

EU Risk Assessment Guidelines

- Part I.** Quality Criteria for Environmental Risk Assessment Software Using the Example of EUSES
Stefan Schwartz, Volker Berding, Stefan Trapp, Michael Matthies
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Volker Berding, Stefan Schwartz, Michael Matthies
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Preamble

In order to realise EU legislation, the environmental risk of new and existing chemical substances has to be assessed. The methods for risk assessment are laid down in the Technical Guidance Documents - TGD (EC 1996A). Basically, risk assessment consists of a comparison of predicted environmental concentrations (exposure assessment) and concentrations which may cause adverse effects (effect assessment). With the European Union System for the Evaluation of Substances - EUSES (EC 1996B) a decision support system is available which integrates the models presented in the TGD into a Windows 95/NT-based software product. Meanwhile, EUSES has attained a far reaching and extensive use in governments, industry, and research institutes.

For exposure assessment, various exposure models (regression equations, simple generic models, multimedia compartment models) are used. One of the objectives is to investigate the validity of model calculations and evaluate uncertainty in models and data arising in model application. Scientific justification of underlying equations, limitations, and respective software are tested and checked for possible errors. The project consists of several work packages: comprehensive data collection and evaluation, conceptual validation, model simulations, sensitivity and uncertainty analyses, comparison of model results with measured values (numerical validation), appropriateness of models (operational validation), comparison with alternative models, and software evaluation. It is determined for which substances and for which environmental segments the models deliver realistic values. Within this project, exposure assessments are carried out for different substances which represent a wide variety of physical-chemical properties. Substances of interest are those which are used in many products or chemical processes and which are frequently found in the environment. Due to their relatively good data availability, typical and well-known pollutants such as dioxins and PCBs are also investigated. For validation studies, in particular to compare measured concentrations with predicted ones, spatially and temporally coherent data sets must be available. Thus, before starting the project, an environmental segment of regional scale had to be chosen. The German state of North Rhine-Westphalia (approximately 34 000 km²) was selected as an environmental segment of regional scale.

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EU Risk Assessment Guidelines, Part III Scenario Analysis of a Level III Multimedia Model Using Generic and Regional Data

Volker Berding, Stefan Schwartz, Michael Matthies

Institute of Environmental Systems Research, University of Osnabrück, D-49069 Osnabrück, Germany

Corresponding author: Volker Berding; e-mail: vberding@usf.uni-osnabrueck.de

Abstract. Regional PECs (Potential Environmental Concentrations) calculated with the software EUSES were compared with measured values using different emission and environmental distribution scenarios. The environmental data set recommended in EUSES (default data set) represents a generic standard region. In different scenarios the parameters of the generic region are replaced by concrete values, and estimated parameters (emissions, degradation rates and partition coefficients) are substituted by measured or investigated values. Deviations with regard to the measured values can be up to three orders of magnitude. Despite the basically conservative approximations, underestimations can occur. However, these are usually due to poor monitoring data

or inappropriate input values. The use of regional data instead of default parameters only slightly ameliorates the results. The use of real emission and degradation rates alone can improve the results significantly.

Keywords: EUSES, Level III multimedia model, Simple Box; measured concentrations, comparison with modelled results; predicted environmental concentrations, water, air, soil, sediment; scenario analysis, generic data, regional data; scenarios, generic region, default data, regional data, North Rhine-Westphalia; substances, Benzene, DEHP, EDC, EDTA, PCDD, HHCb, LAS, EDTA; validation, measured concentrations, modelled results

1 Introduction

This part III of the series "EU Risk Assessment Guidelines" presents the validation of the regional distribution model included in EUSES [1]. The term validation is controversially discussed in science and is not defined consistently. We follow the ideas of Beck et al. [2], who split the model validation into two basic parts: internal and external validation. Internal validation comprises the examination of the appropriateness of models and the scrutiny of theory, i.e. the inner model structure (also often called verification). On the other hand, with external validation the model results are compared with measured values. Furthermore, sensitivity and uncertainty analyses are required (as part of the external validation), in addition to a comparison with alternative models, and, according to [3], a software evaluation.

The software evaluation [4] and part of the internal validation [5] have already been completed. As a contribution to the external validation, the results of a comparison of measured values with modelled results are presented here.

For this purpose, a set of example substances with different characteristics was chosen. The investigated substances are, on the one hand, those that are used in numerous consumer products or as chemical base substances: benzene, linear alkyl benzene sulfonates (LAS), Di(2-ethylhexyl)phthalate (DEHP), 1,2-Dichlorethane (EDC), Ethylendiaminetetra acetic acid (EDTA) and 1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethyl-cyclopenta-(g)-2-benzopyrane (HHCB). On the other hand, polychlorinated dibenzo-*p*-dioxines (PCDD) have also been included in the selection: 2,3,7,8-Cl₄CDD (TCDD), 1,2,3,7,8-Cl₅CDD (PeCDD), 1,2,3,4,7,8-Cl₆CDD (HxCDD-1), 1,2,3,6,7,8-Cl₆CDD (HxCDD-2), 1,2,3,7,8,9-Cl₆CDD (HxCDD-3), 1,2,3,4,6,7,8-Cl₇CDD (HpCDD), and Cl₈CDD (OCDD). In part, these substances differ strongly in their physico-chemical properties (water solubility, lipophilicity, vapour pressure, etc.) as well as in production volume, releases to the environment, and in the amount and type of use. A brief description of the substances can be found in Table 1.

In order to compare measured with calculated values it is necessary to use spatially and temporarily coherent data for the chosen substances. Hence a comparative region is selected which forms the basis of the survey of monitoring data. The chosen region is North Rhine-Westphalia for the year 1990. The aim of the study is to show for which of the selected substances and for which environmental media the regional distribution model delivers realistic values. General statements about the model's applicability and validity are derived from this.

2 Model and Scenarios

EUSES contains numerous models that are related to each other [5]. The regional distribution model *Simple Box* is implemented to calculate background concentrations. It is a 6-box Level III model with the compartments air, water, sediment, agricultural soil, industrial/urban soil and natural soil. The EUSES Simple Box consists of two nested spatial scales (continental and regional). With its parameters the continental scale represents the European Union. The regional scale characterises a fictitious European standard region. However, it is possible to fit the model's parameters to a real environment. The relevant parameters and the altered values are presented in Section 3.

