

Guidance on information requirements and chemical safety assessment

Chapter R.16: Environmental Exposure Estimation



May 2008

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PREFACE

This document describes the information requirements under REACH with regard to substance properties, exposure, use and risk management measures, and the chemical safety assessment. It is part of a series of guidance documents that are aimed to help all stakeholders with their preparation for fulfilling their obligations under the REACH regulation. These documents cover detailed guidance for a range of essential REACH processes as well as for some specific scientific and/or technical methods that industry or authorities need to make use of under REACH.

The guidance documents were drafted and discussed within the REACH Implementation Projects (RIPs) led by the European Commission services, involving stakeholders from Member States, industry and non-governmental organisations. These guidance documents can be obtained via the website of the European Chemicals Agency (http://echa.europa.eu/about/reach_en.asp). Further guidance documents will be published on this website when they are finalised or updated.

This document relates to the REACH Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006¹

¹ Corrigendum to Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC (OJ L 396, 30.12.2006); amended by Council Regulation (EC) No 1354/2007 of 15 November 2007 adapting Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) by reason of the accession of Bulgaria and Romania (OJ L 304, 22.11.2007, p. 1).

Convention for citing the REACH regulation

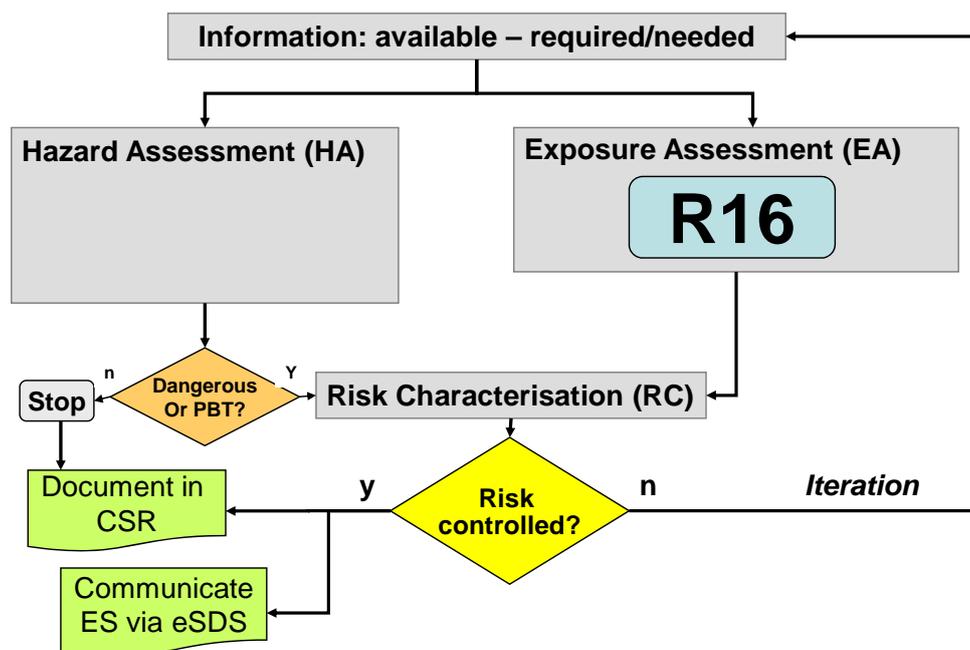
Where the REACH regulation is cited literally, this is indicated by text in italics between quotes.

Table of Terms and Abbreviations

See Chapter R.20

Pathfinder

The figure below indicates the location of Chapter R16 within the Guidance Document.



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R.16 ESTIMATION OF ENVIRONMENTAL EXPOSURE

R.16.1 Introduction

R.16.1.1 Aim of this chapter

Exposure estimation is a critical step in the whole process of environmental exposure assessment. The purpose of carrying out environmental exposure estimation is to derive the predicted environmental concentration (PEC) for environmental compartments of interest, i.e. water, sediment, soil, air and top-predators to be compared with the Predicted No Effect Concentrations (PNEC). The PECs of a chemical are a result of both:

- Releases of the chemical into the environment. Estimation of the releases is part of the development of exposure scenarios (see Section D.5.5).
- So-called fate processes taking place after the release resulting in that the chemical will be distributed in the various environmental compartments (air, soil, water, sediment, biota) at certain concentration levels. These fate processes can for example be passive transport with water and air (i.e. advective exchange between compartments), diffusion, degradation or sedimentation.

For each environmental compartment (air, soil, water, sediment) potentially exposed, the exposure concentrations (Predicted Environmental Concentrations, PECs) should be derived, either by measurement (monitoring data) or by model prediction taking into consideration distribution and fate processes after the chemical has entered the environment. Relevant measured data from substances with analogous use and exposure patterns or analogous properties, if available, should also be considered when applying model calculations.

R.16.1.2 Workflow for environmental exposure estimation

When an exposure scenario is being developed (see Part D) it has to be tested whether the information collected is sufficient to demonstrate that the risks occurring from the manufacture and all identified use(s) are controlled. Exposure estimates (PECs) are compared to the predicted no-effect concentrations (PNECs) at each iteration. It should be kept in mind that the exposure estimate(s) should cover all identified uses described in the exposure scenario.

The following steps are included in the assessment of the releases of a substance to the environment and the resulting PECs for the relevant environmental compartments (air, water, sediment, soil):

1. Select an appropriate method for release estimation based on the information in the ES and determine the appropriate release estimation method (Section [R.16.2](#)) This also includes the use of measured release data. If measurements or emission estimates show that releases into the environment take place then further environmental exposure estimations are needed. More detailed guidance is given in Section [R.16.3](#).
2. Compile the relevant substance properties. For the release estimation you may need the vapour pressure, water solubility and boiling point. For a Tier 1 distribution calculation (Section [R.16.6](#)) you will additionally need the molecular weight, octanol-water partition coefficient, melting point and information on ready biodegradability. In case of an inorganic chemical it is recommended to have information on the partition coefficients (see Section [16.4.3](#)) and possible abiotic transformation products. During the compilation do also consider if substance can be degraded to give stable and/or toxic degradation products.

3. Determine the quantity of the substance which is applied in a process and life cycle stage and other input parameters for the release estimation module (Section [R.16.2](#)).
4. Carry out manual or IT-based calculations to determine the releases at local and regional level based on generic emission equations. The workflow of Section D.5.5.1 can be used to calculate the releases with environmental release categories (ERCs) (Section [R.16.2](#)).
5. Apply the relevant emission rates in the selected tool (see Section [R.16.6](#)), calculate the environmental distribution (Sections [R.16.4](#) and [R.16.5](#)) and derive the PECs (Sections [R.16.5.5](#) and [R.16.5.6](#)).
6. Calculate the exposure for (top-)predators (Section [R.16.5.7](#)) and the indirect exposure to humans via the environment (Section [R.16.5.8](#)).

After step 5 and 6, PECs and human intake levels are determined for each iteration of the environmental exposure estimation. The next two steps then follow, as part of the exposure assessment as a whole.

7. In case control of risks cannot be demonstrated for the environment, refine the default input parameters in the applied release estimation method based on more specific information from the ES and/or refine applied substance property data, and/or introduce additional risk management measures.
8. If control of risks is not confirmed by the iteration in step 7, a higher tier assessment might be needed or the use(s) may be advised against.

R.16.2 Release estimation

Release estimation is the process whereby releases to the environment are quantified during the life cycle stages of a chemical, taking into account the different types of uses during these life cycle stages, the different emission pathways and receiving environmental compartments and the spatial scale of the emissions. To streamline the release estimation and make it accessible for data collection in the supply chain, environmental release classes (ERCs) have been developed. ERCs are a starting point for:

- i. Considering relevant emissions to the environment linked to categories for occupational activities and article categories (see Appendixes R.12-3 and R.12-4).
- ii. Grouping of substance uses from an environmental perspective.
- iii. Carrying out Tier 1 exposure estimates (see Chapter D.5), taking risk management measures into account.
- iv. Communication on emissions and releases in the supply chain.

The ERCs provides the input parameters, together with tonnage and risk management measures, that are needed to calculate releases during the life-cycle of a substance from manufacture to the waste stage. The emission calculations are based on equations discussed in more detail in Sections [R.16.5.5](#) and [R.16.5.6](#). The rationale behind ERCs is based on considerations of

- i. Life cycle stage
- ii. Emission pattern;
- iii. Level of containment;
- iv. Type of use and technical fate;
- v. Dispersion of emission sources;
- vi. Indoor or outdoor use and
- vii. Release potential during service life and waste stage.

The release estimation for the environment is based on generic equations as described in Section [R.16.2.1.13](#). The ERCs contain the relevant inputs (determinants of exposure) with corresponding default values. The name and description of the different release categories and the values for the determinants in the ERCs are documented in [Appendix R.16-1](#). In Sections [R.16.2.1](#) to [R.16.2.2](#), each of the inputs that define emissions and releases are discussed in more detail.

ERCs should be used as a general starting point for emission estimation (see Part D). However, all available information should be used. In particular for identified point sources, specific information on releases may be available (e.g. from permits, etc.). If such is the case these data should be used instead of or complementary to the ERC approach. Emissions may be influenced by risk management (emission reduction) measures, e.g. filters, scrubbers, on-site wastewater treatment etc. RMMs should always be documented in the ES and are discussed in more detail in Section [R.16.2.1.9](#). Examples on how to work with ERCs are given in Part D.

R.16.2.1 Information needed for release estimation

The information that needs to be considered for the release estimation is:

- Tonnage
- Life Cycle Stage
- Type of use in the life cycle stage
- Distribution of production volume in the market
- Emission Pattern – Distribution in time and space
- Emission Pathways (Air, Soil, Water)
- Multiple emissions
- Emission factors
- Risks management measures to reduce emissions.

R.16.2.1.1 Tonnage

The registration tonnage should be used in the release calculations. The tonnage at the different life-cycle stages (except manufacture) should be corrected for losses at previous life-cycle stages and for possible import or export of the same substance during the life-cycle.

R.16.2.1.2 Life cycle stages

The ERCs ([Appendix R.16-1](#)) provide a structure for considering releases at each life cycle stage.

The stages of the life cycle of a substance ([Figure R.16-1](#)) may consist of

Manufacture (production): Chemical synthesis of the substance. Manufacture is the stage where the substance is manufactured, i.e. formed by chemical reaction(s), isolated, purified, drummed or bagged, etc. For intermediates (chemicals used to make other chemicals) a distinction is made between non-isolated, site-limited, and captive intermediates, as shown in [Figure R.16-1](#).

Formulation: Mixing and blending into a preparation. Formulation is the stage where substances are combined in a process of blending and mixing to obtain a product or a preparation. This may be a formulation such as a paint, or a product such as a photographic film. Formulations are applied or used at the next stages of the life-cycle (industrial/professional use, private use).

Industrial use: Application of the substance as such, in a preparation or in an article in an industrial process. Application may have the purpose to incorporate the substance into an article or to technically support the manufacturing process but not intentionally becoming part of the product (processing aid). One example of a processing aid is a developer used in a photographic bath that is disposed of after use.

Professional and private use: Application of the substance or preparation by professionals or the public at large outside industrial installations

- a. Professional use may include the use of substances as such, in preparations or in articles in order to deliver services to business or private customers. This may include sophisticated equipment and specialised, trained personal.
- b. Private use includes the use of substances as such, in preparations or in articles. It is assumed that the user is not trained. Use can take place in closed systems (lubricants for vehicles or hydraulic systems) or open systems (lubricants for bicycles). It may also include processing of material.

Service life: Use of articles or the polymer matrix of a preparation (paints, adhesives) containing the substance over a period > 1 year. Such activities include for example wearing and maintenance of textiles, housing, using and maintenance of vehicles, use and maintenance of sport articles, etc.

Waste treatment: Final stage where substances, preparations or articles are disposed of after their service life, like for example used lubricants or solvents, old tyres or home appliances. Also unintended losses of preparations may enter into the waste life stage, like e.g. overspray from coating, surplus of dyes, inks or residues from cleaning of machinery. Treatment includes incineration or landfilling, or recovery of the basis material or substance takes place.

At each of the life-cycle stages a larger or smaller fraction of the substance is lost via emissions and will therefore not enter the next life cycle stage. When applying emission factors in more precise emission calculation, this should be taken into account. However for the following release estimates the emission factors are always applied to the total production volume of M/I regardless the life cycle stage under assessment.

Between the various life cycle stages *transport, storage, and handling* may occur. This stage has not been indicated in [Figure R.16-1](#). Emissions due to storage, handling, repacking and filling, including local transfer, are assumed to be included within the relevant life cycle stage.

Transport is not considered under REACH.

R.16.2.1.3 Type of use in the life cycle stage

The type of use is considered in the ERCs, since the fate of the substance is influenced by the technical process and the consequences for the remaining part of the life-cycle after the process. The following main distinctions can be made:

1. Processing aid: Processing aids are substances facilitating a process; often they will not be consumed (reacted) during the process (detergents in cleaners, solvents in paints) and will be emitted during processing to waste water, waste air and/or waste.

2. Inclusion into/onto matrix: Manufacturing into/onto an article matrix means all processes where chemicals are incorporated into materials. These materials are subsequently used to manufacture products or articles, and hence emission during processing will be limited. Substances enter into service life stage, either as part of an article or as part of a dried/reacted preparation.

