0.00959
600	19.20	0.00958
800	19.10	0.00956
1000	19.10	0.00955
1200	19.10	0.00953
1400	19.00	0.00952
1600	19.00	0.00950
1800	19.00	0.00949
2000	18.90	0.00947
2200	18.90	0.00945
2400	18.90	0.00944
2600	18.80	0.00942
2800	18.80	0.00941
3000	18.80	0.00939
3200	18.80	0.00938
3400	18.70	0.00936
3600	18.70	0.00935
3800	18.70	0.00933
4000	18.60	0.00932
4200	18.60	0.00930
4400	18.60	0.00929
4600	18.50	0.00927
4800	18.50	0.00926
5000	18.50	0.00924

APPENDIX F. MODULE FOR CALCULATION OF A LOCAL PEC IN SOIL

For a more realistic estimation of the concentration in soil a module was developed, which estimates the steady state concentration after many years of exposure via aerial deposition and sludge application, balanced by elimination processes. This results in a PEC_{local}, calculated for a point source. The basic assumptions made for this module are given in Section 4.3.4. The details of calculation are outlined below.

Yearly average concentration in the air

In order to estimate this concentration it is assumed, that:

- emission takes place at a height of 10 meters;
- an emission of 1 g/s results in a yearly average immission concentration of 1 $\mu g/m^3$ at a distance between 100 and 2000 meter. This has been derived from calculations on the basis of the Dutch National Air Dispersion Model (RIVM, VROM, WVC, 1994).

Deposition from air to soil

The deposition velocity in m/h is dependent on the physical state of the substance in the air, that means as aerosol or as gas. The deposition velocity is dependent on the Henry coefficient for substances as vapour.

The fraction of the compound bound to aerosol in the air is estimated from:

$$F_{ab} = \frac{0.00017}{0.00017 + P} \qquad (3)$$

where:-

F_{ab} = fraction aerosol bound
P = vapour pressure pure compound [Pascal]

The deposition velocity of the aerosol bound fraction is assumed to be 36 m/h.

The deposition velocity of the vapour fraction is assumed to be related to the Henry coefficient according to Table F.1 below (RIVM, VROM, WVC, 1994).

Table F.1 Deposition Velocity of Vapours

$^{10}\log H$	deposition velocity (Dpv-gas) meter/hour
≤ -2	1.8
$> -2 \; < 2$	1.44
≥ 2	1.08

The Henry coefficient H is calculated according to Equation 4.

$$H = \frac{P \cdot Mw}{Sb} \tag{4}$$

where:-

H = Henry coefficient
P = vapour pressure of the substance [Pascal]
M_w = molecular mass [g/Mol]
S_b = solubility in water [g/l]

The deposition rate D_{pr} in $\mu g/(m^2 \cdot h)$ can be easily estimated from:

$$D_{pr} = D_{pv} \cdot C_a \tag{5}$$

Where:-

C_a = Emis $\cdot$ 1000 / 3600 [$\mu g/m^3$]
Emis = emission [kg/h]

The deposition velocity D_{pv} in m/h is given by Equation 6:

$$D_{pv} = D_{pv\text{-}part} \cdot F_{ab} + (1 - F_{ab}) \cdot D_{pv\text{-}gas} \tag{6}$$

Estimation of the steady state concentration in soil

The preferred local model aims to estimate a steady state concentration in soil. It should be realised that such a steady state concentration will be achieved only after many years of aerial deposition and/or sludge application.

The steady state concentration in soil is controlled by:

- deposition rate from air; this can be estimated on the basis of the equations above;
- application of sludge of about 2 tons per ha per year. This results in a soil load Sl_{Appl} of the substance in $\mu g / m^2 \cdot h$ given by:

$$Sl_{Appl} = \frac{2 \cdot 10^6 \cdot Sl_{Co}}{10^4 \cdot 365 \cdot 24} \tag{7}$$

Where:-

Sl_{Co} = sludge concentration of substance in ppm.

- removal by evaporation, leaching and degradation.

Removal by evaporation

Mass transfer by evaporation takes place at the following sites:

- from soil surface to air via an air boundary layer. The mass transfer coefficient for this process MTC_a is 5 m/h;
- from soil air to the soil surface via diffusion. The mass transfer coefficient for this process MTC_{sa} is 0.02 m/h.
- from soil water to the soil surface via diffusion. The mass transfer coefficient for this process MTC_{sw} is 0.00001 m/h.