For an external validation it is necessary to detect all input and output variables:

- The output parameters of Simple Box are the continental and regional PECs (Predicted Environmental Concentrations) for air, water, sediment, the three soils and pore water of agricultural soil.
- The input values are, on the one hand, substance parameters like the physico-chemical properties (PC-data), the use and production categories, amounts of production, import and export, and, on the other hand, the regional and environmental parameters.

Most of these parameters are also input values for other models in EUSES.

Table 1: Brief description of the investigated substances (according to [6])

Substance	Description
Polychlorinated dibenzo- <i>p</i> -dioxines (PCDD)	Non-polar, barely water soluble, lipophilic compounds with high persistence. They have never been produced, but can result as the spin-off in the production of organic chloro compounds (e.g. Pentachlorophenol) or in combustion processes.
Benzene	Hydrocarbon produced and emitted in high amounts which, due to its volatility, is a typical air pollutant.
Di(2-ethylhexyl)phthalate (DEHP)	A substance with a high lipophilicity produced in high amounts, mainly used as a softener in plastics.
1,2-Dichlorethane (EDC)	A substance with high volatility and water solubility, used in the chemical industry as a solvent or base substance for further syntheses.
Ethylendiaminetetra acetic acid (EDTA)	Chelating agent used in many sectors, especially as a bonding substance and preservative.
1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethyl-cyclopenta-(g)-2-benzopyrane (HHCB)	Polycyclic musk fragrance used in perfumes, cosmetics, detergents and cleaning agents. It is mainly emitted into water by sewage treatment plants. Recently, this substance became controversial because of its high bioaccumulation potential.
Linear alkyl benzene sulfonates (LAS)	Mixture of anionic surfactants, produced in high amounts and mainly used as sodium salt in cleaning and washing detergents. It is mainly emitted into water by sewage treatment plants. Because of its slight volatility, high water solubility and use pattern it is a typical water pollutant.

Using the substance parameters, the emissions into air and surface water, to agricultural soil, and to industrial/urban soil are estimated. A distinction is made between direct emissions from industrial plants and indirect emissions from sewage treatment plants. By default, the direct emissions are estimated with the help of emission tables (A-tables). Indirect emissions are calculated with the sewage treatment plant (STP) model *Simple Treat*. Hence, an external validation has to take into consideration the uncertainties in the emission tables and in the STP model. It is obvious that if the model's input data are initially incorrect, this model can consequently not deliver realistic results, even if all the underlying processes are represented correctly. The same applies to the partition coefficients that are calculated with regression equations (e.g. BCF and K_{OC} from K_{OW}). Thus, an external validation of Simple Box alone is only possible if all its input parameters (and therefore emissions and partition coefficients, too) are known and are not the result of previous estimations, regressions or modelled calculations. Due to the facility in EUSES to overwrite almost every intermediate result it is possible to replace the estimated values with measured or investigated data.

Some of the regional and environmental parameters characterise the region, like area and fractions for different land uses, number of inhabitants, fraction connected to sewer systems,

wind speed, precipitation, etc. The majority of these parameters must be changed if a real region has to be represented. According to this, several scenarios can be formed, each based on a different data set. Here, three scenarios are elaborated: the scenarios *Default*, *NRW standard* and *NRW realistic*. The *Default* scenario only uses the minimum of necessary input data, such as physico-chemical properties, tonnages, imports, use categories and characterisation of biodegradability. All other parameters either have default values or are calculated from other parameters. In the scenario *NRW standard* the regional and environmental parameters are changed to values representative of the Rhinish-Westphalian region (\rightarrow Table 2). The most realistic scenario is *NRW realistic*. Here, in addition to *NRW standard*, all known values for this substance are used. These are real emissions (by changing emission factors or directly the release rates), measured values for partition coefficients like the Henry coefficient and K_{OC} and measured degradation rates. Brief information on the characteristics of the used scenarios is given in Table 3.

As previously mentioned, the PCDDs are a special case. Since they have never been produced, the emissions cannot be estimated in the usual way and must be investigated directly. For North Rhine-Westphalia these data are available for direct emissions into the air [12]. However, they have to be estimated from the via International Toxicity Equivalents

Table 2: Regional and environmental parameters used in the scenarios

Parameter	Standard Scenario	NRW Scenario
Constant of Junge equation [Pa m]	0.01	0.172 [7]
Environmental temperature [°C]	12	11 [8]
Surface area of particles [m ² /m ³]	0.01	1.5E-4 [7]
Number of inhabitants feeding one STP	10 000	17 225.7 [9]
Sewage flow [l/(eq*d)]	200	200.47 [10]
BOD [g/d]	54	60 (German value for calculation of inhabitant equivalent)
Area of regional system [km ²]	40 000	34 400 [11]
Number of inhabitants of region	20 000 000	17 816 100 [10]
Area fraction of water of the regional system	0.03	0.018 [11]
Area fraction of natural soil	0.6	0.26 [11]
Area fraction of industrial/urban soil	0.1	0.202 [11]
Area fraction of agricultural soil	0.27	0.52 [11]
Fraction of water flow from continental scale to region	0.034	0.029 (AREA reg/AREA EU*DEPTHwater)
Wind speed in the system at the height of 10 m [m/s]	3	3.1 [8]
Average annual precipitation [mm/yr]	700	679 [8]
Fraction connected to sewer systems	0.7	0.92 [10]
Sewage treatment: Mode of aeration	surface	bubble

Table 3: Overview of the used scenarios; (R) pre-set regional data are replaced with realistic data, (P) estimated substance-specific parameters and emissions are replaced with measured or investigated values, respectively

Scenario	R	P	Characterisation
Default			Only the minimum of substance-specific data was inserted. The values given by EUSES were not changed.
NRW standard	•		The parameters of the EUSES standard region were replaced by values representing the region North Rhine-Westphalia.
NRW realistic	•	•	The same as NRW standard, but the estimated emissions, partition coefficients and degradation rates were substituted by measured ones.

(I-TEQs [13]) and typical congener patterns. There are also PCDD emissions to waste water that arise from washing clothes contaminated with Pentachlorophenol (PCP) [14,15]. According to [14] and [15] a per capita emission of each congener via waste water can be estimated. Measured or otherwise obtained values for K_{OC} and the Henry coefficient are available [16], but not taken into consideration because they vary widely (uncertainty and variability analyses could consider these variations) and the EUSES estimations are near the mean of the range of these values. Thus, the scenarios for PCDD differ from the other substances' scenarios since all three scenarios use inputted emissions and estimated partition coefficients.

3 Data Basis

In the following, we present which data are required for the external validation of the regional distribution model. These are monitoring data, production volumes and emissions, as well as further substance-specific parameters.