3. Substances reacting in use: Substances intended to be consumed on use (chemically reacted to another substance, either monomer unit in a polymer), and hence emissions during processing will be limited. Only a residual fraction of the original substance will enter into the service life stage. A few examples are:

- Intermediate (being consumed in creating a new substance which will be again an intermediate or will be sold to formulation and further uses)
- Reactive processing aid (for instance bleaching agents in paper production)
- Monomers for polymers (polymerisation processes: monomers, initiators)
- Monomers for thermosets (polymer processing: curing agents, cross-linking agents)

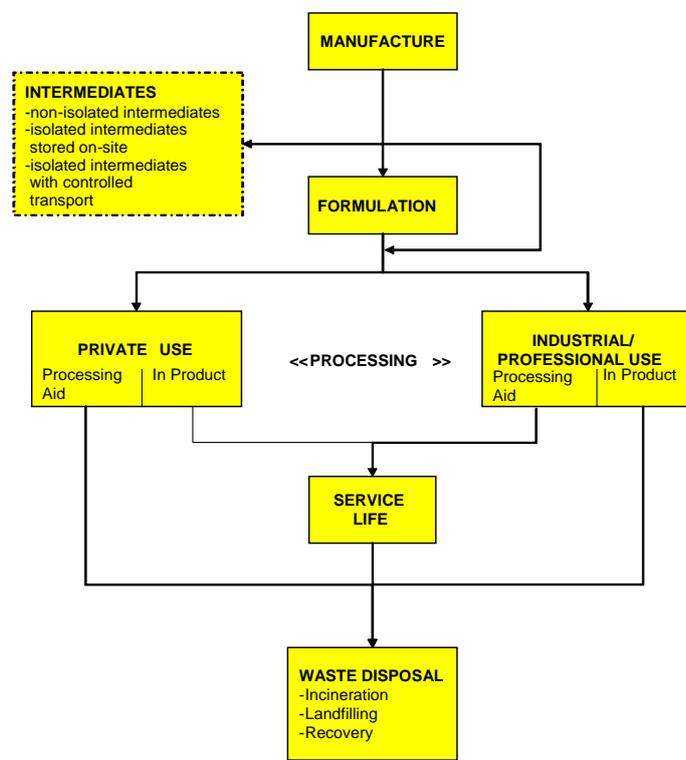


Figure R.16-1 Life-cycle stages of chemicals

R.16.2.1.4 Distribution of production volume in the market

The manufacturer's annual production volume of a substance or the importer's annual imported volume of a substance will be distributed in the EU market and flow down the supply chains. The registrant usually knows his own production volume and the markets to which he sells the substance. However, often he has little information on annual or daily volumes used by the downstream users at the local scale.

For use with the ERCs, the M/I needs to consider his own manufacturing and use, and the downstream uses including formulation and industrial uses. For each downstream use, whether formulator or further down the supply chain, the '*largest customer approach*' (largest fraction of main source) can be used. This assumes that at each life-cycle stage, the largest volume that appears in the overall volume marketed by an MI is protective for all smaller customers at each life-cycle stage. Other approaches can also be used, but provisions must then be taken to ensure control of risks for all actors in the supply chain, whether they use a large or a small volume. Another approach is the '*representative customer approach*' where at each life-cycle stage, the mean or representative volume in a life-cycle step is used. Scaling up or scaling down to a larger or smaller customer to show control of risks can be done using so called 'scaling equations', see Appendix G-1.

R.16.2.1.5 Emission pattern – distribution in space and time

Local scale

Distribution on the local scale is assessed in the vicinity of point sources. Each identified use of the substance at each stage of the life cycle is assumed to occur at another point source. Therefore, in principle, a local assessment has to be performed for each identified use and each relevant life-cycle step that is described by ERCs.

In case of point source emissions associated with production, formulation or use, the emission into a local environment needs to be calculated based on ERCs for each life-cycle step or further iterations of the defaults in it. For the life cycle stage professional use of substances (in preparations) and private use of substances or preparations, substances will usually be released into the central public sewage system and be locally released after treatment. Emissions to water could be treated in an on-site sewage treatment plant (STP; in many cases, these treatment plants are not biological treatment plants but physico-chemical treatment plants) or in a public STP. STPs are available as an RMM for local industrial emissions. See Section [R.16.5.5](#) for more detail on the calculations for STPs. Substances or preparations used directly in the environment (e.g. loss lubricants in chain saws) will possibly not pass any kind of abatement technique before entering the environmental media. Hence there is no connection to sewer.

The temporal scale is the daily average concentration. A ‘standard’ environment for the local scale has been defined for each environmental compartment (see Section [R.16.5.3.1](#)). In case of diffuse emissions, the local concentration in fresh water is calculated based on a standard scenario. Diffuse emissions to water are processed in a default sewage treatment (number of inhabitants and sewage flow per inhabitant). A fixed dilution factor is applied to the effluent concentration. Dilution factors are dependent on flow rates and the industry-specific discharge flow.

For further iterations, more specific assessments may be appropriate. The actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate of the STP. This approach should be used for rivers only and not for estuaries or lakes. In other cases, the calculation of PEC_{local} can be carried out using actual environmental conditions around the source. Local PECs are based on the concentrations from the local distribution model, adding the concentrations from the regional scale as background.

Regional scale

Regional emissions are calculated from the emissions of a substance from a single registration volume (corrected for import and export) for all of its life-cycle stages, released from point and diffuse sources in a larger area. In its default settings, the regional distribution module represents a typical densely populated EU-area located in Western Europe (~ 20 million inhabitants).

The regional scale takes into account the further distribution and fate of the chemical upon release, resulting in steady-state concentrations in the environmental compartments. The regional concentrations are used as background concentrations in the calculation of the local concentrations. Regional exposure estimation is based on year-averaged emissions to air, water, and soil.

For those life-cycle stages with diffuse emissions, e.g. use, service-life and waste, the ERC default is that 10% of the market volume goes into the regional scale calculation. This accounts for the fact that substances are usually formulated into preparations and products that are marketed and used throughout Europe. The regional scale then only accounts for 10% of the overall diffuse emissions in Europe (known as the continental scale). For substances without diffuse emissions, the assumption is that 100% of the emissions are allocated to the regional scale.

For each stage, the losses in the previous stage are accounted for. Losses due to release during production are not taken into account for subtraction to the other stages, as these releases will generally already be accounted for in the final reported production volume. After losses during the life cycle have been accounted for, the part of the tonnage remaining is assumed to end up entirely in waste streams. Quantitative methods for estimating emissions at the waste treatment (disposal) stage are included in the ERCs, as explained in Chapter R.18.

For the life-cycle stages ‘use, service-life and waste’ (ERCs 8-11), local emissions to water are based on a scenario for a ‘standard town’ where 80% of the wastewater is treated in a biological STP and the remaining 20% is released directly into surface waters. This split is accounted for in the total regional emissions but not in the regional release per life-cycle stage.

In case all local emission rates are known, further iterations can override the generic assumptions on regional distribution of emissions in the ERCs. The ERC tables assume that for the life cycle stages production, formulation and non-dispersive use (ERC 1-7), 100% of all local emissions are emitted into the regional scale. Information on market volumes can be used to refine this assumption, e.g. when at some life-cycle stages, a part of the market volume is exported or imported. The regional environmental distribution module calculates PECs for the compartments air, surface water, sediment, natural soil, agricultural soil, and industrial soil.

The releases from point sources are regarded as continuous or intermittent. Continuous releases are characterized by an almost constant release rate over a prolonged period (e.g. 220 working days). The number of days at which a substance is used (and released) may vary from branch to branch or product to product. In the absence of better knowledge conservative assumptions must be made (see the ERC tables in [Appendix R.16-1](#)). Intermittent releases are defined as occurring infrequently, i.e. less than once per month and for no more than 24 hours. The emission rate is given averaged per day (24 hours). This implies that, even when an emission only takes place a few hours per day, the emission will be averaged over 24 hours. Emissions to air and water will be presented as release rates during an emission episode.

Releases from the service life of long-lived products are to be considered as well. Here it is assumed that the release to the environment continuously takes place over the total service life. It has to be taken into account, that the “market history” and “market future” of a substance plays a role here, since the release from one marketing year will add to the releases from marketing volumes of previous years and future years. Hence the registrant should make himself aware whether the product-cycle of his substance has reached steady state which means that the annual marketed volume is driven by the replacement of products at the end of their service life (becoming waste) or by losing or winning market shares from competitors. In such case the current annual production volume can be taken to estimate the annual releases by multiplying it with the emission factor of the article over service life.

R.16.2.1.6 Emission pathways

Emissions can occur via air, water and soil and are estimated for every environmental compartment and each relevant stage of the life cycle separately. The direct release to soil is only considered at a regional scale. The split of releases depends on the physico-chemical properties of the substances in combination with the process parameters in the relevant uses.

The ERCs consider different aspects of emission sources and pathways:

Dispersion of emission sources, divided in two main categories:

- Industrial point sources refers to a limited number of industrial points sources where only certain groups of workers, with knowledge of the process, come into contact with these chemicals.
- Wide dispersive use refers to many small point sources or diffuse release by for instance the public at large or sources like traffic

Location of emission sources. This aspect is included to consider the potential for wide dispersive use and the options for different types of risk management measures. Industrial manufacture, processing and formulation is usually related to controlled indoor use and outdoor facilities, while wide dispersive use can also relate to both indoor and outdoor use.

Release potential during service life. This relates to type of use and type of article. It refers to the degree of release (low, high, intended) related to the type of article and use during service life.

- Intended release (technical performance of product is geared to release of substances)
- Unintended release (technical quality of product includes limitation or prevention of substance or material losses).
 - Conditions of use promote significant emissions during service life
 - Conditions of use do not promote emission from service life.

Release potential from waste treatment and recycling: The release from waste stage depends inter alia on the following determinants (see Chapter R.18):

- fraction of substance volume entering into the waste life stage (fraction which is not already emitted to air, water or soil or has reacted on use in the previous life cycle stages)
- The dispersion and size of treatment facilities (driving the emission in the local scenario)
- the technical type of treatment process (including abatement techniques) and
- type of recovery (e.g. in form of construction and building material) potentially leading to wide disperse emission during a second service life (regional scenario)

R.16.2.1.7 Multiple emissions

Emissions of a substance may take place from multiple sources at the same time. This results from the manufacturers own production/market volume and the production/market volume of his competitors. Hence single source assessment must take into account that other releases of the same substance may take place at the same time in a near or far distance. However, REACH does not require the registrant to take into account the market volumes of his competitors even if a Consortium performs a joint registration under REACH. But the single manufacturer or importer he is obliged to take account of his total market volume and the possibility that total releases may lead to significant higher exposure than calculated or measured at a local single source. There are a number of ways to address this aspect of safety assessment, i.a.:

- Carry out a very conservative local assessment covering already a situation that several sites emit the substance into the same environment. Unless it is a seasonal use pattern, assume 365 release days, since not all sites will use the substance at the same time.
- Carry out a regional background assessment, assuming that 100% of the registrant's market volume is manufactured and applied in the EU standard region as defined in Section [R.16.5.4](#) and sum up the emission factors at the different life stages. Unless it is a seasonal use pattern, assume 365 release days since the use will be spread over the whole year.

R.16.2.1.8 Emission factors

Emission factors express the fraction of the used amount being emitted to the environmental compartment of consideration.

Emission factors from processes and products

The emission of a substance from a certain use (e.g. technical processes in installations or vehicles, application of preparations in private households) depends on the operational conditions of use, like e.g. temperature, pressure, level containment of machinery, level of internal regeneration of processing fluids, dry or wet process, dipping or spraying. Also, the chemical-physical properties of the substance play a role here (e.g. water solubility, vapour pressure). Section [R.16.2.1.10](#) presents methods for deriving the emission factors.

Emission factors from service life long-life articles

Special considerations have to be put on the derivation of the emission factors from service life of long-life articles, see Chapter R.17.

Emission factors from waste disposal

Special considerations apply to the derivation of the emission factors from waste disposal, see Chapter R.18.

R.16.2.1.9 Risk management measures to reduce emissions

The substance losses (emissions) from a process or product do not necessarily enter into the environment, depending on the type and extent of applied risk management measures, e.g. biological or chemical waste water treatment, detoxification of metal salt solutions or waste gas treatment. It might also be possible that a certain emission pathway can be excluded, e.g. when sludge from a waste water treatment is incinerated and not spread on agricultural soil. If a certain RMM is applied in current standard practice and the efficiency of such technique is known, emission factors can be reduced accordingly and taken into account in the development of the ES (see Section D and Chapter R.13). Since biological sewage treatment is current standard practice in Europe, the environmental exposure estimation includes the calculation of the partitioning and degradation of organic substances in the sewage treatment, driven by the degradability, the volatility and octanol-water partition coefficient of a substance. This is described in much more detail in Section [R.16.5.5](#).

For other abatement techniques, the RMM library² (see <http://www.cefic.org/files/downloads-/Guidance%20on%20REACH%20-%20Dec%202007.pdf>) can be consulted. Also EU BREF Documents under the EU Directive on Integrated Pollution Prevention and Control (IPPC) are a valuable source of information.

R.16.2.1.10 Selection of an appropriate release estimation method

Several release estimation methods are available and suitable for Tier 1 assessments:

1. Environmental release classes (ERC). In a first tier CSA this step, based on input from generic ESs, will help to identify which substances cannot be used safely under the conditions specified

² The RMM library will become available via the CEFIC website

in the ES. The information in the ERCs can be used as a basis for more reliable or precise emission estimates (with additional RMMs to reduce emissions).

2. If reliable measured release data are available these might be used instead of the ERCs. Before using measured data, consider if they cover the use to be covered by the ES. For example, if developing a generic ES, the measured data may not represent all uses covered by the generic ES.
3. If the uses are covered by branch-specific OECD and EU emission scenario documents (ESDs) including generic scenarios by US EPA (US EPA OPPT Generic Scenarios (<http://www.epa.gov/oppt/exposure>)). These might be used instead of the ERCs ([Appendix R.16-1](#)).
4. Use specific information on emission; either based on measurements (see Section [R.16.3](#)) or DU information, or more precise process descriptions.
5. More specific scenarios are available for the life cycles steps related to service-life (see Chapter R.17) and waste disposal (see Chapter R.18).

Relevant information to be used in the release estimation should be provided in Sections 1 to 7 of the ES template. Which method should be used depends on the specificity and quality of the information in the exposure scenario.

R.16.2.1.11 Compile relevant substance information

The ERC method does not require any explicit substance information for an initial Tier 1 estimate. To refine the default emission factors, branch-specific ESDs or other sources are needed to improve the initial exposure estimate and substance parameters such as vapour pressure, water solubility, and boiling point are needed.

R.16.2.1.12 Compile relevant information

[Table R.16-1](#) indicates the core determinants which shall be available to use an appropriate Tier 1 release estimation method (column 1 and 2). Once the method is selected the additional determinants of the release estimation module have to be extracted (column 3).