The removal rate by evaporation K_{evap} in h^{-1} for arable and natural soil can be formulated by means of the fugacity modelling of Mackay *et al* (1992):

$$K_{evap[ar]} = \frac{1}{\left(\dfrac{1}{MTC_a \cdot Z_a} + \dfrac{1}{(MTC_{sa} \cdot Z_a + MTC_{sw} \cdot Z_w)}\right) \cdot Z_{soil} \cdot H_{soil[ar]}} \qquad (8)$$

$$K_{evap[nat]} = \frac{1}{\left(\dfrac{1}{MTC_a \cdot Z_a} + \dfrac{1}{(MTC_{sa} \cdot Z_a + MTC_{sw} \cdot Z_w)}\right) \cdot Z_{soil} \cdot H_{soil[nat]}} \qquad (9)$$

Where:-

$K_{evap[ar]}$ = evaporation rate arable soil [1/h]
$K_{evap[nat]}$ = evaporation rate natural soil [1/h]
$H_{soil[ar]}$ = arable soil depth = 0.2 m
$H_{soil[nat]}$ = natural soil depth = 0.05 m
Z_{soil} = $Va \cdot Za + Vw \cdot Zw + Vs \cdot Zs$ [Mol/(m^3·Pa)]
MTC = Mass Transfer Coefficient
MTC_a = soil air boundary layer MTC = 5 m/h
MTC_{sa} = soil air phase diffusion MTC = 0.02 m/h
MTC_{sw} = soil water phase diffusion MTC = 10^{-5} m/h
Z_a = 1/RT [Mol/(m^3·Pa)]
Z_w = 1/H [Mol/(m^3·Pa)]
Z_s = $K_{sol} \cdot$ Dens / H [Mol/(m^3·Pa)]
R = 8.314 Pa·m^3/Mol·°K
T = 293 °K
H = $P \cdot Mw / Sb$ [Pa·m^3/Mol]
M_w = molecular mass [g/Mol]
S_b = solubility in water [g/m^3]
K_{sol} = $0.41 \cdot F_{oc} \cdot K_{ow}$ [l/kg]
F_{oc} = fraction organic carbon soil
K_{ow} = octanol water partition coefficient
D_{ens} = density solids in soil = 2.4 kg/l
V_a = air volume in soil = 0.2 m^3/m^3
V_w = water volume in soil = 0.3 m^3/m^3
V_s = solids volume in soil = 0.5 m^3/m^3

Removal by leaching

It is assumed, that the annual rain excess is 0.3 meter per year. The removal rate by leaching is now formulated by:

$$K_{leach[ar]} = \frac{0.001 \cdot R_{pex} \cdot Z_w}{Z_{soil} \cdot H_{soil[ar]} \cdot 365 \cdot 24} \qquad (10)$$

$$K_{leach[nat]} = \frac{0.001 \cdot R_{pex} Z_w}{Z_{soil} \cdot H_{soil[nat]} \cdot 365 \cdot 24} \qquad (11)$$

Where:-

R_{pex} = rain precipitation excess [mm/y]
$K_{leach[ar]}$ = leaching rate arable soil [1/h]
$K_{leach[nat]}$ = leaching rate natural soil [1/h]
Z_w = 1/H [Mol/(m^3·Pa)]
Z_{soil} = Va ·Za + Vw · Zw + Vs · Zs [Mol/(m^3·Pa)]
$H_{soil[ar]}$ = arable soil depth = 0.2 m
$H_{soil[nat]}$ = natural soil depth = 0.05 m

Removal by (bio)degradation

The (bio)degradation half life in soil ($T_{½soil}$) is of decisive influence on the concentration of a substance in the soil. Assuming a first order degradation rate, the (bio)degradation rate constant K_{deg} expressed in h^{-1} can be derived as follows:

$$K_{deg} = \frac{\ln 2}{T_{½\,soil}} \qquad (12)$$

The concentration in arable and natural soil

The concentration in arable soil is controlled by:

- deposition from the air;
- sludge (or fertiliser etc.) application;

- removal by evaporation, leaching and biodegradation;
- the arable soil depth.

It is calculated according to Equation 13, expressed in µg/kg:

$$C_{soil[ar]} = \frac{D_{pr} + SI_{Appl}}{(K_{deg} + K_{leach} + K_{evap}) \cdot H_{soil[ar]} \cdot Den_{soil}} \tag{13}$$

The concentration in natural soil is controlled by:

- deposition from the air;
- removal by evaporation, leaching and biodegradation;
- the natural soil depth.

It is calculated according to Equation 14, expressed in µg/kg:

$$C_{soil[nat]} = \frac{D_{pr}}{(K_{deg} + K_{leach} + K_{evap}) \cdot H_{soil[nat]} \cdot Den_{soil}} \tag{14}$$

Where:-

D_{pr} = deposition rate [$\mu g/(m^2 \cdot h)$]
SI_{Appl} = substance application rate via activated sludge [$\mu g/(m^2 \cdot h)$]
$H_{soil[ar]}$ = arable soil depth [m]
$H_{soil[nat]}$ = natural soil depth [m]
Den_{soil} = density of soil = $V_a \cdot Den_a + V_w \cdot Den_w + V_s \cdot Den_s$ [kg/m^3]
Den_a = density air in soil = 1.2 kg/m^3
Den_w = density water in soil = 1000kg/m^3
Den_s = density solids in soil = 2400 kg/m^3
V_a = air volume in soil = 0.2 m^3/m^3
V_w = water volume in soil = 0.3m^3/m^3
V_s = solids volume in soil = 0.5m^3/m^3

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