3.1 Monitoring data

Validating a regional model is problematical because the model delivers background concentrations while measured data can be local top values that are much higher than the background concentrations. In the TGD [17], p. 257, the following demands are made to regional measured values: "Data from a prolonged monitoring program, where seasonal fluctuations are already included, are of special interest. If available, the 90-percentile values of the measured data are of highest preference. If only maximum concentrations are reported, they should be considered as a worst-case assumption, whereas using the average concentrations can result in an underestimation of the existing risk, because temporal and/or spatial concentrations do not reflect periods and/or locations of high exposure." The TGD [17], p. 258, also proposes how measured values can be assigned to regional PECs: "If there is no spatial proximity between the sampling site and point sources of emission (e.g. from rural regions), the data represent a background concentration ($PEC_{regional}$) (...)."

Environmental concentrations of the relative substances have been investigated for the realisation of the external validation. Complete monitoring programmes were rarely obtainable. As a result of this, often only a few data were available for comparison. The minimum, median and maximum were calculated from these values and used for the numerical values. Table 5 (Section 6, p. 156) shows the accessible data. A sufficient data set for every substance could not be obtained for any of the compartments. Most data could be found for PCDD, where only water concentrations are missing. The other substances have usually been measured in water, but only rarely or even not at all in the other compartments.

3.2 Productions and emissions

EUSES contains emission tables that serve to estimate releases by means of the substance's tonnage, use and main category, and a number of PC parameters. This information has to be

detected for each of the chosen substances. The release estimations represent a great uncertainty for the calculation of environmental concentrations. Hence, for a consistent validation it is useful to know the real releases for the year of the measurement. In fact, these are obtainable for almost every selected substance. The releases are listed in Table 6 (Section 6, p. 156). However, it must be considered that only the total regional emissions are presented, although they are the sum of emissions taking place at any of five possible life cycle steps.

Since productions, etc. are, of course, not available for PCDD they have to be inputted directly at the appropriate place in EUSES. The required emissions could not be gained for several substances and media for North Rhine-Westphalia, but only for Germany. In such a case they were estimated from the available emissions.

3.3 Substance-specific parameters

Physico-chemical properties and partition coefficients had to be detected for each of the used substances. Required input parameters are the molecular weight, melting and boiling point, vapour pressure, water solubility and the partition coefficient Octanol/water (K_{OW}). The Henry coefficient and partition coefficient organic carbon/water (K_{OC}) can often be found in the literature, but are calculated in EUSES, too. The investigated and the calculated parameter values are presented in Table 7 (Section 6, p. 157). It should be noted that many different equations exist to calculate the K_{OC} [16], [17]. In the scenarios used here only the EUSES estimations and measured values are taken, but not results of other calculations. Additionally, it is possible to input substance-specific degradation rates for air, water, soil and sediment. Table 8 (Section 6, p. 157) shows the used values. It must be taken into consideration that the chosen degradation rates for PCDD are highly uncertain since they are quite difficult to measure. The chosen values from [16] may probably be too high, but the assumption that PCDD are not degraded is already considered in the *Default* scenario.

4 Results and Discussion

In the following the model results are presented in a comparison of calculated with measured regional concentrations for air, water, sediment and agricultural soil. The scenario results and the measured values are shown in Fig. 1 to 4 (pp. 151-155). A summarising assessment is listed in Table 4 (p. 154). The following criteria have been developed to evaluate the results:

"Good" are modelled results between the median and maximum of the measured concentrations or less than half an order of magnitude above the measured maximum.

The modelled results are "fair" if they are less than half an order of magnitude below the measured minimum and less than one order of magnitude above the maximum. These results are already further beyond the measured values. Since an underestimation is beyond the scope of a conservative estimation, the underestimation must not be higher than half an order of magnitude, while the overestimation may be up to one order of magnitude.

Higher over- or underestimations are classified as "poor".

4.1 Water

Regional concentrations were available for the water compartment for all substances apart from the dioxins.

The water concentrations are estimated well for the majority of the chosen substances.

For dioxins comparative values are derived from air concentrations using the partition coefficients. This is why they cannot be utilised to evaluate the validity of Simple Box, but can only serve for orientation purposes. The assumption of degradation in the scenario *NRW realistic* leads to a much more considerable decrease of the predicted concentrations than the use of realistic regional instead of default values.

The estimations for benzene are only slightly too high and thus are classified as good. The modelled results improve, i.e. they are nearer to the median, when realistic values are inserted. But altogether they differ only negligibly (< 0.5 orders of magnitude).

The measured DEHP concentrations are exceeded in the standard scenarios by slightly more than half an order of magnitude. These overestimations decrease in the realistic NRW-scenario to under half an order of magnitude. Hence the estimations are conservative, but nevertheless good when realistic values are used.

The model clearly overestimates the measured EDC concentrations. Bad monitoring data (only single values) or wrong emissions could be the reasons for this error. The emissions could only be estimated because real data were not available. This is why the modelled results are not easy to assess for this substance, and are rather poor.

The scenario outcomes for EDTA barely differ. A slight increase of water concentration can be noticed when real regional parameters are used. This results from a lower area fraction for water and a regional area reduction with otherwise unchanged emission data. Inserting realistic degradation rates decreases the concentrations again to the results of the *Default* scenario. Altogether, EDTA is estimated rather conservatively, but well. The same applies for LAS. The measured concentrations are estimated well from the scenarios. The results of the standard scenarios are between the measured median and maximum. With more realistic degradation rates and emissions the modelled slightly underestimate the measured median. The reason for the good estimations of EDTA and LAS could be their "unequivocal" environmental behaviour: They are scarcely volatile and are exclusively emitted into water. The degradation rates of both substances are well known, and the supposed emissions seem to be near to the real numbers.

A similar situation applies for HHCB. The modelled values of this substance are between the measured median and maximum or (NRW realistic) just slightly below the median, even though the difference between the measured minimum and maximum is only one order of magnitude. More exact scenario analyses for HHCB were carried out by Schwartz et al. [18].

Altogether it can be stated that the regional PECs for water are estimated quite well. The modelled results are only worse when no real emissions are available and monitoring data are sparse. The estimations are best for substances that can typically be found in water (EDTA, LAS, HHCB). Underestimations only take place with dioxins, but it has to be considered that the only comparative values are estimations, which are thus unsuitable.