Table R.16-1 Overview of ES information and core determinants for release estimation at Tier 1

Information source in ES	Basic determinants derived from ES information	Dependent determinants derived from basic determinants
Environmental release classes IT-tool: Standard Excel file available		
Registration dossier Short title of use of ES Description of activities /processes covered by ES	Exposure category Amount of substance produced/imported by M/I	Amount of substance used as input to emission calculation Release spatial Fraction of amount used at main source (largest customer) Release time in days per year STP connection Default release to air Default release to water from process (before abatement) Dilution to be applied for PECwater derivation → for exposure estimation
Branch-specific ESDs IT-tool: ESDs partly in EUSES; further available tools³		
Registration dossier Short title of use of ES Description of activities /processes covered by ES Operational conditions of use Risk Management Measures	Possible determinants (varies between ESDs): Life cycle stage* Industrial category* Use category* Specific information on the use pattern of the substance Certain physico-chemical properties (water solubility, vapour pressure etc.) etc.	Possible determinants (varies between ESDs): Branch-specific uses / techniques Typical application amounts in branch Emission factors to the environment Abatement techniques (branch-specific) etc.

The terms “main category (MC)”, “industrial category (IC)”, and “use category (UC)” are used in the Guidance Document for carrying out risk assessment for existing substance (EU, 2003). IC described the industrial category (16 categories are defined), and UC describes how the substance is used (55 categories), and MC is introduced to describe more specifically the use condition (open/closed system, widely dispersed)..

³ EU / OECD ESDs: IT-prototypes implementing ESDs are available for:

- textile finishing processes (“Screening tool supporting environmental exposure assessment under REACH for substances used in textile finishing” <http://www.reach-info.de/expoanalyse.htm>)
- plastic additives, and partly photochemicals (<http://emissiontool.com>)

US EPA OPPT Generic Scenarios (<http://www.epa.gov/oppt/exposure/>): partly Excel Spreadsheets by Environment Canada available on request

R.16.2.1.13 Carry out a manual or IT-based calculation of the environmental release

The following basic equations are usually applied to estimate the releases to the environment on local and regional scale. The generic input parameters are described in [Table R.16-2](#). Variations of the equations might be necessary for specific cases:

Estimation of local releases (single point sources)

$$E_{local_{i,j,u}} = \frac{Q_{chemical} \cdot F_{emission} \cdot (1 - F_{abatement})}{T_{emission}}$$

**EQUATION
R. 16-1**

with:

i: environmental compartment (water, air, soil)

j: life cycle stage (from production to waste treatment/recovery)

u: use or process in a specific life cycle stage

$Q_{chemical}$: quantity of the substance of concern that is applied in a use or a process and life cycle stage per year [mass per year]

$F_{emission}$: emission factor: the fraction of the substance emitted from the process or use considered to (waste) water, (waste) air, soil, or (solid) waste before onsite or offsite abatement measures [dimensionless]

$F_{abatement}$: efficiency of any abatement or control technology (onsite or offsite) that reduces the emission to air, water, soil or (solid) waste [dimensionless]

$T_{emission}$: duration of emission (e.g. working days per year) [days per year]

Attention:

If the emission factor or the efficiency of an abatement technique is given in the unit [percent] please divide the value by 100 % in order to derive a dimensionless parameter.

Estimation of regional background releases

The regional background release for each environmental compartment is calculated from the sum of releases from all uses in all life cycle stages of the substance in a particular region. The emissions are assumed to be a constant and continuous flux during the year. The result of this calculation is to derive the regional background concentration ($PEC_{regional_background}$), which should be added to the local PEC related to the emissions from a single site or a single use:

$$E_{regional_background_{i,j,u}} = \frac{\sum_{i,j,u} [Q_{chemical} \cdot F_{emission} \cdot (1 - F_{abatement})]}{365d}$$

EQUATION
R.16-1

Table R.16-2 Input parameters for the generic equations

Parameter	Description	Possible source information ⁴
Tonnage _{M/I}	The whole amount of a substance produced or imported by one manufacturer or importer [mass per year]	M/I information solely
Q _{chemical}	The quantity of the substance of concern that is applied in a use or a process and life cycle stage per year [mass per year]	M/I or DU own information, calculation based on production or import volume, further refinement options or according to environmental release classes or defaults of ESDs
Q _{product}	The quantity of product (preparation or article), in which the substance of concern is processed or used per year [mass per year]	M/I own information in case of speciality substances (for concentration), DU information
C _{chemical}	The concentration or fraction of the substance in the product [dimensionless]	
F _{emission}	The emission factor: the fraction of the substance emitted from the process or use to (waste) water, (waste) air, soil or (solid) waste before onsite or offsite abatement measures [dimensionless]	DU information, defaults of environmental release classes or ESDs
F _{abatement}	Efficiency of any abatement or control technology that reduces the emission to air, water, soil or (solid) waste [dimensionless] It can be on-site or off-site emission abatement.	BREFs, ESDs or DU information, standard Sewage Treatment Plant (STP) (see section R; Simple Treat)
T _{emission}	The duration of emission (e.g. working days per year) [days per year]	DU information, defaults of environmental release classes or ESDs
F _{use}	The fraction of the registrants market volume entering into different supply chains or into an identified use or category of use [dimensionless].	M/I own information and DU information

The output of the release calculations are release rates, mainly measured in mass per time, for the different uses in various life cycle stages. These release rates are subsequently used to derive the exposure levels (see Section [R.16.5](#)).

⁴ Information available in the registration dossier or exposure scenarios are not listed in detail.

Table R.16-3 Summary of release rates according to the basic equations

Parameter	Description	Destination
$E_{local,i,j,u}$	Emission of a local point source for life cycle stage j to compartment i in use u measured in [mass per time], mostly [kg per day]	Local distribution and local PECs
$E_{regional,i,j,u}$	Regional (diffuse) emission for life cycle stage j to compartment i in use u measured in [mass per time], mostly [kg per day]	Regional distribution and regional PECs
$E_{regional_background,i}$	Sum of emissions from all uses and life cycle stages to compartment i in [mass per time], mostly [kg per day]	Regional distribution and regional PECs to be added for background exposure

R.16.2.2 Refinement options

Release estimation which is based on Environmental Release Classes can be regarded as a first conservative approach. If a risk is indicated in a tentative ES built on conservative release estimates, the assessment of the release rates may be refined by using more precise data. In general, the following refinement options of the environmental release classes can be considered:

- Reduce the emission factor based on information about current standard practise in a certain area of industry, including RMMs.
- Substitute the assumption that the emission in the region s_i based on 100% of the registrants market volume by the actual percentage of the total M/I tonnage used in the region based on supply chain evidence.
- Adapt the number of release days based on the actual operational conditions (as described in the exposure scenario) based on a more frequent or continuous use (= spreading the emission over a longer period of time).
- Adapt the fraction of main source to the fraction of market volume that is actually used in a local environment by the largest customer(s).

An example(s) is provided elsewhere to explain the use of the ERCs and to illustrate the possible refinement options (see the introduction on ERCs in D4.4, D.5.5.1, Appendix D-2).

If no further information is readily available the M/I may seek more precise knowledge about the use of the substances, e.g. by entering into a dialogue with his customers.

If detailed information on the identified uses is available, a higher Tier assessment may be performed by using specific information on marketing, use, release or exposure of the substance (e.g. data obtained from M/I, product registers or open literature).

How to derive and refine the applied amount of substance ($Q_{chemical}$)?

In general, $Q_{chemical}$ may be calculated from the applied amount of a preparation/article [mass per year] times the concentration of the chemical in the product [mass per mass]:

$$Q_{chemical} = Q_{product} \cdot C_{chemical}$$

EQUATION
R.16-2

$Q_{chemical}$ depends on the spatial emission (local and regional), the use or process as well as on the life cycle stage. In absence of detailed knowledge, some general options can be followed to derive and refine $Q_{chemical}$.

Life cycle stage: The most conservative assumption is that 100 % of the manufacturer’s or importer’s tonnage per year is applied at one site (local scenario for production, formulation, industrial use):

$$\text{CONSERVATIVE ASSUMPTION (LOCAL): } Q_{\text{chemical}} = \text{Tonnage}_{M/I} \quad \text{EQUATION R.16-3}$$

where $\text{Tonnage}_{M/I}$ is the tonnage of the manufacturer or importer [mass per year].

If it is known that the production or processing sites are numerous, various in size and randomly distributed over Europe, a “10 % rule” can be applied by assuming that 10 % of the amount produced or imported is used at the local scale:

$$\text{REFINEMENT OPTION (LOCAL AND REGIONAL): } Q_{\text{chemical}} = 0.1 \cdot \text{Tonnage}_{M/I} \quad \text{EQUATION R.16-4}$$

Alternatively, it can be decided to apply more specific values if sufficient information is available. For the regional scenario it is generally assumed that 10 % of the total $\text{Tonnage}_{M/I}$ is marketed in the region. However, this percentage can be adapted based on information on the specific substance.

Main local emission source: The ‘fraction of main source’ ($F_{\text{mainsource}}$ [dimensionless]) is only applied for local release estimation. The ‘fraction of main source’ describes the share of the production or imported volume which is used by the main or average downstream user. This should be identified by communication in the supply chain. By multiplying the $\text{Tonnage}_{M/I}$ with the fraction of main source, the size of the main local emission source is assumed.

$$\text{REFINEMENT (LOCAL): } Q_{\text{chemical}} = \text{Tonnage}_{M/I} \cdot F_{\text{mainsource}} \quad \text{EQUATION R.16-5}$$

Different uses at the same life cycle stage: If the produced or imported volume is applied in different uses or processes at the same life cycle stage or enters different supply chains the total $\text{Tonnage}_{M/I}$ may be divided between these uses/processes or supply chains before the fraction of main source is determined.

$$\text{REFINEMENT (LOCAL AND REGIONAL): } Q_{\text{chemical}} = \text{Tonnage}_{M/I} \cdot F_{\text{use}} \quad \text{EQUATION R.16-6}$$

When combining the refinement options of i) splitting the $\text{Tonnage}_{M/I}$ between different uses and ii) determining the fraction of main source for each use it should be taken into account that markets may shift. Therefore it could be reasonable to assume for a first estimation 100 % of $\text{Tonnage}_{M/I}$ for each use.

R.16.2.2.1 ESD

An Emission Scenario Documents (ESD) is a document that describes the sources, production processes, pathways and use patterns with the aim of quantifying the emissions (or releases) of a chemical into water, air, soil and/or solid waste. An ESD should ideally include all life cycle stages. Some European countries have their own ESDs. The US-EPA has developed a number of generic scenarios to be used as default release scenarios in risk assessment. Information on ESDs used in national or regional contexts is compiled in the OECD Database on Use and Releases of Chemicals (<http://appli1.oecd.org/ehs/urchem.nsf>). [Appendix R.16-2](#) presents an overview of available ESDs developed by the OECD.

R.16.2.3 Use of release measurements

Due to the in-house information of companies, the measured release information of substances might be easily obtained for the first three life cycle stages (LCSs): (i) Production, (ii) Formulation, and (iii) Industrial Use. Manufacturer/Importer of the first three LCSs will usually have the required knowledge on the (possible) release estimation of substances because this information usually have to be laid down in the licence(s) supplied by the authorities. For reasons such as the use of actual and updated abatement techniques it will be beneficial that these data will be the input in the ES.

For the remaining LCSs the availability of measured data is expected to be quite limited. Examples for using the ERCs and possible further refinement are given below.

R.16.3 Measured data

R.16.3.1 Introduction

A general introduction on the use of measured exposure data can be found in Section D.5.2. Measurements encompasses both actual measured concentrations and measured values that can be used to refine the exposure calculation, e.g. measured release fractions or emission rates, measured removals in sewage treatment facilities.

Measurements can be used

- as part of carrying out exposure estimation by the M/I
- as part of the DU → M/I communication. This could happen if the DU has relevant measured data, e.g. on measured emission fractions of a substance, which can be used in the exposure estimation.

For some substances measured data will be available for air, fresh or saline water, sediment, biota and/or soil. These data have to be carefully evaluated for their adequacy and representativeness according to the criteria below. They are used together with calculated environmental concentrations in the interpretation of exposure data.

The evaluation should follow a stepwise procedure:

- reliable and representative data should be selected by evaluation of the sampling and analytical methods employed and the geographic and time scales of the measurement campaigns ([Section R.16.3.2](#));
- the data should be assigned to local or regional scenarios by taking into account the sources of exposure and the environmental fate of the substance ([Section R.16.3.3](#));

- the measured data should be compared to the corresponding calculated PEC. For naturally occurring substances background concentrations have to be taken into account. For risk characterisation, a representative PEC should be decided upon based on measured data and a calculated PEC (Section [R.16.5.6.9](#)).

R.16.3.2 Selection of adequate measured data

The available measured environmental concentrations have to be assessed first. The following aspects could be considered in order to decide if the data are adequate for use in the exposure estimation and how much importance should be attached to them:

- Quality of the applied measuring techniques
- Selection of representative data for the environmental compartment of concern

R.16.3.2.1 Quality of the applied measuring techniques

The applied techniques of sampling, sample shipping and storage, sample preparation for analysis and analysis must consider the physico-chemical properties of the substance. Measured concentrations that are not representative as indicated by an adequate sampling programme or are of insufficient quality should not be used in the exposure estimation.

The limit of quantitation (LOQ) of the analytical method, which is normally defined by the analytical technique being used, should be suitable for the risk assessment and the comparability of the measured data should be carefully evaluated. For example, the concentrations in water may either reflect total concentrations or dissolved concentrations according to the sampling and preparation procedures used. The concentrations in sediment may significantly depend on the content of organic carbon and particle size of the sampled sediment. The soil and sediment concentrations should preferably be based on concentrations normalised for the particle size (i.e. coarsest particles taken out by sieving). All measurements below the LOQ constitute a special problem and should be considered on a case-by-case basis. One approach that could be considered would be to use a value corresponding to LOQ/2 before estimating a mean or standard deviation (EC, 1999). As this method could heavily influence the mean and standard deviation, other methods may also be considered (e.g. assuming same distribution of data below and above the LOQ).

The aim is to obtain as much useful information on exposure from a data set as possible, but there is inherent danger for inappropriate use of the data for risk assessment purposes. To address this problem, two quality levels for existing data are given in [Table R.16-4](#) (taken from OECD, 2000). In recommending this table the OECD stressed “...these criteria should be applied in a flexible manner. For example, data should not always be discounted because they do not meet the criteria. Risk assessors should make a decision to use the data or not, on a case-by-case basis, according to their experience and expertise and the needs of the risk assessment”. The most important factors to be addressed are the analytical quality control and the representativeness of the sample. Clearly at concentrations approaching the LOQ of an analytical method, percentage errors will be greater than at higher concentrations.