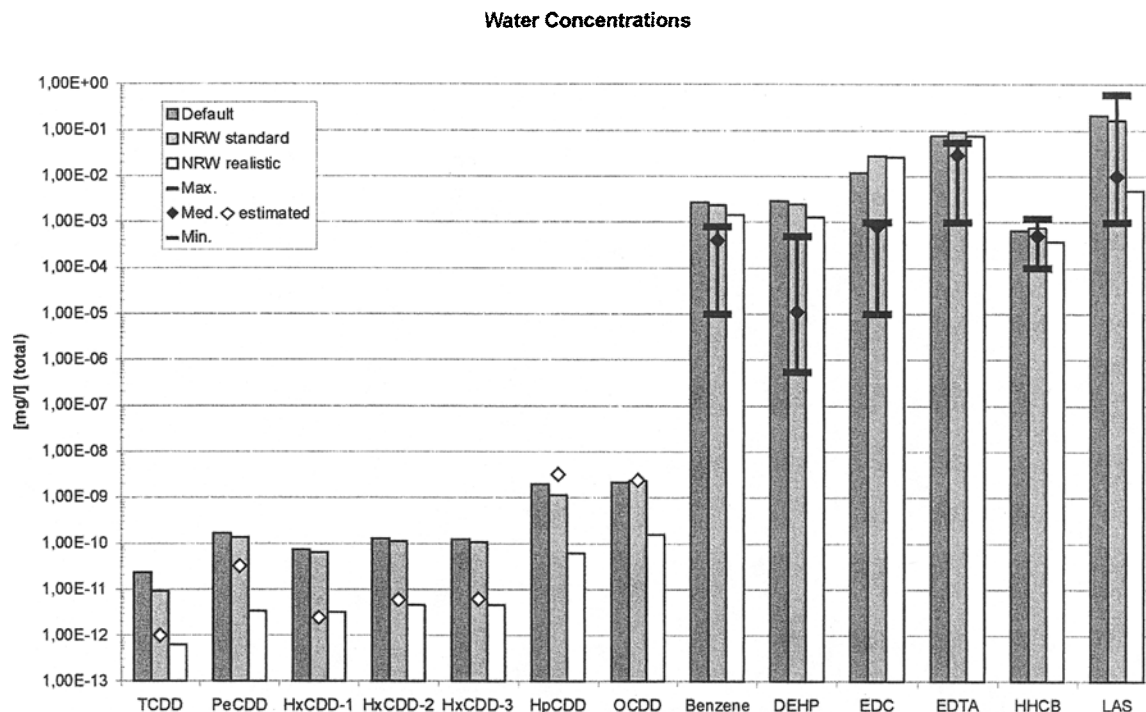


Fig. 1: Comparison of calculated water concentrations with measured values; comparative concentrations for PCDD are estimated from air concentrations

4.2 Air

No measured values of EDTA and LAS exist for the compartment air since these substances are not volatile. Nevertheless, EUSES delivers PECs for these substances because a vapour pressure larger than 0 has to be inputted, even though it is not measurable for these substances. The minimum that can be set without a warning for this parameter in EUSES is $1\text{E-}6$ Pa. With the scenario *NRW realistic* EUSES calculates infinitely small PECs (EDTA $6\text{E-}21$ mg/m^3 , LAS $5\text{E-}19$ mg/m^3) what is assumed to be the most realistic estimation. Here, the calculated emissions to air are additionally set to 0 kg/d , and the Henry coefficient is set to the minimum ($4\text{E-}10$ Pa m^3/mol), too. At this point the advised parameter ranges must be questioned. It is possible to use lower values than the advised minima that are nearer to 0, which of course produces lower air concentrations. As a consequence, the *Default scenario* would already lead to qualitatively different results if the advised minima were lower or ignored by the user. It is not evident why the vapour pressure's minimum has to be $1\text{E-}6$ Pa and the Henry's minimum $4\text{E-}10$ Pa m^3/mol since mathematically correct results are possible with lower values. The reason to exclude 0 as the minimal value is to prevent division by zero, but the set ranges should be discussed.

There are no measured air concentrations for HHCB either. This can be attributed to the low total number of measurements of this substance to date. In any case, the likeliest occurrence is in water and thus the main focus so far has been concentrated on that compartment. For this substance the difference between the two standard scenarios is negligible. But replacing the estimated degradation rate for air by a measured one decreases the predicted concentration by more than one order of magnitude.

The modelled results for typical air pollutants (benzene, EDC) are good, since they are between the measured medians and maximums. A distinct enhancement of the modelled results for benzene, i.e. an approach to the median, can be noticed in the scenario *NRW realistic* with set emissions and degradation rates. The reason for this is the high overestimation of benzene emissions into air using the emission tables.

The regional model predicts the PCDD concentrations worse with increasing lipophilicity. While TCDD and PeCDD are estimated nearly to the measured median, the results are fair for HxCDDs and HpCDD (slight underestimations). The results for OCDD are poor because of the clear underestimation by nearly one order of magnitude. The reason for these different estimations could be the difficulty in approximating emissions (from I-TEQs and the appropriate congener patterns shown in [12]). It is noticeable that the use of degradation rates for air only marginally decreases the predicted concentrations. This can result from the very low mass fraction of PCDD in the air and the fact that advective processes are much more important loss paths than degradation.

It is wrong to conclude from this that very lipophile substances are always underestimated: Even though DEHP's K_{ow} is between PeCDD and HxCDD, the predicted concentration is even more than one order of magnitude higher than the measured maximum. An explanation for this high deviation could be that monitoring data were only obtainable from clean air (rural areas). The use of investigated partition coefficients, degradation rates and emissions leads to a slight improvement, even though the estimated emissions are lower than in reality. The improvement could be caused by the relatively high degradation rate for air that is assumed

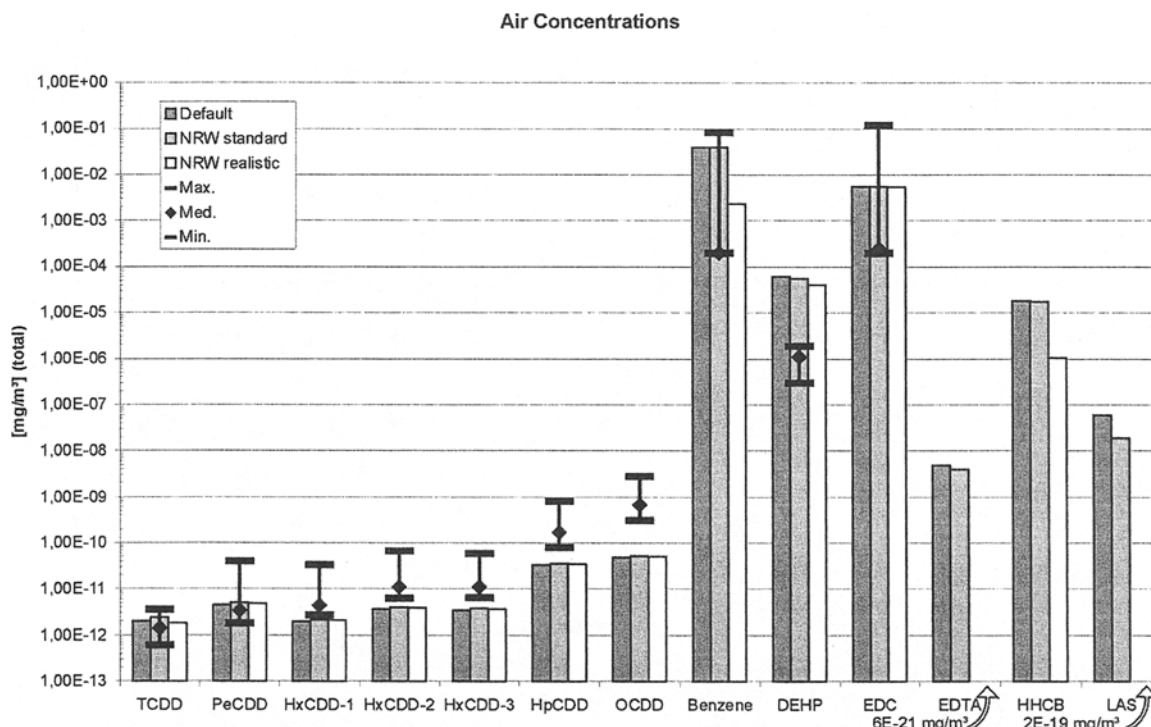


Fig. 2: Comparison of calculated air concentrations with measured values

in the realistic scenario. Nevertheless, the underestimation of emissions to air is remarkable because the emission tables usually calculate releases very conservatively. However, the modelled results do not differ by more than half an order of magnitude from one another.

4.3 Soil

Assessing the modelled results for the compartment soil is difficult since monitoring data are poor (exception: PCDD) and emissions have to be estimated. Any monitoring data used are related to agricultural soil. Hence the PEC for agricultural soil is taken for the comparison. When evaluating these results, it must be taken into consideration that EUSES assumes a continuous sewage sludge application rate on agricultural soil. The STP model calculates fractions for indirect emissions, substances remaining in the sludge and degradation. It uses PC data, biodegradability, STP properties and environmental parameters. The calculated fractions are multiplied by the emissions to waste water. Thus, the emission rate to agricultural soil is the emission rate to waste water multiplied by the fraction directed to sludge. Hence, measured concentrations from agricultural soil with sludge application were chosen if available.

Sufficient measured values were only obtainable for PCDD. These substances are estimated well in the standard scenarios, even though the emissions are based on approximated releases to waste water. The calculated values do not diverge by more than one order of magnitude from the measured medians and are, with the exception of TCDD, between the median and maximum or slight above the maximum. The use of regional data decreases the calculations slightly. The difference is only larger for TCDD because changing the parameters for particle content and properties has a more serious effect on the fraction associated with aerosol particles. This leads to a lower deposition rate and consequently to lower emissions to soil. The use of degradation rates leads to a high underestimation of the measured soil concentrations. This shows that the used rates [17] may still be too high, even if the half-lives are between 17,000 h (TCDD) and 55,000 h (OCDD). One generally has to bear in mind that degradation rates for PCDD can hardly be measured, especially for soil, and any value used is worth discussing. Additionally, it must be considered that in the regional model each soil is treated as a homogenous compartment, i.e. degradation is assumed to take place in the whole soil at the given rate, although PCDDs are best degraded at the thin top layer while the rest in the deeper soil is degraded much more slowly.

The calculated soil concentrations for benzene are near the detection limit (about half an order of magnitude above in the standard scenarios and marginally below in the realistic scenario) but nearly two orders of magnitude lower than the only measured value. Since benzene can not usually be found in soil, except for local hot spots, these results well represent the real circumstances. The clear difference between the standard scenarios and the realistic scenario comes from the strongly changed emissions.

The data available for DEHP enable the modelled results to be assessed. The two standard scenarios overestimate the concentrations considerably (about 2.5 orders of magnitude). The use of realistic emissions and degradation rates leads to a marginal underestimation of the measured minimum, i.e. a clear improvement of the predicted concentration. As the measured values have a narrow range the underestimation is only slight. Due to this the result for the realistic scenario is fair, and the standard scenarios must be considered poor.

No statements are possible for EDC because the only comparative value is the detection limit. But the clearly increasing modelled result in the scenario "NRW realistic" is noticeable. Since the K_{OC} is raised by a factor of 10, the degradation rate in the sewage treatment plant decreases evidently and hence the emissions to agricultural soil increase.

The only value obtainable for EDTA is an estimation after sludge application. Hence, no comparison is possible for this substance either. In any case, the considerable difference between the standard scenarios and the realistic scenario is significant. This results from the very low air concentration, which leads to a lower deposition rate and hence to decreasing soil concentrations. Even though EDTA is not biodegraded in sewage treatment plants, input via sludge does not play a significant role. Because of its very low lipophilicity ($\log K_{OW} = -3,34$) EDTA is chiefly dissolved in water, but not bound to sludge.

No classification is possible for HHCb either, since no measured values are available. The several scenarios barely differ from each other.

The monitoring situation for LAS is poor. There are only single values for agricultural soil after sludge application. These are maximal values which are, as expected, underestimated. Indeed, the explicitness of the underestimation is noticeable (minimum/median about 2.5 orders of magnitude, maximum about 5 orders of magnitude). The realistic scenario does not produce significantly reduced soil concentrations because, for LAS, deposition is a less important process in comparison with indirect emissions via STP sludge. LAS is readily biodegradable, but there is also a significant fraction of the non-degraded substance that is bound to sludge.

Altogether the monitoring data are only sufficient for PCDD and DEHP. For the other substances the measured concentrations are rather maximum values than regional background concentrations. Furthermore, one has to bear in mind that the estimation of the agricultural soil concentration is based on the results of the STP model Simple Treat (which is expressly left disregarded here) which calculates the indirect emissions. Hence the statements on the validity of Simple Box only have little weight for this compartment.