Table R.16-4 Quality criteria for use of existing data (OECD, 2000)

Criteria	Study category	
	1	2
	Valid without restriction – may be used for measured PEC	Valid with restrictions - May be used to support Exposure estimation (data interpretation difficult)
What has been analysed? ¹⁾	x	X
Analytical method ²⁾	x	X
Unit specified ³⁾	x	X
Limit of quantitation ⁴⁾	x	X
Blank concentration ⁵⁾	x	
Recovery ⁶⁾	x	
Accuracy ⁷⁾	x	
Reproducibility ⁸⁾	x	
Sample collection ⁹⁾	x	
One shot or mean ¹⁰⁾	x	X
Location ¹¹⁾	x	X
Date dd/mm/yy ¹²⁾	x	Minimum is knowledge of year
Compartment characteristics ¹³⁾	x	
Sampling frequency and pattern	x	X
Proximity of discharge points ¹⁴⁾	x	X
Discharge emission pattern and volume ¹⁵⁾	x (for local scale)	x (for local scale)
Flow and dilution or application rate	x (for local scale)	x (for local scale)
Explanation of value assigned to non-detects if used in a mean	x	X

Notes to Table R.16-4:

- 1) Precisely what has been analysed should be made clear. Details of the sample preparation, including for example whether the analysis was of the dissolved fraction, the suspended matter (i.e. adsorbed fraction) or the total (aqueous and adsorbed) should be given.
- 2) The analytical method should be given in detail or an appropriate reference cited (e.g. the relevant ISO/DIN method or standard operating procedure).
- 3) Units must be clearly specified and information given whether it has been normalised to e.g. organic carbon, lipid etc.
- 4) The limit of quantitation and details of possible known interfering substances should be quoted.
- 5) Concentrations in system blanks should be given.
- 6) Recovery of standard additions (spikes) should be quoted.
- 7) Results of analysis of standard “reference samples”, containing a known quantity of the substance should be included. Accuracy is connected to the analytical method and the matrix.
- 8) The degree of confidence (e.g. 95% confidence interval) and standard deviation in the result from repeat analysis should be given. Reproducibility is also connected to the analytical method and the matrix.
- 9) Whether the sampling frequency and pattern relate to the emission pattern, or whether they allow for effects such as seasonal variations need to be considered.

- 10) The assessor needs to know how the data have been treated, e.g. are the values reported single values, means, 90-percentile, etc.
- 11) The monitoring site should be representative of the location and scenario chosen. If data represent temporal means, the time over which concentrations were averaged should be given too.
- 12) The time, day, month and year may all be important depending upon the release pattern of the chemicals. Time of sampling may be essential for certain discharge/emission patterns and locations. For some modelling and trends analysis, the year of sampling will be the minimum requirements.
- 13) Compartment characteristics such as lipid content, content of organic carbon and particle size should be specified.
- 14) For the local aqueous environment, detailed information on the distance of other sources in addition to quantitative information on flow and dilution are needed.
- 15) It is necessary to consider whether there is a constant and continuous discharge, or whether the chemical under study is released as a discontinuous emission showing variations in both volume and concentration with time.

When a substance is used in materials (e.g. polymers) it may be released to the environment enclosed within the matrix of small particles of the material formed e.g. by weathering or abrasion. In such cases it would be useful to know if the analytical method used is able to detect also the fraction of substance that is associated with these particles. The availability for analysis can be expected to be reduced for resistant materials and/or large particles. Depending on use pattern, particles may end up in STP sludge/agricultural soil, sediments affected by storm water outflows, industrial/urban soil and indoor dust.

R.16.3.2.2 Selection of representative data for the environmental compartment of concern

There are two distinct aspects to consider:

1. The level of confidence in the result, i.e. the number of samples, how far apart and how frequently they were taken. The sampling frequency and pattern should be sufficient to adequately represent the concentration at the selected site.
2. Whether the sampling site(s) represent a local or regional scenario. Samples taken at sites directly influenced by an emission should be used to describe the local scenario, while samples taken at larger distances may represent the regional concentrations.

It has to be ascertained if the data are results of sporadic examinations or if the substance was detected at the same site over a certain period of time. Measured concentrations caused by an accidental spillage or malfunction should not be considered in the exposure estimation.

Outliers

Where outliers have been identified their inclusion/exclusion should be discussed and justified. The data should be critically examined to establish whether high values reflect an increased or new release, a recent change in emission pattern or a newly discovered occurrence in a specific environmental compartment. The data should also be examined to check that the analytical methodology was appropriate.

If many data are available, the following statistical approach for defining outliers may be used:

$$\log(X_i) > \log(p_{75}) + K(\log(p_{75}) - \log(p_{25}))$$

EQUATION
R.16-7

Where X_i is the concentration, above which a measured value may be considered an outlier, p_i is the value of the i^{th} percentile of the statistic and K is a scaling factor. This filtering of data with a scaling $K = 1.5$ is used in most statistical packages, but this factor can be subject dependent.

Data from a prolonged monitoring programme, where seasonal fluctuations are already included, are of special interest. If available, the distribution of the measured data could be considered for each monitored site, to allow all the information in the distribution function to be used. For regional PEC assessment, a further distribution function covering several sites could be constructed from single site statistics (for example, median, or 90th percentile if the distribution function has only one mode), and the required 90th percentile values, mean or median values of this distribution could be used in the PEC prediction. The mean of the 90th percentiles of the individual sites within one region is recommended for regional PEC determination. Care should be taken that data from several sites obtained with different sampling frequencies should not be combined, without appropriate consideration of the number of data available from each site. If individual measurements are not available then results expressed as means and giving standard deviation will be of particular relevance because in most instances a log normal distribution of concentrations can be assumed and a 90th percentile concentration may be calculated. If only maximum concentrations are reported, they should be considered as a worst-case assumption, providing they do not correspond to an accident or spillage. However, use of only the mean concentrations can result in an underestimation of the existing risk, because temporal and/or spatial average concentrations do not reflect periods and/or locations of high exposure.

For intermittent release scenarios, even the 90-percentile values may not properly address emission episodes of short duration but of high concentration discharge. In these cases, mainly for PEC_{local} calculations, a more realistic picture of the emission pattern can be obtained from the highest value of average concentrations during emission episodes.

Representative measured data from monitoring programmes or from literature, for comparison with calculated PECs should be compiled as tables and annexed to the risk assessment report. The measured data should be presented in the following manner:

Location	Substance	Concentration	Period	Remark	Reference
Country location	substance or metabolite	Units: [$\mu\text{g/L}$], [ng/L] [mg/kg], etc Data - mean - average - range - percentile - daily - weekly - monthly - annual - etc.	month, year	limit of quantitation (LOQ) relevant information on analytical method analytical quality control	Literature reference

When emissions of a substance from waste treatment or disposal stages are significant, measured data may be important along with model calculations in the assessment of the release of the substance from the waste life stage. Besides measured data on concentrations in leachate and landfill gases it is important that flows of water and, when appropriate, gases and solids, from principal treatment or disposal processes and facilities are measured to obtain flow-weighted concentrations. As a surrogate and complement, average time trend data on real runoff or landfill

gas production data can be used, also to extend flux measures to long-term estimates. Emission data of higher quality may become available when the European Pollutant Emissions Register is fully implemented.

However, for release scenarios from waste disposal operations including landfills, the measured concentration may underestimate the environmental concentration that might occur once a substance has passed through all the life-cycle stages including the possible delays. In selecting representative data for waste related releases, consideration should be given to the question whether or not production/import of the substance is in steady state with the occurrence of substance in the waste streams and/or releases from waste treatment and/or releases from landfills.

In a similar manner, if the amount of a substance in use in the society in long-life articles has not reached steady state and the accumulation is ongoing, only a calculated PEC will represent the future situation. This should be considered when comparing such a PEC with measured data representing a non-steady-state.

For the evaluation of measured concentration in biota additional information on season, sex, and dimension could be useful.

R.16.3.3 Allocation of the measured data to a local or a regional scale

The measured data should be allocated to a local or regional scale in order to define the nature of the environmental concentration that is derived. This allows a comparison with the corresponding calculated PEC to be made to determine which PEC should be used in the risk characterisation (Section [R.16.5.6.9](#)).

R.16.3.4 Evaluation of the geographical relation between emission sources and sampling site

If there is no spatial proximity between the sampling site and point sources of emission (e.g. from rural regions), the data represent a regional concentration (PEC_{regional}) that has to be added to the calculated PEC_{local}. If the measured concentrations reflect the releases into the environment through point sources, they are of a PEC_{local}-type. In a PEC_{local} based on measured concentrations, the regional concentration (i.e. PEC_{regional}) is already included.

R.16.3.5 Measured concentrations in biota

Samples of living organisms may be used for environmental monitoring. They can provide a number of advantages compared to conventional water and sediment sampling especially with respect to sampling at large distances from an emission source or on a regional scale. Furthermore they can provide a PEC_{biota} and consequently an estimation of the body burden to be considered in the food chain.

R.16.4 Partitioning and degradation

In this section the derivation of the substance's fate and distribution characteristics is described.

After entering the environment, chemicals are transported within a compartment, such as in air or in soil, or between several compartments (between air and water, air and soil or water and soil). Some xenobiotics are taken up by organisms. Bioaccumulation produces higher concentrations of a chemical in an organism than in its immediate environment, including food. Chemicals may also be transformed into other chemicals ('metabolites'). Transformation ('fate') includes both biotic and abiotic degradation processes.

To assess the environmental exposure, the following processes should be considered:

- Adsorption to aerosol particles (gas-aerosol partitioning) (detailed in Section [R.16.4.3.1](#))
- Partitioning between air and water (volatilisation) (detailed in Section [R.16.4.3.2](#))
- Partitioning between solids and water in soil, sediment and suspended matter (adsorption and desorption) (detailed in Section [R.16.4.3.3](#) and [R.16.4.3.4](#))
- Partitioning between water/solids and biota (bioconcentration and biomagnification) (detailed in Section [R.16.4.3.5](#))
- Transformation processes in the environment. Both biological (biotic, detailed in Sections [R.16.4.4.4](#), [R.16.4.4.5](#)) and abiotic (detailed in Sections [R.16.4.4.1](#), [R.16.4.4.2](#), [R.16.4.4.3](#)) should be considered. If stable and/or toxic degradation products are formed, these should be assessed as well.

In this section the derivation of the substance fate and distribution characteristics is described.

R.16.4.1 Information needed for assessing the partitioning and degradation behaviour

The following minimum information are required: molecular weight, water solubility, vapour pressure, octanol-water partition coefficient and information on ready biodegradability for the substance. For an inorganic substance, it is also advised to provide information on the abiotic degradation, and solid-water partition coefficients and the water-biota partition coefficients. Information requirements on physico-chemical properties are discussed in detail in Section R.7.1.

R.16.4.2 Output from the calculations

The output from the calculations is a number of substance characteristics, mainly expressed as partition coefficients and degradation rates (or half-lives) to be used in the further modelling of the exposure levels.

R.16.4.3 Partition coefficients

Once released into the environment, the chemicals will be transported between the compartments, for example by water and air movements (advection). In addition, the chemicals will by diffusion seek to be in equilibrium with the various compartments. The latter is mainly driven by the partition properties of the chemical.

Basically, all needed partition coefficients can be calculated just from information on the octanol-water partition coefficient, the water solubility and vapour pressure. As these basic calculations are developed for organic substances, care should be taken when dealing with inorganic substances.

In this section, the following processes are described:

- fraction of substance in air associated with aerosol;
- partitioning between air and water;
- partitioning between solids and water in soil, sediment and suspended matter;
- partitioning between water/solids and biota (bioconcentration and biomagnification).

It should be noted that for ionising substances, partitioning behaviour between air-water and solids-water is dependent on the pH of the environment. Section [R.16.4.3.6](#) gives more specific guidance for the assessment of these compounds.

Estimates based on “partitioning” are limited to distribution of a substance in molecular form. However, substances may also be distributed in the environment as particles (caused by abrasion/weathering of anthropogenic materials) extrapolation based on partitioning may not be relevant. In such a case the partitioning method may underestimate exposure of soil and sediment environments and overestimate the exposure of water. If the particle size is small also air distribution may occur, at least in the local perspective. There are no estimation methods available for particle distribution so this has to be dealt with on a case-by-case basis.

R.16.4.3.1 Adsorption to aerosol particles (gas-aerosol partitioning)

The fraction of the substance associated with aerosol particles can be estimated on the basis of the substance's vapour pressure, according to Junge (1977). In this equation, the sub-cooled liquid vapour pressure should be used.

$$F_{ass_{aer}} = \frac{CON_{junge} \cdot SURF_{aer}}{VPL + CON_{junge} \cdot SURF_{aer}} \quad \text{EQUATION R.16-8}$$

Explanation of symbols

CON _{junge}	constant of Junge equation	[Pa · m]	*
SURF _{aer}	surface area of aerosol particles	[m ² · m ⁻³]	*
VP	vapour pressure	[Pa]	data set
F _{ass_{aer}}	fraction of the substance associated with aerosol particles	[-]	

* as a default the product of CON_{junge} and SURF_{aer} is set to 10-4 Pa (Van de Meent, 1993; Heijna-Merkus and Hof, 1993).

Alternatively the octanol-air partition coefficient could be used as described by Finizio et al. (1997).

For solids, a correction of the vapour pressure is required to derive the sub-cooled liquid vapour pressure (Mackay, 1991):

$$VPL = \frac{VP}{e^{6.79 \cdot (1 - \frac{TEMP_{melt}}{TEMP})}} \quad \text{EQUATION R.16-9}$$

Explanation of symbols

TEMP	environmental temperature	[K]	285
TEMP _{melt}	melting point of substance	[K]	data set
VPL	sub-cooled liquid vapour pressure	[Pa]	
VP	vapour pressure	[Pa]	data set

R.16.4.3.2 Volatilisation (air-water partitioning)

The transfer of a substance from the aqueous phase to the gas phase (e.g. stripping in the aeration tank of a STP, volatilisation from surface water) is estimated by means of its Henry's Law constant. If the value is not available in the input data set, the required Henry's Law constant and the *K_{air-water}* (also known as the “dimensionless” Henry's Law constant) can be estimated from the ratio of the

vapour pressure to the water solubility (Equation R.16-11). For water miscible compounds, direct measurement of the Henry's Law constant is recommended. For detailed information, see Section R.7.1.22.

$$HENRY = \frac{VP \cdot MOLW}{SOL} \quad \text{EQUATION R.16-10}$$

$$K_{air-water} = \frac{HENRY}{R \cdot TEMP} \quad \text{EQUATION R.16-11}$$

Explanation of symbols			
VP	vapour pressure	[Pa]	data set
MOLW	molecular weight	[g · mol ⁻¹]	data set
SOL	solubility	[mg · l ⁻¹]	data set
R	gas constant	[Pa · m ³ · mol ⁻¹ · k ⁻¹]	8.314
TEMP	Temperature at the air-water interface	[K]	285
HENRY	Henry's law constant	[Pa · m ³ · mol ⁻¹]	
K _{air-water}	air-water partitioning coefficient	[-]	

If no reliable data for vapour pressure and/or solubility can be obtained, QSPRs are available, see Sections R.7.1.5.3 and R.7.1.22.