The trend for the estimation of the agricultural soil concentration is an underestimation. The over-estimations of emissions in the standard scenarios compensate the general under-estimations, thus these results are nearer to the measured values than those of the realistic scenario.

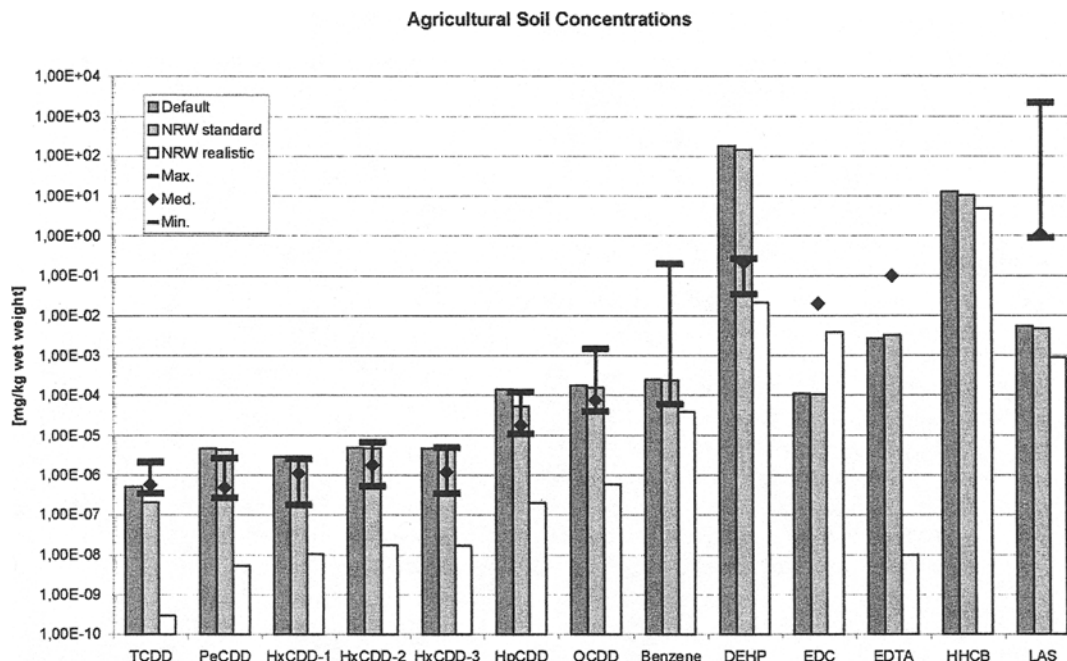


Fig. 3: Comparison of calculated agricultural soil concentrations with measured values

4.4 Sediment

There are no direct emissions into sediment. Hence the concentration depends on the emissions into water (direct, indirect, deposition) and the sedimentation rate, combined with the fraction of substance associated to suspended matter. Analogue to soil there were only a few measured values for sediment.

Although the monitoring data for PCDD are sparse (eight measuring points at the Rhine and Elbe), it is possible to carry out a rough comparison. Overall, the concentrations of PCDD in sediment are underestimated. The difficult estimation of PCDD emissions to water could be a reason for this. However, the estimations are only poor for TCDD and OCDD. The other considered dioxins are estimated fairly in the standard scenarios. With the presumed degradation rates the predicted concentrations decrease considerably. As already discussed in the context with soil, the degradation rates for sediment may be too high. Difficulties arise in three fields which may explain this phenomenon: the measurement of PCDD-degradation rates is problematical; it is not certain whether they are degraded in sediment at all; the consideration of the sediment as one homogeneous compartment.

Even if there are measured values for benzene, they can only serve as an orientation because the data were taken in Japan and the USA. Nevertheless, the modelled results of the three scenarios are between these two, only slightly differing, values. This is a good result from a more formal point of view albeit questionable with respect to the available data.

Sufficient measured values exist for DEHP. But because of the very high variation of these data (factor 1,000,000 between minimum and maximum), a classification of the modelled results is not feasible. One can only state that the modelled results are within the measured values. The use of

realistic values for emissions, degradation and partition coefficients leads to a distinct reduction (one order of magnitude) of the predicted concentrations in sediment.

There are no monitoring data for EDC, so a comparison of the model and reality is impossible. But it is worth noting that the modelled results increase from the scenario *Default* to *NRW realistic*, although the standard scenario should deliver the most conservative prediction.

Table 4: Summarising assessment

Substance	Compartment			
	Water	Air	Soil	Sediment
TCDD	#	+	+	-
PeCDD	#	+	+	o
HxCDD-1	#	o	+	o
HxCDD-2	#	o	+	o
HxCDD-3	#	o	+	o
HpCDD	#	o	+	o
OCDD	#	-	+	-
Benzene	+	+	#	#
DEHP	+	-	o	#
EDC	#	+	#	#
EDTA	+	#	#	#
HHCB	+	#	#	#
LAS	+	#	#	-

+: good (modelled results between median and maximum or <0.5 orders of magnitude (OoM) above maximum)

o: fair (modelled results <0.5 OoM below minimum and <=1 OoM above maximum)

-: poor (modelled results >=0.5 OoM below minimum or >1 OoM above maximum)

#: not assessable (no sufficient monitoring data)