R.16.4.3.3 Adsorption/desorption (solids-water partitioning)

In addition to volatilisation, adsorption to solid surfaces is the main partitioning process that drives distribution in soil, surface waters, and sediments. The adsorption of a substance to soil, sediment, suspended matter and sludge can be obtained from experimental data or estimated. More explanation and information on the requirements for this property is given in Section R.7.1.15.

For water soluble, highly adsorptive substances the use of K_{ow} as input into Simple Treat model (see Section R.16.5.5) may lead to an overestimation of the aquatic exposure concentration. SimpleTreat will predict a low elimination on the basis of the log K_{ow} (and small Henry's Law constant), while adsorption onto sludge may be a significant elimination mechanism for these substances.

The solid-water partition coefficient (K_p) in each compartment (soil, sediment, suspended matter) can be calculated from the K_{oc} value, and the fraction of organic carbon in the compartment. Initially, the fraction of organic carbon in the standard environment should be used, as given in [Table R.16-11](#).

$$K_{p,comp} = F_{oc,comp} \cdot K_{oc} \quad \text{with } comp \in \{soil, sed, susp\} \quad \text{EQUATION R.16-12}$$

Explanation of symbols

K _{oc}	partition coefficient organic carbon-water	[l · kg ⁻¹]	data set/Ch. 4
F _{oc,comp}	weight fraction of organic carbon in compartment <i>comp</i>	[kg · kg ⁻¹]	Table R.16-11
K _{p,susp}	partition coefficient solid-water in suspended matter	[l · kg ⁻¹]	
K _{p,sed}	partition coefficient solid-water in sediment	[l · kg ⁻¹]	
K _{p,soil}	partition coefficient solid-water in soil	[l · kg ⁻¹]	

K_p is expressed as the concentration of the substance sorbed to solids (in mg_{chem} · kg_{solid}⁻¹) divided by the concentration dissolved in porewater (mg_{chem} · l_{water}⁻¹). The dimensionless form of K_p , or the total compartment-water partitioning coefficient in (mg · m_{comp}⁻³)/(mg · m_{water}⁻³), can be derived from the definition of the soil in three phases:

$$K_{comp-water} = \frac{C_{total,comp}}{C_{porew,comp}}$$

$$K_{comp-water} = F_{air,comp} \cdot K_{air-water} + F_{water,comp} + F_{solid,comp} \cdot \frac{K_{p,comp}}{1000} \cdot RHO_{solid}$$

EQUATION
R.16-13

with $comp \in \{soil, susp, sed\}$

Explanation of symbols

F _{water,comp}	fraction water in compartment <i>comp</i>	[m ³ · m ⁻³]	Table R.16-11
F _{solid,comp}	fraction solids in compartment <i>comp</i>	[m ³ · m ⁻³]	Table R.16-11
F _{air,comp}	fraction air in compartment <i>comp</i> (only relevant for soil)	[m ³ · m ⁻³]	Table R.16-11
RHO _{solid}	density of the solid phase	[kg · m ⁻³]	2,500
K _{p,comp}	solids-water part. coeff. in compartment <i>comp</i>	[l · kg ⁻¹]	Equation R.16-12
K _{air-water}	air-water partitioning coefficient	[-]	Equation R.16-11
K _{soil-water}	soil-water partitioning coefficient	[m ³ · m ⁻³]	
K _{susp-water}	suspended matter-water partitioning coefficient	[m ³ · m ⁻³]	
K _{sed-water}	sediment-water partitioning coefficient	[m ³ · m ⁻³]	

R.16.4.3.4 Partition coefficients in the marine environment

This section only highlights some specific issues related to the marine environmental conditions.

Measured partition coefficients between water and a second compartment, if available, are usually derived from studies using non-saline water (freshwater or distilled/deionised water). In the absence of measured data, the relevant partition coefficients must be extrapolated from the primary data listed in Section [R.16.4.3](#). However, the techniques that allow such an extrapolation are also largely based on freshwater data sets. Therefore, to assess the distribution of chemicals in the marine environment, it is necessary to consider the extent to which partition coefficients may differ between seawater and freshwater.

The ionic strength, composition, and pH of seawater, compared with freshwater, have potential effects on the partitioning of a chemical with other compartments. To a large extent, these effects

are associated with differences in water solubility and/or speciation of the chemical, compared with freshwater. The relatively high levels of dissolved inorganic salts in seawater generally decrease the solubility of a chemical (referred to as ‘salting-out’), by about 10-50% for non-polar organic compounds but by a smaller fraction for more polar compounds (Schwarzenbach et al., 1993). A recent review found a typical reduction factor of 1.36 (Xie et al., 1997).

For non-ionisable organic substances, the decreased solubility in seawater, compared with freshwater, is expected to result in proportional increases in the partition coefficients between water and octanol, organic carbon and air. However, considering the uncertainty in measured partition values and the uncertainty associated with the frequent need to predict some or all of the partition coefficients, the differences attributable to the seawater environment (less than a factor of 2) are unlikely to be significant in risk assessment. Thus, unless measured seawater data of equal reliability are available, freshwater data can be used for non-ionisable organic compounds without adjustment for the marine environment.

For ionisable organic compounds, as for freshwater, the pH of the environment will affect the water solubility and partitioning of the substance. There is some evidence that the degree of dissociation may also be directly affected by the ionic strength of seawater (Esser and Moser, 1982). However, the resulting shift in the dissociation curve is relatively small compared with that which can occur due to pH for substances with dissociation constants close to the marine water pH. It may, therefore, be preferable to obtain realistic measurements by use of seawater instead of deionised water. Because the pH of seawater (approximately 8) tends to be more constant than that of freshwater, the procedure to correct partition coefficients for ionisable substances, as described in Section R.7.1.20, may however be considered sufficiently reliable for marine conditions.

For inorganic chemicals such as metals, the form or speciation of the substance can be directly affected by the ionic composition of seawater, which may have a considerable influence on both solubility and partitioning. On a case-by-case basis, there may be sufficient information available to allow the relevant partition coefficient in seawater to be calculated from the freshwater data; otherwise, measurements under marine conditions may be necessary.

R.16.4.3.5 Bioconcentration and biomagnification (biota-water/solids partitioning)

Bioconcentration and bioaccumulation may be of concern for lipophilic organic chemicals and some metal compounds as both direct and indirect toxic effects may be observed upon long-term exposure. Secondary poisoning is concerned with toxic effects in organisms in higher trophic levels of the food web, either living in the aquatic or terrestrial environment, which result from ingestion of organisms from lower trophic levels that contain accumulated substances. The subject of bioaccumulation and the corresponding information requirements is discussed in Section R.7.10.1.

Bioaccumulation in aquatic species is described by the Bioconcentration Factor (BCF). The static bioconcentration factor is the ratio between the concentration in the organism and the concentration in water in a steady-state (sometimes also called equilibrium) situation. When uptake and depuration kinetics are measured, the dynamic bioconcentration factor can be calculated from the quotient of the uptake and depuration rate constants:

$$BCF_{org} = \frac{C_{org}}{C_{water}} \text{ or } \frac{k_1}{k_2}$$

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Explanation of symbols

C_{org}	concentration in aquatic organism	$[mg \cdot kg^{-1}]$
C_{water}	concentration in water	$[mg \cdot l^{-1}]$
k_1	uptake rate constant from water	$[l \cdot kg^{-1} \cdot d^{-1}]$
k_2	Elimination rate constant	$[d^{-1}]$
BCF_{org}	bioconcentration factor	$[l \cdot kg^{-1}]$

The testing strategy for bioaccumulation is described in Section R.17.10.1.

A distinction is made between the methodology used to assess the effects of substances whose effects can be related directly to bioconcentration (direct uptake via water) and those where also indirect uptake via the food may contribute significantly to the bioaccumulation. Bioaccumulation of metallic species is not considered explicitly in this section.

Indication of bioaccumulation potential

The most important and widely accepted indication of bioaccumulation potential is a high value of the n-octanol/water partition coefficient (K_{ow}), see Section R.17.1.8. In addition, if a substance belongs to a class of chemicals, which are known to accumulate in living organisms, it may have a potential to bioaccumulate. However, some properties of a substance may preclude high accumulation levels even though the substance has a high $\log K_{ow}$ or has a structural similarity to other substances likely to bioaccumulate. Alternatively there are properties, which may indicate a higher bioaccumulation potential than that suggested by a substance's low $\log K_{ow}$ value. A survey of these factors is given below.

Summary of indications of bioaccumulation potential

If, at production/import volumes between 1-100 tonnes per year, a substance:

- has a $\log K_{ow} \geq 3$ and a molecular weight below 700 g/mol; or;
- is highly adsorptive; or;
- belongs to a class of substances known to have a potential to accumulate in living organisms; or;
- there are indications from structural features;
- and there is no mitigating property such as of hydrolysis (half-life less than 12 hours);

there is an indication of bioaccumulation potential. See Section R.7.10.3 for more information on indicators for bioaccumulation and their interpretation and use.

Experimentally derived bioconcentration factors

REACH Annex IX indicates that information on bioaccumulation in aquatic – preferably fish - species is required for substances manufactured or imported in quantities of 100 t/y or more. For substances that are produced or imported at tonnages of 100 t/y or more. an experimentally derived BCF will be present (unless mitigating factors apply, see Section R.7.10.3.1 on testing data for bioaccumulation).

Calculation of BCF_{fish}

If measured BCF values are not available, the BCF for fish or other organisms can be predicted from the relationship between K_{ow} and BCF (QSARs), see Section R.7.10.3.2 on non-testing data.

Calculation of BCF_{earthworm}

When measured data on bioconcentration in worms is available, the measured BCF earthworm can be used. If data are not available, the BCF can be estimated with a QSAR. For more information on terrestrial bioaccumulation and biomagnification, see Section [R.16.5.7](#).

Biomagnification factor

In a relatively simple food chain with 1 or 2 trophic levels, the concentration in the fish (i.e. the food for the fish-eater) ideally should take account of all possible exposure routes, but in most instances this will not be possible because it is not clear what contribution each potential exposure route makes to the overall body burden of a contaminant in fish species. Therefore for very hydrophobic substances a simple correction factor for potential biomagnification on top of the bioconcentration through the water phase can be applied. For a more in-depth discussion on biomagnification, see Section R.7.10.

The biomagnification factor (BMF) should ideally be based on measured data. However, the availability of such data is usually very limited and therefore, the default values given in [Table R.16-5](#) can be used (see also Section R.7.10.4.4). For further explanation, see [Section R.16.5.7](#) on secondary poisoning. When measured BCF values are available, these should form the basis for deciding on the size of the BMF_1 .

It is realised that food chains of the marine environment can be very long and complex and may consist of 5 or more trophic levels. Since very hydrophobic substances may biomagnify in the tissue and organs of the predator, for the calculation of the internal concentration of the predator an additional biomagnification factor (BMF_2) must be applied. Default values for BMF_2 is given in [Table R.16-5](#) as well.

The possible extent of bioaccumulation in marine food chains with more than the above three to four trophic levels should be evaluated case by case if necessary input data for such an evaluation is available, using the principles for the shorter food chain. Also if further data are available it may be possible to refine the assessment of secondary poisoning via marine food chains by employing more advanced modelling that takes the differences in for instance uptake and metabolic rates into account for the different trophic levels.

Table R.16-5 Default BMF values for organic substances with different log K_{ow} or BCF in fish

log K_{ow}	BCF (fish)	BMF ₁	BMF ₂
<4.5	< 2,000	1	1
4.5 - < 5	2,000-5,000	2	2
5 – 8	> 5,000	10	10
>8 – 9	2,000-5,000	3	3
>9	< 2,000	1	1

The derivation of appropriate default BMFs can only, at this stage, be considered as preliminary for use in screening of chemicals for the purposes of identifying those that need further scrutiny. In reviewing the appropriateness of the BMF applied in any particular assessment, it should be recognised that factors other than the log K_{ow} and BCF should also be taken into account. Such factors should include the available evidence that may indicate a potential for the substance to metabolise or other evidence indicating a low potential for biomagnification. Evidence of a potential for significant metabolism may include:

- data from in vitro metabolism studies;
- data from mammalian metabolism studies;
- evidence of metabolism from structurally similar compounds;
- a measured BCF significantly lower than predicted from the log K_{ow} , indicating possible metabolism.

Where evidence exists suggesting that such metabolism may occur, the BMF detailed above may be reduced. Where such reductions are proposed, a detailed justification should be provided.

R.16.4.3.6 Ionising substances

The degree of ionisation of an organic acid or base greatly affects both the fate and the toxicity of the compound. The water solubility, the adsorption and bioconcentration, as well as the toxicity of the ionised form of a substance may be markedly different from the corresponding neutral molecule.

When the dissociation constant (pKa/pKb) of a substance is known, the percentage of the dissociated and the neutral form of the compound can be determined. See Section R.7.1.17 for more details and explanation on the information requirements.

Every time when partitioning of a substance between water and air or solids is concerned, a correction needs to be made in order to take only the undissociated fraction of the compound into account at a given pH. See Section R.7.1.20 for the equations for the correction factor.

R.16.4.4 Degradation rates in the environment

The degradation in all environmental compartments and the sewage treatment plant can be predicted using information on the ready biodegradability of the substance. It should be emphasized here, that the calculations using information on ready biodegradability only, are very conservative.

So, improved information on the actual degradation rates in the environment can be used as a part of the iteration strategy. In this situation and in case of dealing with inorganic substances, guidance on how to deal with information on degradation is given in this section.

In this section, the following processes are described:

- hydrolysis in surface water;
- photolysis in surface water and in the atmosphere;
- biodegradation in the sewage treatment plant;
- biodegradation in the environmental compartments (surface water, soil, sediment).

In general, the assessment of degradation processes should be based on data, which reflect the environmental conditions as realistically as possible. For an in-depth discussion on the information requirements on degradation, see Section R.7.9.

R.16.4.4.1 Hydrolysis

Values for the hydrolytic half-life (DT50) of a hydrolysable substance can be converted to degradation rate constants, which may be used in the models for calculating PEC_{local} and especially $PEC_{regional}$. The results of a ready biodegradability study will show whether or not the hydrolysis products are themselves biodegradable. Similarly, for substances where hydrolytic DT50 is less than 12 hours, environmental effects are likely to be attributed to the hydrolysis products rather than to the parent substance itself. These effects should also be assessed. See Chapter R.6 and Sections R.7.9 and R.7.1.7 for more details on hydrolysis.

For many substances, the rate of hydrolysis will be heavily dependent on the specific environmental pH and temperature and in the case of soil, also moisture content. For risk assessment purposes for fresh water, sediment and soil, a pH of 7 and a temperature of 12°C (285 K) will normally be established which conform to the standard environmental parameters of [Table R.16-11](#). However, for some substances, it may be necessary to assume a different pH and temperature to fully reflect the potential of the substance to cause adverse effects. This may be of particular importance where the hydrolysis profile shows significantly different rates of hydrolysis over the range pH 4 - 9 and the relevant toxicity is known to be specifically caused by either the stable parent substance or a hydrolysis product.

Rates of hydrolysis always increase with increasing temperature. When hydrolysis half-lives have been determined in standard tests, they should be recalculated to reflect an average EU outdoor temperature by the equation:

$$DT50(X^{\circ}C) = DT50(t) \cdot e^{(0.08 \cdot (T-X))} \quad \text{EQUATION R.16-15}$$

where $X = 12^{\circ}C$ for fresh water. When it is documented for a specific substance that the typical pH of the environmental compartment to be assessed also affects the hydrolysis rate in addition to temperature, the most relevant hydrolysis rate should be taken or extrapolated from the results of the standard test in different pH values. Thereafter the temperature correction is to be applied, where relevant.

When the use of an alternative pH will affect the environmental distribution and toxicity by changing the nature of the soluble species, for example with ionisable substances, care should be taken to ensure that this is fully taken into account when making a final PEC/PNEC comparison.

The half-life for hydrolysis (if known) can be converted to a pseudo first-order rate constant:

$$k_{hydr_{water}} = \frac{\ln 2}{DT50_{hydr_{water}}} \quad \text{EQUATION R.16-16}$$

Explanation of symbols

$DT50_{hydr_{water}}$	half-lifetime for hydrolysis in surface water	[d]	data set
$k_{hydr_{water}}$	first order rate constant for hydrolysis in surface water	[d ⁻¹]	

R.16.4.4.2 Photolysis in water

In the vast majority of surface water bodies dissolved organic matter is responsible for intensive light attenuation. Thus photolysis processes are normally restricted to the upper zones of water bodies. Indirect processes like photo-sensitisation or reaction with oxygen transients (1O₂, OH-radicals, ROO-radicals) may significantly contribute to the overall breakdown rate. Photochemical degradation processes in water may only become an important fate process for substances, which are persistent to other degradation processes (e.g. biodegradation and hydrolysis). For more details on this property, see Section R.7.9.4.

The following aspects have to be considered when estimating the photochemical transformation in natural water bodies:

- the intensity of the incident light depends on seasonal and geographic conditions and varies within wide ranges. For long-term considerations average values can be used while for short-term exposure an unfavourable solar irradiance (winter season) should be chosen;
- in most natural water bodies, the rate of photoreaction is affected by dissolved and suspended matter. Since the concentration of the substance under consideration is normally low compared to the concentration of e.g. dissolved humic acids, the natural constituents absorb by far the larger portion of the sunlight penetrating the water bodies.

Using the standard parameters of the regional model (i.e. a water depth of 3 m and a concentration of suspended matter of 15 mg/l), the reduction in light intensity is higher than 98% through the water column.

Indirect (sensitised) photochemical reactions should only be included in the overall breakdown rate of water bodies if there is clear evidence that this pathway is not of minor importance compared to other processes and its effectiveness can be quantified. For facilitating the complex calculation of phototransformation processes in natural waters computer programs have been developed (See Section R.7.9). In practice it will not be possible to easily demonstrate that photodegradation in water is significant in the environment.

A value for the half-life for photolysis in water (if known) can be converted to a pseudo first-order rate constant:

$$k_{photo_water} = \frac{\ln 2}{DT50_{photo_water}} \quad \text{EQUATION R.16-17}$$

Explanation of symbols

DT50 _{photo_{water}}	half-lifetime for photolysis in surface water	[d]	data set
k _{photo_{water}}	first order rate constant for photolysis in surface water	[d ⁻¹]	

R.16.4.4.3 Photochemical reactions in the atmosphere

Although for some substances direct photolysis may be an important breakdown process, the most effective elimination process in the troposphere for most substances results from reactions with photochemically generated species like OH radicals, ozone and nitrate radicals. The specific first order degradation rate constant of a substance with OH-radicals (k_{OH} in $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$) can either be determined experimentally or estimated, see Sections R.7.9.3 and R.7.9.4.

By relating k_{OH} to the average OH-radical concentration in the atmosphere, the pseudo-first order rate constant in air is determined:

$$KDEG_{AIR} = K_{OH} \cdot OHCONC_{AIR} \cdot 24 \cdot 3600 \quad \text{EQUATION R.16-18}$$

Explanation of symbols

k_{OH}	specific degradation rate constant with OH-radicals	$[\text{cm}^3 \cdot \text{molec}^{-1} \cdot \text{s}^{-1}]$	data set/Ch.4
OHCONC _{air}	concentration of OH-radicals in atmosphere	$[\text{molec} \cdot \text{cm}^{-3}]$	$5 \cdot 10^5 *$
k _{deg_{air}}	pseudo first order rate constant for degradation in air	$[\text{d}^{-1}]$	

*The global annual average OH-radical concentration can be assumed to be $5.105 \text{ molecules} \cdot \text{cm}^{-3}$ (BUA, 1992).

Degradation in the atmosphere is an important process and it is essential to consider whether it can affect the outcome, particularly for high tonnage substances when the regional concentration may be significant. Photodegradation data in the atmosphere must be evaluated with some care. Highly persistent substances may be reported as rapidly degraded in air under environmental conditions where the chemical could be in large amounts in the gas phase. In the real environment, most of the substance may be associated to particles or aerosol and the real atmospheric half-life could be orders of magnitude higher.

R.16.4.4.4 Biodegradation in a sewage treatment plant

The assessment of biodegradability and/or removal in sewage treatment plants should preferably be based on results from tests simulating the conditions in treatment plants. For further guidance on use of STP simulation test results, see Section R.7.9.3.

The ready biodegradability tests that are used at the moment are aimed at measuring the ultimate biodegradability of a substance. They do not give a quantitative estimate of the removal percentage in a wastewater treatment plant. Therefore, in order to make use of the biodegradation test results that are available and requested in the present chemical legislation, it is necessary to assign rate constants to the results of the standard tests for use in STP-models. Because direct measurements of degradation rates at environmentally relevant concentrations are often not available, a pragmatic solution to this problem has been found. For the purpose of modelling a sewage treatment plant (STP), the rate constants of [Table R.16-6](#) were derived from the biodegradation screening tests. All constants in Table R.16-6 have the following prerequisites:

- they are only used for the water-dissolved fraction of the substance. Partitioning between water and sludge phases should be calculated prior to the application of the rate constant
- sufficiently valid data from internationally standardised tests are preferred

Data from non-standardised tests and/or tests not performed according to the principles of GLP may be used if expert judgement has confirmed them to be equivalent to results from the standardised degradation tests on which the calculation models, e.g. SimpleTreat⁵, are based. The same applies to STP-measured data, i.e., in-situ influent/effluent measurements.

Table R.16-6 Elimination in sewage treatment plants:

Extrapolation from test results to rate constants in STP model (SimpleTreat)

Test result	Rate constant $k \cdot (\text{h}^{-1})$
Readily biodegradable	1
Readily, but failing 10-d window	0.3
Inherently biodegradable, fulfilling specific criteria	0.1
Inherently biodegradable, not fulfilling specific criteria	0
Not biodegradable	0

R.16.4.4.5 Biodegradation in surface water, sediment and soil

The rate of biodegradation in surface water, soil and sediment is related to the structure of substances, adequate concentration to induce microbial enzyme systems, microbial numbers, organic carbon content, and temperature. These properties vary spatially and an accurate estimate of the rate of biodegradation is very difficult even if laboratory or field data are available. Fate and exposure models normally assume the following simplifications:

- the kinetics of biodegradation are pseudo-first order;
- only the dissolved portion of the substance is available for biodegradation.

For many substances available biodegradation data is restricted to aerobic conditions. However, for some compartments, e.g. sediment or groundwater, anaerobic conditions should also be considered. In deeper sediment layers anaerobic conditions normally prevail. The same applies to anaerobic

⁵ SimpleTreat is incorporated in the EUSES and TGD excel sheet. See Sections R.16.6.1 and R.16.6.2 for more details on how to get the tools

conditions in landfills and treatment of sewage sludge. Salinity and pH are other examples of environmental conditions that may influence the degradation.

Normally, specific information on biodegradability in sediment or soil is not available. Hence, rate constants for these compartments have to be estimated from the results of standardised tests. For an in-depth discussion of biodegradation testing strategies, see Section R.7.9.

Temperature influences the activity of microorganisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives have been determined in simulation tests, it should be considered to recalculate the degradation rates obtained to reflect an average EU outdoor temperature by [Equation R.16-15](#). When it is documented for a specific substance that a difference between the temperature employed in the test and the average outdoor temperature has no influence on the degradation half-life, no correction is needed.

When results from biodegradation tests simulating the conditions in surface waters are not available, the use of results from various screening tests may be considered. [Table R.16-7](#) gives a proposal for first order rate constants for surface water to be used in local and especially, regional models, based on the results of screening tests for biodegradability. The proposal is based on general experience in relation to available data on biodegradation half-lives in surface waters of readily and not readily biodegradable substances.

The assigned degradation half-lives of an inherently biodegradable substance of 150 days in surface water ([Table R.16-7](#)) and 300 – 30,000 days in soil and sediment ([Table R.16-8](#)) will only affect the predicted regional concentration provided that the residence time of the substance is much larger than the assigned half-life (i.e. only for substances present in soil compartment and sediment).

It is noted that the conditions in laboratory screening tests are very different from the conditions in various environmental compartments. The concentration of the test substance is several orders of magnitude greater in these screening tests than the concentrations of xenobiotic substances generally occurring in the environment and thus the kinetic regimes are significantly different. The temperature is also higher in screening tests than those generally occurring in the environment. Furthermore the microbial biomass is normally lower under environmental conditions than those occurring in these screening tests, especially in the tests for inherent biodegradability. These factors are taken into account in the proposed degradation rates and half-lives in [Table R.16-7](#) and [Table R.16-8](#).

Table R.16-7 First order rate constants and half-lives for biodegradation in surface water

based on results of screening tests on biodegradability^{a)}

Test result	Rate constant k (d ⁻¹)	Half-life (d)
Readily biodegradable	$4.7 \cdot 10^{-2}$	15
Readily, but failing 10-d window ^{b)}	$1.4 \cdot 10^{-2}$	50
Inherently biodegradable ^{c)}	$4.7 \cdot 10^{-3}$	150
Not biodegradable	0	∞

Notes to Table.R.16-7:

a) For use in exposure models these half-lives do not need to be corrected for different environmental temperatures.

b) The 10-day time window concept does not apply to the MITI test. The value obtained in a 14-d window is regarded as acceptable in the Closed Bottle method, if the number of bottles that would have been required to evaluate the 10-d window would cause the test to become too unwieldy.

c) Only those inherently degradable substances that fulfil the criteria described in note b) to [Table R.16-6](#) above. The half-life of 150 days reflects a present "best expert judgement".

The general experience is that a substance passing a test for ready biodegradability may under most environmental conditions be rapidly degraded and the estimated half-lives for such substances (cf. [Table R.16-7](#)) should therefore be regarded as a "the realistic worst-case concept". An OECD guidance document for classification of chemicals hazardous for the aquatic environment (OECD, 2001) contains a chapter on interpretation of degradation data. Even though this guidance relates to hazard classification and not risk assessment, many of the considerations and interpretation principles may also apply in a risk assessment context. One difference is of course that in the risk assessment context not only a categorisation of the substance (i.e. a classification) is attempted, but instead an approximate half-life is estimated. Another difference is that for risk assessment, the availability of high quality test data is required in virtually all cases and further testing may therefore be required in the case of low quality data.

In distribution models, calculations are performed for compartments each consisting of homogeneous sub-compartments, i.e. surface water containing dissolved organic carbon and suspended matter, sediment containing porewater and a solid phase, and soil containing air, porewater and a solid phase. Since it is assumed that no degradation takes place in the sorbed phase, the rate constant for the surface water, bulk sediment or soil in principle depends on the suspended matter/water, sediment/water or soil/water partition coefficient of the substance. With increasing hydrophobicity (sorption) of the substance, the freely dissolved fraction present in the water phase available for degradation decreases, and therefore the overall rate constant should also decrease. However, for surface waters the influence of sorption is already comprised in the degradation rates when they are determined for bulk water in simulation tests employing the same conditions as in the aquatic environment. Neither is it needed to consider the influence of sorption processes when rate constants are established from screening test results due to the well-established practice to conclude on biodegradability in the environment from such data.

When no data from tests simulating the conditions in soil or sediment are available, the use of screening test data may be considered (see Section R.7.9). The guidance for use of such data is based on the general recognition that for substances with low K_p values at present not enough empirical data are available to assume some sort of dependence of the soil biodegradation half-life on the solids/water partition coefficient. Nevertheless, for substances with high K_p -values there is evidence that some sort of K_p dependence exists. Therefore degradation half-life classes for (bulk) soil, partly based on K_p are presented in [Table R.16-8](#). If a half-life from a surface water simulation test is available it may, in a similar manner, form the basis for the establishment of a half-life in soil. The half-lives indicated in the table are considered conservative.