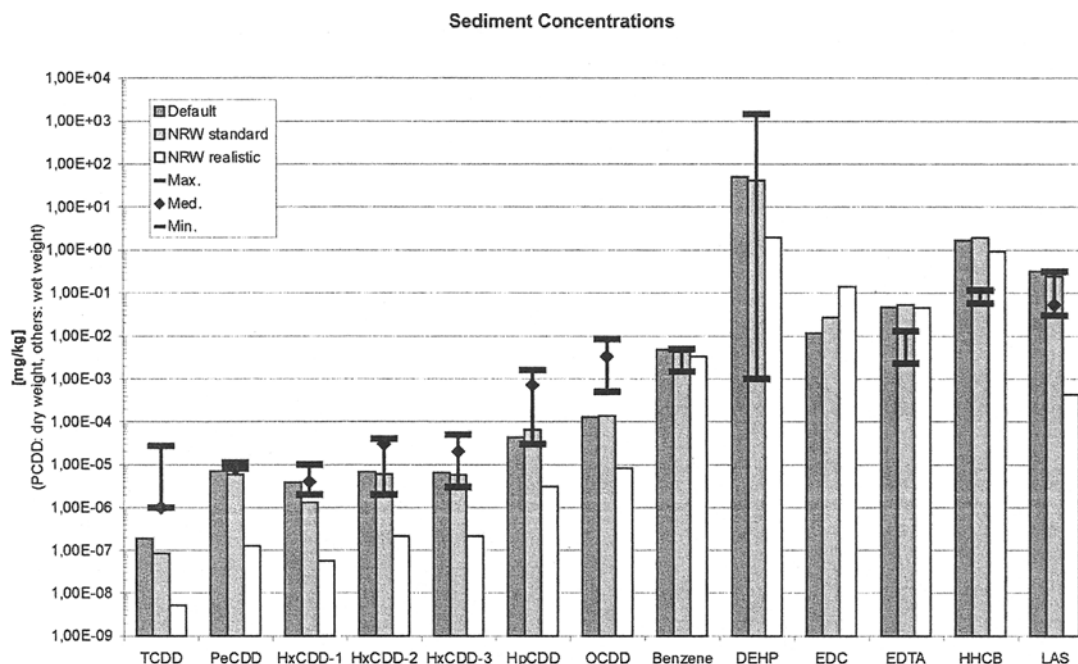


Fig. 4: Comparison of calculated sediment concentrations with measured values

EDTA has not been measured sufficiently either. The two values from Japan and USA can only serve as an orientation. They are overestimated by about one to 1.5 orders of magnitude. The scenarios do not differ very much.

The monitoring data for HHCb are also poor since there are only single values which are overestimated by about one order of magnitude.

LAS concentrations are estimated well with the standard scenarios. The use of realistic values, i.e. lower emissions and higher degradation rates for water and sediment, leads to an underestimation of more than two orders of magnitude. Consequently, the results have to be classified as poor.

5 Conclusions

The evaluation has shown that the use of regionally specific values instead of the defaults of the generic standard region only leads to small deviations of the predicted environmental concentrations. There could be two reasons for this that have to be further evaluated: On the one hand, the sensitivity of the regional parameters could be very low so that changes only slightly affect the results. On the other hand, the slight differences between the first two scenarios could result from the similarity of the standard region and the chosen comparative region.

More serious changes are effected by inserting measured and investigated values for degradation rates, partition coefficients and emissions. If these parameters are known without having to be estimated, the results of the scenario *NRW realistic* approach the median of the measurements. The predicted concentrations decrease in the scenario *NRW realistic* with only a few exceptions (these are: DEHP air, EDC soil, EDC sediment). Since underestimations are possible, this can even lead to a weakening of the model results. How-

ever, underestimations can usually be attributed to inapplicable measured data or insufficient degradation and emission rates. Consequently, EUSES can still be viewed as a conservatively working model system.

Because of the particularly poor availability of monitoring data it is not easy to judge the applicability of the regional fate model for the different substances and environmental media. In principle, it can be stated that the modelled results depend strongly on the quality of the used input data, which is not surprising. An evaluation of Simple Box irrespective of the whole EUSES system is almost impossible since preliminary calculations are indispensable. This particularly concerns the results of the STP model. It is the only facility to quantify the emissions to agricultural soil, since investigated data are not obtainable for this parameter. With a good monitoring data set and good – or well estimated – input data the regional model delivers realistic results.

The worst results are achieved with very lipophilic substances (higher chlorinated PCDD, DEHP). However, it must be considered that the estimation of congener-specific PCDD emissions from I-TEQ-values is problematic and involves considerable uncertainties. It is remarkable that the results are very near to the measured values for substances whose physico-chemical properties are such that they can typically be found in one medium (e.g. benzene and EDC in air, EDTA, HHCb, LAS in water, and PCDD in soil when no degradation is supposed). In other media the model results may deviate more clearly from the measured values. One point to discuss is the assumption that soil and sediment are simple homogenous compartments without different layers. Using degradation rates for the bulk compartment can, as seen for the PCDD, lead to under-estimations that could be avoided with a more detailed model structure. Bennett et al. [19] suggested using the soil penetration depth which is specific

for each substance, instead of a fixed soil depth. Presuming or calculating an average degradation rate that includes the different degradations in the several soil layers could also be a solution to this problem. This confirms the presumption that many uncertainties are usually based on poor data and that the model is altogether applicable to calculate regional background concentrations.

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6 Data Tables: Tables 5 – 8

Table 5: Sources of monitoring data

Substance	Water	Air	Soil	Sediment
PCDD	Estimated from air concentrations	Chloraromatenprogramm 1990 [20]	Chloraromatenprogramm 1990 [20]	8 measuring points river Rhine and river Elbe 1987 [21]
Benzene	Single measured values Rhine 1990-1994 [22]	Rural areas BRD 1988 [23]	Detection limit (min.) and contaminated soil (max.) [22], [23]	USA, Japan [24]
DEHP	Measured values for Rhine between Honnef and Bingen, 4 measuring points with 83 measured values 1991-1992 [25]	Reinluftgebiete 1985 [24], no NRW or coherent data	German soils 1995 [26]	Rhine [25]
EDC	Single measured values river Rhine 1987-1992 [27]	Only single values [24]	Detection limit [27]	No data
EDTA	Single measured values river Rhine and tributaries 1980-1994 [28]	No data (not volatile)	Estimated values after application of fertilisers [28]	Japan 1979, only Min. and Max. (ECDIN) [29]
HHCB	30 measured values river Ruhr 1994/1995 [30], [31]	No data	No data	Single measured values river Ruhr 1994/1995 [30], [31]
LAS	Measured values between 1989 and 1992 for river Rhine [32]	No data (not volatile)	Agricultural soils after sludge application [33], [34]	River Lippe [35]