Table R.16-8 Half-lives (days) for (bulk) soil based on results from standardised biodegradation test results

Kp_{soil} [l · kg ⁻¹]	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
≤ 100	30	90	300
>100, ≤ 1000	300	900	3,000
>1000, ≤ 10,000	3,000	9,000	30,000
etc.	etc.	etc.	etc.

The following equation can be used to convert DT50 to a rate constant for biodegradation in soil:

$$k_{bio_{soil}} = \frac{\ln 2}{DT50_{bio_{soil}}} \quad \text{EQUATION R.16-19}$$

Explanation of symbols

$DT50_{bio_{soil}}$	half-life for biodegradation in bulk soil	[d]	Table R.16-8
$k_{bio_{soil}}$	first order rate constant for degr. in bulk soil	[d ⁻¹]	

The extrapolation of results from biodegradation tests to rate constants for sediment is problematic given the fact that sediment in general consists of a relatively thin oxic top layer and anoxic deeper layers. For the degradation in the anoxic layers a rate constant of zero (infinite half-life) can be assumed unless specific information on degradation under anaerobic conditions is available. For the oxic zone, similar rate constants as the ones for soil can be assumed. For the present regional model, a 3 cm thick sediment compartment is assumed with aerobic conditions in the top 3 mm. The sediment compartment is assumed to be well mixed with respect to the substance concentration. This implies that the total half-life for the sediment compartment will be a factor of ten higher than the half-life in soil. The degradation half-life for sediment is given by:

$$k_{bio_{sed}} = \frac{\ln 2}{DT50_{bio_{soil}}} \cdot Faer_{sed} \quad \text{EQUATION R.16-20}$$

Explanation of symbols

$DT50_{bio_{soil}}$	half-life for biodegradation in bulk soil	[d]	Table R.16-8
$Faer_{sed}$	fraction of the sediment compartment that is aerobic	[m ³ · m ⁻³]	0.10
$k_{bio_{sed}}$	first order rate constant for degr. in bulk sediment	[d ⁻¹]	

The remarks in the section on soil biodegradation regarding use of half-lives derived in surface water simulation tests may also apply for sediments.

R.16.4.4.6 Overall rate constant for degradation in surface water

In surface water, the substance may be transformed through photolysis, hydrolysis, and biodegradation. For calculation of the PEC_{regional}, the rate constants for these processes can be summed into one, overall degradation rate constant. It should be noted that different types of degradation (primary and ultimate) are added. This is done for modelling purposes only. It should also be noted that measurements on one degradation process might in fact already include the effects of other processes. For example, hydrolysis can occur under the conditions of a biodegradation test or a test of photodegradation, and so may already be comprised by the measured rate from these tests. In order to add the rates of different processes, it should be determined that the processes occur in parallel and that their effects are not already included in the rates for other processes. If exclusion of hydrolysis from the other degradation rates cannot be confirmed its rate constant should be set to zero. The equation below relates to primary degradation. If the primary degradation is not the rate-limiting step in the total degradation sequence and degradation products accumulate, then also the degradation product(s) formed in the particular process (e.g. hydrolysis) should be assessed. If this cannot be done or is not practical, the rate constant for the process should be set to zero.

$$k_{deg_{water}} = k_{hydr_{water}} + k_{photo_{water}} + k_{bio_{water}} \quad \text{EQUATION R.16-21}$$

Explanation of symbols

k _{photowater}	first order rate constant for hydrolysis in surface water	[d ⁻¹]	Equation 16-17
K _{hydrwater}	first order rate constant for photolysis in surface water	[d]	Equation R.16-17
k _{biowater}	first order rate constant for biodegradation in surface water	[d]	Table R.16-7
K _{degwater}	Total first order rate constant for degradation in surface water	[d]	

R.16.4.4.7 Biodegradation in the marine environment

The rate of biodegradation in the various marine environments depends primarily on the presence of competent degraders, the concentration and the intrinsic properties of the chemical in question, the concentration of nutrients and organic matter and the presence of molecular oxygen. These factors vary significantly between various marine environments.

In estuarine environments, the supply of xenobiotics, nutrients and organic matter is much higher than in more distant marine environments. These factors enhance the probability that biodegradation of xenobiotics occurs with a greater rate in estuaries than is the case in more distant marine environments. Furthermore, estuarine and coastal environments are often turbulent and characterised by a constant sedimentation and re-suspension of sediment particles including microorganisms and nutrients, which increase the biodegradation potential in these environments compared to marine environments with a greater water depth. The presence of suspended particles and surfaces for attachment may favour the degradation of xenobiotics in estuarine environments. For more information on (bio)degradation in marine environments, see Section R.7.9.

Use of marine biodegradation screening test data

For many chemicals, no test data from marine simulation tests are yet available. For many chemicals only data from screening tests are available. This may be data from marine biodegradation screening tests or freshwater biodegradation screening tests (see Section R.7.9.4.1).

When only results from marine or freshwater biodegradation screening tests are available, it is recommended to use the default mineralisation half-lives for the pelagic compartment as specified in [Table R.16-9](#).

**Table R.16-9 Recommended mineralisation half-lives (days)
for use in marine risk assessment when only screening test data are available**

	Freshwater ¹⁾	Estuaries ⁴⁾	Other marine environments ⁵⁾
Degradable in marine screening test	N.a.	15	50
Readily degradable ²⁾	15	15	50
Readily degradable, but failing 10-d window	50	50	150
Inherently degradable ³⁾	150	150	∞
Persistent	∞	∞	∞

Notes to [Table R.16-9](#):

- 1) Half-lives from [Table R.16-9](#).
- 2) Pass level >70% DOC removal or > 60% ThOD in 28 days. Not applicable for freshwater.
- 3) A half-life of 150 days may be used only for those inherently degradable substances that are quickly mineralised in the MITI II or the Zahn Wellens Test (see Section R.7.9). The half-life of 150 days is not fully scientifically justifiable (see Section R.7.9), but reflects a “guesstimate consensus” between a number of experts.
- 4) Also including shallow marine water closest to the coastline
- 5) The half-lives mentioned under this heading are normally to be used in the regional assessment (coastal model) as described in Section [R.16.5.6.8](#).

The half-lives for the marine environments that are described in [Table R.16-9](#) are provisional recommendations, which should be reconsidered, when sufficient data for degradation of different substances in screening tests and simulation tests have been evaluated. The basis for the recommendation is the assumption that the degradation of xenobiotics in freshwater and estuarine waters in general can be described by similar degradation rates, whereas the degradation rates are lower in other marine environments more distant from the coastline (Here the half-life is suggested to be increased by a factor of three relative to estuaries for readily biodegradable substances and even more for more slowly degradable substances, see [Table R.16-9](#)).

R.16.5 Exposure and intake estimation

Exposure of the environment is the result of the release of substances (Section [R.16.2](#)), which may partly be degraded/removed due to treatment facilities (Section [R.16.5.3.4](#)), subsequent distribution and degradation within the environment (Section [R.16.4](#)). Secondary poisoning (section [R.16.5.7](#)) of predators and intake of man via the environment (Section [R.16.5.8](#)) is calculated based on the environmental exposure concentrations in water, air, soil.

R.16.5.1 Output from the exposure and intake calculations

The output from the distribution and exposure calculations are the following PECs:

For inland risk assessment:

- microorganisms in sewage treatment systems;
- atmosphere
- aquatic ecosystem (including sediment);
- terrestrial ecosystem (including groundwater to be used for man-indirect calculations);
- top predators via the food chain (secondary poisoning);

For marine risk assessment:

- aquatic ecosystem (including sediment);
- top predators via the food chain (secondary poisoning)

A survey of the PEC values to be derived is given in the table below.

In addition, intake by man via the environment is calculated (Section [R.16.5.8](#)).

Table R.16-10 Derivation of PEC-values

Target	Medium of exposure	Exposure scenario			Section
		regional	local	Section	
Aquatic compartment (incl. Marine environment)	surface water	steady-state concentration in surface water	concentration during emission period taking into account dilution, sorption, and, if relevant, sedimentation, volatilisation and degradation	R.16.5.6.2	
	sediment	steady-state concentration in sediment	equilibrium concentration in freshly deposited sediment, related to the local surface water concentration	R.16.5.6.3	
Terrestrial compartment	agricultural soil	steady-state concentration in agricultural soil	concentration in agricultural soil averaged over 30 days, fertilised with STP sludge over 10 years and receiving input through continuous aerial deposition	R.16.5.6.6	
	ground water	steady-state concentration in groundwater under agricultural soil	concentration in groundwater under agricultural soil.	R.16.5.6.7	
Air compartment	air	steady-state concentration in air	concentration in air, at 100 m from point source or STP	R.16.5.6.1	
Microorganisms	STP aeration tank	-	concentration during emission period	R.16.5.6.2	

R.16.5.2 Input to exposure estimation calculations

Input into the exposure estimation calculations are:

- Substance properties as described in Section [R.16.4.1](#)
- Emission rates as described in Section [R.16.2](#),
- Removals and distribution in waste treatment systems derived in Section [R.16.5.5.4](#),
- Partition coefficients and degradation rates derived in Section [R.16.4](#)

For full details, read Section [R.16.5](#) and Section [R.16.6](#)

R.16.5.3 Principles

Two types of PEC-values are derived to be used in the further risk assessment: the regional concentration (PEC_{regional}) and the local concentration (PEC_{local}). In addition, continental PEC-values are derived, but they are not used in the risk assessment. The continental PEC-values are used to account for the chemical exchange - due passive transport of the chemical with air and water - with the surrounding area of the regional area. These three types of concentrations differ in temporal and spatial scale.

The regional concentration mainly serves as estimates for background levels, and the estimate of these are so-called steady-state concentration, i.e. the concentration obtained at emissions and fate processes taking place over infinite time. The estimated values are thus considered worst-case estimates. How conservative the estimate is depends on the rate of the fate processes, being most conservative for chemicals where the fate processes take place very slowly. The size of the regional scale is a default set at 10% of the size of the EU. This will be described in more details in Section [R.16.5.6.8](#).

The local concentration is calculated for each identified local point source. The temporal scale is in days, i.e. for discharges with varying magnitude over the day, the daily average concentration is typically used in the further assessment. Also a “standard” environment for the local scale has been defined, e.g. operating with a default dilution of 10 in fresh water systems. This does not exclude that for specific industrial point sources that the calculation of PEC_{local} can be carried out using actual environmental conditions around the source.

A number of environmental properties have impact on the exposure level, e.g. temperature, concentration of organic matter in the soil and sediment. In Section [R.16.5.4](#) the main generic characteristics of the ‘standard’ environments are presented.

The environmental distribution estimation of a chemical is considered on a local scale (in proximity of a production or processing site) and a regional scale (to assess the distribution in a larger area with several sources), detailed below and in Sections [R.16.5.6.8](#).

Three spatial scales are used in the distribution calculations: continental, regional and local. The local scale receives the background concentration from the regional scale; the regional scale receives the inflowing air and water from the continental scale. [Figure R.16-2](#) illustrates the relationships between the three scales.

This implies that the continental, regional, and local calculations must be done sequentially. It should be noted that the use of regional data as background for the local situation may not always be appropriate. If there is only one source of the substance, this emission is counted twice at the local scale: not only due to the local emission, but the same emission is also responsible for the background concentration of the region.

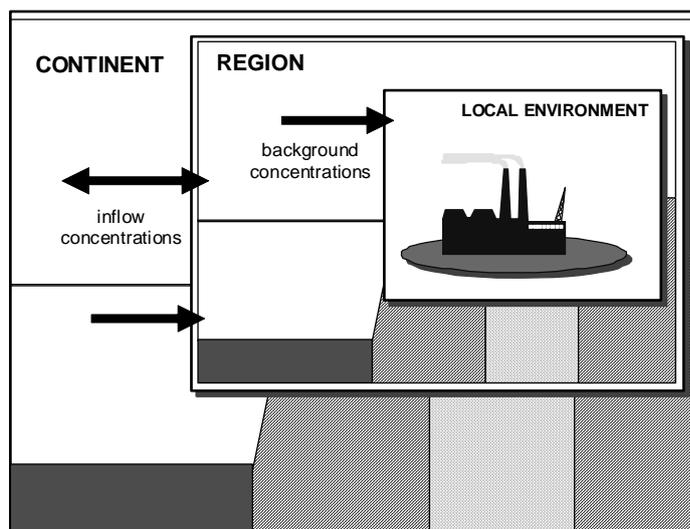


Figure R.16-2 The relationship between the continental, regional, and local scale

R.16.5.3.1 Local environmental distribution

Distribution on the local scale is assessed in the vicinity of point sources. (Figure R.16-3) shows the relationship between the local emission routes and the subsequent distribution processes modelled for the different environmental compartments. Each application of the substance and each stage of the life cycle are assumed to occur at different point sources. Therefore, in principle, a local assessment has to be performed for each relevant application and each relevant life-cycle step (which can be summed if several steps occur on the same location). A generic standard environment is defined to allow for a risk assessment on the European level. As it is impossible to characterise an 'average European environment', default parameter values are chosen which reflect typical, or reasonable worst-case, settings. Dedicated modelling approaches are used to calculate the concentrations in air, surface water and soil. The sediment and groundwater concentrations are estimated from the surface water and soil concentration respectively.

In defining the standard environments, a number of assumptions have been made with respect to spatial and time scale, which are described in Section [R.16.5.4](#).