Table 6: Production and emissions

Substance	EU Prod. / Imp.[t/a]	Direct emissions ^a (Default / NRW Standard / NRW realistic)				Indirect emissions ^b (Default / NRW Standard / NRW realistic)		
		Emissions to air [kg/d] ^c	Emissions to waste water [kg/d] ^d	Emissions to water [kg/d]	Emissions to industrial soil [kg/d]	Emissions to air by STP [kg/d]	Emissions to water by STP [kg/d]	Emissions to agr. soil [kg/d]
TCDD	-	7.4E-5	1.88E-7	1.63E-8	0	1.77E-10	1.63E-8	1.71E-7
PeCDD	-	2.65E-4	3.16E-7	2.75E-8	0	8.51E-12	2.44E-8	2.92E-7
HxCDD-1	-	1.18E-4	4.2E-6	3.65E-7	0	7.98E-10	3.13E-7	3.89E-6
HxCDD-2	-	2.2E-4	4.19E-6	3.64E-7	0	7.96E-10	3.12E-7	3.88E-6
HxCDD-3	-	2.09E-4	4.2E-6	3.65E-7	0	7.98E-10	3.13E-7	3.89E-6
HpCDD	-	2.04E-3	9.57E-5	8.32E-6	0	4.31E-10	7.06E-6	8.86E-5
OCDD	-	2.96E-3	7.23E-4	0	0	1.13E-8	5.3E-5	6.7E-4
Benzene	6.1E6 / 0 [29]	1.12E6 / 1.12E6 / 3.42E4 [36] ^e	8.16E3 / 1.07E4 / 3.42E3 ^f	3.66E3 / 1.09E3 / 1.09E3	2.12E3 / 2.12E3 / 2.12E3	3.75E3 / 2.41E3 / 750	476 / 818 / 263	48.4 / 64.3 / 28.7
DEHP	1E6 / 0 [25]	688 / 688 / 3333 [37]	2.49E3 / 3.27E3 / 1.45E3 [37]	1070 / 284 / 126 [37]	82 / 82 / 0 [37]	4.65 / 3.77 / 37.6	209 / 249 / 186	2.27E3 / 3.01E3 / 1.23E3
EDC	8.5E6 [30] / 0 [28]	1.28E5	2.09E4 / 2.74E4 / 2.74E4	8.94E3 / 2.39E3 / 2.39E3	692 / 692 / 692	1.43E4 / 1.05E4 / 1.07E4	6.48E3 / 1.69E4 / 1.6E4	40.5 / 61.7 / 684
EDTA	2.65E4 / 0 [29]	883 / 883 / 0	3.35E3 / 4.4E3 / 4.4E3	1.44E3 / 393 / 393	49.2 / 49.2 / 49.2	3.67E-5 / 5.05E-5 / 3.45E-8	3.35E3 / 4.4E3 / 4.4E3	1.04E-3 / 1.42E-3 / 1.42E-3
HHCB	0 / 2400 [39]	0 / 0 / 0	456 / 599 / 295	195 / 52.1 / 25.7	6.58 / 6.58 / 0	6.6 / 7.07 / 3.63	70.1 / 85.6 / 43	379 / 506 / 248
LAS ^g	5E5 / 0 [40]	344 / 344 / 0	9.5E4 / 1.25E5 / 6.24E4	4.07E4 / 1.09E4 / 5.43E3	1.39E3 / 1.39E3 / 695	1.22E-4 / 1.57E-4 / 9.91E-8	1.2E4 / 1.44E4 / 7.19E3	435 / 571 / 286

^a: NRW realistic emission calculated from tonnages with set emission factors.

^b: emissions are calculated with SimpleTreat.

^c: PCDD: emissions to air (I-TEQ) and congener pattern from [12].

^d: PCDD: Emissions to waste water / water according to [14] and [15].

^e: The emissions for the whole of Germany are given. 25 % of this value has been assumed for NRW.

^f: Estimated: 10% of the emissions to air.

^g: Regional emissions are estimated too high; based on the per-capita use of 3.8 g/d [41], the factor 0.05 instead of 0.1 of the EU-production volume is used for the region; thus all emissions are halved; besides, it is assumed that no emissions to air take place.

Table 7: Overview of PC data used

Substance ^a	Molecular weight [g/mol]	Boiling point [K]	Melting point [K]	Vapour pressure [Pa]	Henry coefficient set by user / estimated [Pa m ³ /mol]	log K _{ow} [-]	log K _{oc} set by user / estimated [l/kg]	Water solubility [mg/l at 25°C]
TCDD [40]	322	720 [16]	578	2E-7	- / 3.39	6.8	- / 5.6	1.9E-5
PeCDD [40]	356.4	738 [16]	469	8.8E-8	- / 0.261	7.4	- / 6.09	1.2E-4
HxCDD [40]	391	761 [16]	546	5.1E-9	- / 0.45	7.8	- / 6.41	4.4E-6
HpCDD [40]	425.2	780 [16]	538	7.5E-10	- / 0.133	8	- / 6.58	2.4E-6
OCDD [40]	460	783 [16]	608	1.1E-10	- / 0.684	8.2	- / 6.74	7.4E-8
Benzene [24]	78.12	353	279	1.27E4	548.43 / 564	2.12	1.96 / 1.82	1.76E3
DEHP [24]	390.56	- [41]	233	1.9E-3	0.045 [25] ^b / 25.6	7.48	4.94 [26] / 6.16	0.029
EDC [27]	98.96	356	238	1.13E4 [24]	149 / 130	1.46	2.3 / 1.3	8.6E3
EDTA [39]	292.25	-	493	1E-6 ^c	4E-10 ^c / 5.84E-7	-3.34	- / 2.48E-3	500
HHCB [38]	258.4	605	-	0.0727	11.3 / 10.7	5.9	4.86 / 4.88	1.75
LAS [24]	348.48	-	263 [39]	1E-6 ^c	4E-10 ^c / 3.17E-7	1.96	- / 1.69	1.1E3

^a: The data relating to a substance are taken from the source given in the first column; exceptions are marked accordingly.

^b: Data range from 0.045 to 64.1; since the estimated value is near the mean, the lowest value is chosen for the validation.

^c: Should be 0; values used are the lowest in the advised range.

Table 8: Degradation rates

Substance ^a	Biodegradability from 0 (not biodegr.) to 4 (readily biodegr.)	half-life air [h]	half-life water [h]	half-life soil [h]	half-life sediment [h]
TCDD [16]	0	170	550	17 000	55 000
PeCDD [16]	0	550	550	17 000	55 000
HxCDD [16]	0	550	1700	55 000	55 000
HpCDD [16]	0	550	1700	55 000	55 000
OCDD [16]	0	550	5500	55 000	55 000
Benzene [29]	4	240	191	720 ^b	7200 ^b
DEHP [29]	1	17.5 ^c	360	1663	7200
EDC [27]	0	2772	2 380 000	2160	2.4E8 ^b
EDTA [43]	0	rate: 0 h ^{-1b}	11 880	2.4E7 ^b	2.4E8 ^b
HHCB [38]	0	3.22	1.2E6 ^b	2.4E7 ^b	2.4E8 ^b
LAS	4 [39]	24 [39]	12 [44]	336 [45]	24 [46]

^a: The data relating to a substance are taken from the source given in the first column; exceptions are marked accordingly.

^b: Standard value assumed for the given biodegradability; i.e. no other data are available.

^c: Calculated from the molecular structure [42].

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