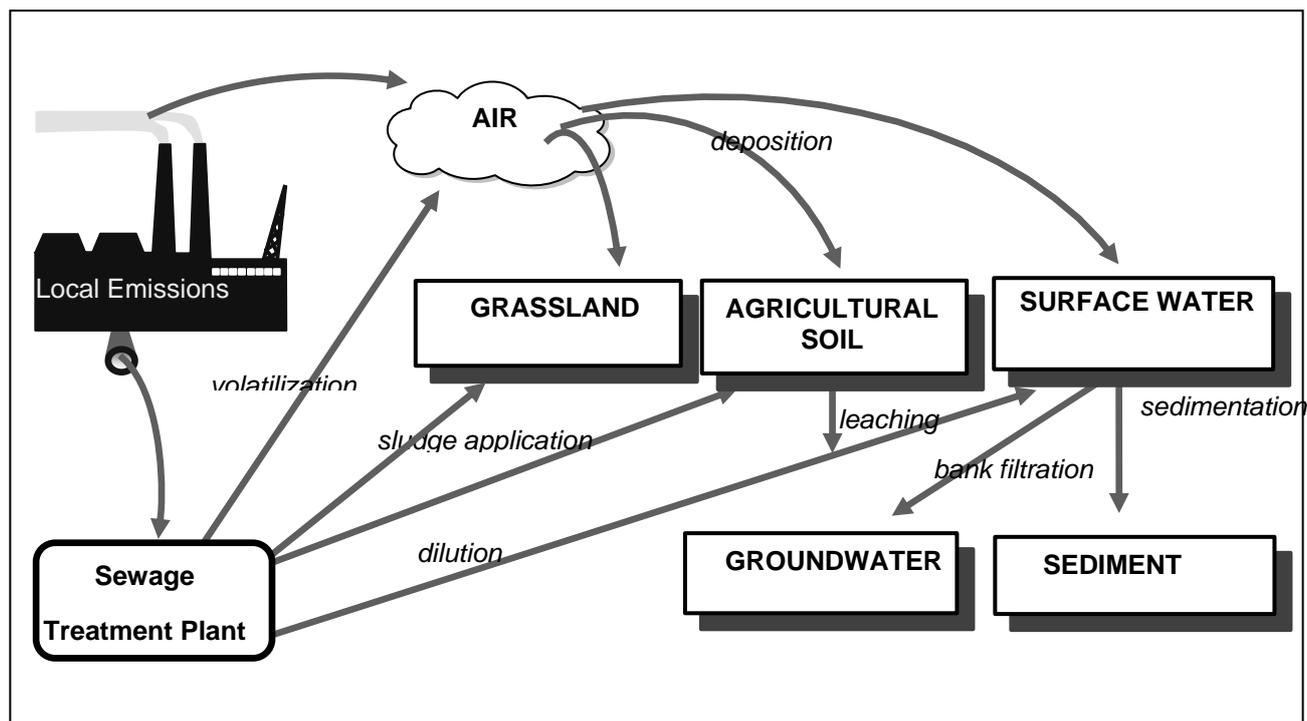


Figure R.16-3 Local distribution calculation

R.16.5.3.2 Regional distribution

For calculating the regional PEC, the multi-media fate-model SimpleBox⁶ is used. The basic characteristics of this model are shown in [Figure R.16-4](#). A description of the assumptions made is given in Section [R.6.5.6.8](#).

In the multi-media model used, the environmental media are represented by the following homogeneous and well-mixed compartment 'boxes':

- Atmosphere;
- Surface water (freshwater and marine environment);
- Sediment (freshwater and marine environment);
- Soil;

⁶ SimpleBox is incorporated in the tools EUSES and TGD Excel (see Sections R.16.6.1 and R.16.6.2)

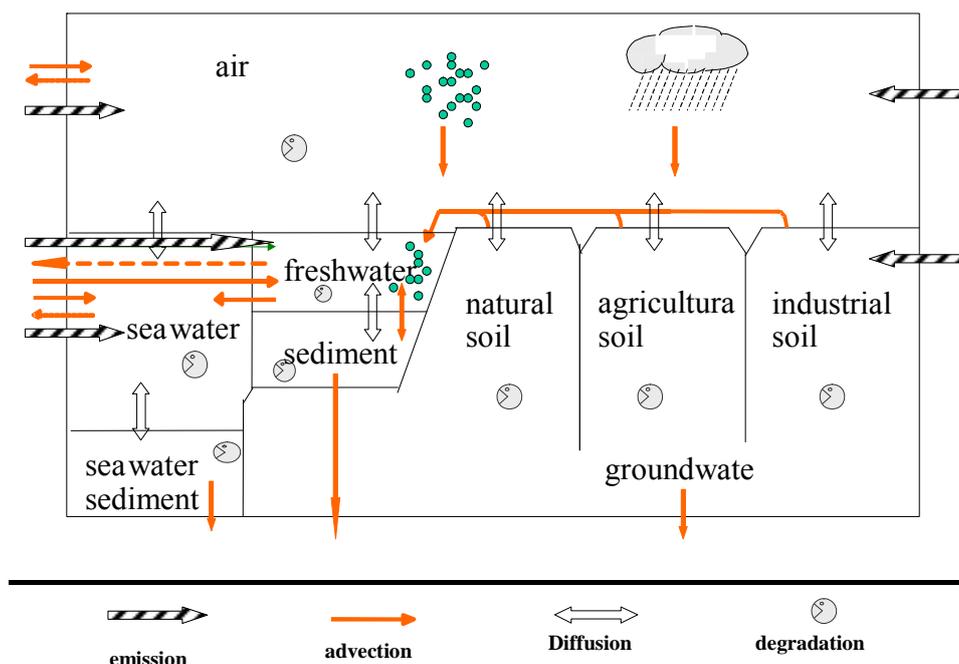


Figure R.16-4 Schematic representation of the model for calculating the regional PECs

R.16.5.3.3 Continental distribution

Concentrations in air and water are also estimated at a continental scale (Europe) to provide inflow concentrations for the regional environment. These concentrations are also derived using the SimpleBox model. The continental concentrations are not used as endpoints for exposure in the risk characterisation.

R.16.5.3.4 Distribution in a sewage treatment plant

The degree of removal in a wastewater treatment plant is determined by the physico-chemical and biological properties of the substance (biodegradation, adsorption onto sludge, removal due to sludge withdrawal, volatility, and the operating conditions of the plant).

For estimation of fate in an STP, the model SimpleTreat 3.10 is recommended. The model is also implemented in the recommended tools (see Sections [R.16.6.1](#) and [R.16.6.2](#)).

Sewage treatment takes place at the local, regional and continental scale.

On a local scale, it is assumed that wastewater will pass through a STP before being discharged into the environment. On a regional scale, it is assumed that 80% of the wastewater is treated in a biological STP and the remaining 20% released directly into surface waters. Typical characteristics of the standard sewage treatment plant are used. At a higher tier in the risk assessment process more specific information on the biodegradation behaviour of a chemical may be available that can be used to refine the assumptions for the STP. The default dilution factor for sewage from municipal treatment plants emitted to a freshwater environment is 10. A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case. Higher dilution factor can be applied if this can be founded by site-specific information. Sludge from an STP is assumed to be spread on agricultural soil for 10 consecutive years.

Further description of the distribution calculation in sewage treatment plants is given in Section [R.16.5.5](#).

R.16.5.4 Characterization of environmental compartments

In this section, the following parameters are derived:

- definition of the standard environmental characteristics ([Table R.16-1](#));
- bulk densities for soil, sediment, and suspended matter.

For the derivation of PECs at the local and regional scale, one standardised generic environment needs to be defined since the general aim is to obtain conclusions regarding risks of the substance at EU level. The characteristics of the real environment will, obviously, vary in time and space. In [Table R.16-11](#), average or typical default values are given for the parameters characterising the environmental compartments (the values are chosen equal on all spatial scales). The standard assessment needs to be performed with the defaults, as given in [Table R.16-11](#). When more specific information is available on the location of the emission sources, this information can be applied in refinement of the PEC by deviating from the parameters of [Table R.16-11](#).

Several other generic environmental characteristics, mainly relevant for the derivation of PEC_{regional} (e.g. the sizes of the environmental compartments, mass transfer coefficients) are given in Section [R.16.5.6.8](#), [Table R.16-14](#) and [Table R.16-16](#).

Table R.16-11: Characterisation of environmental compartments.

Parameter	Symbol	Unit	Value
General			
Density of the solid phase	RHOsolid	[kg _{solid} · m _{solid} ⁻³]	2,500
Density of the water phase	RHOwater	[kg _{water} · m _{water} ⁻³]	1000
Density of air	RHOair	[kg _{air} · m _{air} ⁻³]	1.3
Temperature (12°C)	TEMP	[K]	285
Surface water			
Concentration of suspended matter (dry weight)	SUSP _{water}	[mg _{solid} · l _{water} ⁻¹]	15
Suspended matter			
Volume fraction solids in susp. Matter	Fsolid _{susp}	[m _{solid} ³ · m _{susp} ⁻³]	0.1
Volume fraction water in susp. Matter	Fwater _{susp}	[m _{water} ³ · m _{susp} ⁻³]	0.9
Weight fraction organic carbon in susp. solids	Foc _{susp}	[kg _{oc} · kg _{solid} ⁻¹]	0.1
Sediment			
Volume fraction solids in sediment	Fsolid _{sed}	[m _{solid} ³ · m _{sed} ⁻³]	0.2
Volume fraction water in sediment	Fwater _{sed}	[m _{water} ³ · m _{sed} ⁻³]	0.8
Weight fraction organic carbon sediment solids	Foc _{sed}	[kg _{oc} · kg _{solid} ⁻¹]	0.05
Soil			
Volume fraction solids in soil	Fsolid _{soil}	[m _{solid} ³ · m _{soil} ⁻³]	0.6
Volume fraction water in soil	Fwater _{soil}	[m _{water} ³ · m _{soil} ⁻³]	0.2
Volume fraction air in soil	Fair _{soil}	[m _{air} ³ · m _{soil} ⁻³]	0.2
Weight fraction organic carbon in soil solids	Foc _{soil}	[kg _{oc} · kg _{solid} ⁻¹]	0.02
Weight fraction organic matter in soil solids	Fom _{soil}	[kg _{om} · kg _{solid} ⁻¹]	0.034

Each of the compartments soil, sediment, and suspended matter is described as consisting of three phases: air (only relevant in soil), solids, and water. The bulk density of each compartment is thus defined by the fraction and bulk density of each phase. Both the fractions solids and water, and the total bulk density are used in subsequent calculations. This implies that the bulk density of a compartment cannot be changed independently of the fractions of the separate phases and vice versa.

The bulk densities of the compartments soil, sediment, and suspended matter are defined by the fractions of the separate phases:

$$RHO_{comp} = Fsolid_{comp} \cdot RHOsolid + Fwater_{comp} \cdot RHOwater + Fair_{comp} \cdot RHOair \quad \text{EQUATION R.16-22}$$

with comp ∈ {soil, sed, susp}

Explanation of symbols

$F_{x_{comp}}$	fraction of phase x in compartment comp	$[m^3 \cdot m^{-3}]$	Table R.16-11
RHO_x	density of phase x	$[kg \cdot m^{-3}]$	Table R.16-11
RHO_{comp}	wet bulk density of compartment comp	$[kg \cdot m^{-3}]$	

Application of the formulas above for the values mentioned leads to the following bulk densities of each standard environmental compartment:

Total bulk density of the environmental compartments

RHO_{susp}	Bulk density of (wet) suspended matter	$[kg \cdot m^{-3}]$	1,150
RHO_{sed}	Bulk density of (wet) sediment	$[kg \cdot m^{-3}]$	1,300
RHO_{soil}	Bulk density of (wet) soil	$[kg \cdot m^{-3}]$	1,700

R.16.5.5 Wastewater treatment – estimation of PEC_{stp}

In this section, the following parameters are derived:

- emission from a sewage treatment plant to air (to be further used in PEC_{air} estimation);
- concentration in sewage sludge (to be further used in PEC_{soil} estimation);

concentration in effluent of a sewage treatment plant (to be further used in PEC_{water} estimation).

Elimination refers to the reduction in the concentration of substances in gaseous or aqueous discharges prior to their release to the environment. Elimination from the water phase may occur by physical as well as chemical or biochemical processes. In a sewage treatment plant (STP), one of the main physical processes is settling of suspended matter which will also remove adsorbed material. Physical processes do not degrade a substance but transfer it from one phase to another e.g. from liquid to solid. In the case of volatile substances, the aeration process will enhance their removal from the water phase by “stripping” them from the solid/liquid phases to the atmosphere. Substances may be removed from exhaust gaseous streams by scrubbing e.g. by adsorption on a suitable material or by passing through a trapping solution.

R.16.5.5.1 Wastewater treatment

One of the critical questions to answer in determining the PEC for the aquatic environment is whether or not the substance will pass through a wastewater treatment plant and if yes, through which kind of treatment plant before being discharged into the environment. The situation in the Member States concerning percentage connection to sewage works is quite diverse (see [Appendix R.16-4](#)). The percentage connection rate across the Community is subject to improvement due to the implementation of the Urban Waste Water Treatment Directive (UWWTD, 91/271/EEC). This directive requires Member States (via transposition into national legislation) to ensure that wastewater from all agglomerations of > 2,000 population equivalents is collected and treated minimally by secondary treatment. The time limit for implementation of the directive is 31/12/98, 31/12/2000 or 31/12/2005 dependent on the size of the agglomeration and the sensitivity of the receiving water body. An interim figure of 80% connection to wastewater treatment is proposed for the regional standard environment. This value is thought to be representative for the actual situation in large urban areas at the time of revision of the Guidance Document. Article 6 of the UWWTD allows Member States to declare non sensitive areas for which discharged wastewater from agglomerations between 10,000 and 150,000 population equivalents, which are located at the sea

and from agglomerations between 2,000 and 10,000 population equivalents located at estuaries does not have to be treated biologically but only mechanically (primary treatment). It is notable that 4 Member States have applied this article, corresponding to < 9% of the organic load (in terms of population equivalents).

The situation with respect to wastewater treatment at industrial installations can vary. Many of the larger industrial installations are usually connected to a municipal wastewater treatment plant or have treatment facilities on site. In many cases, these treatment plants are not biological treatment plants but often physico-chemical treatment plants in which organic matter is flocculated by auxiliary agents e.g. by iron salts followed by a sedimentation process resulting in a reduction of organic matter measured as COD of about 25-50%. The above-described situation is taken into account as follows:

- on a local scale, wastewater may or may not pass through a STP before being discharged into the environment. Depending on the exposure scenarios, an aquatic PEC_{local} with or without STP can be calculated. In some cases, both may be needed if it cannot be ascertained that local emissions will pass through the STP. The PEC without considering a STP-treatment will only be used in the exposure estimation, when the substance considered has a specific identified use where direct discharge to water is widely practised;
- for a standard regional scale environment (for definition, see Section [R.16.5.6.8](#)) it is assumed that 80% of the wastewater is treated in a biological STP and the remaining 20% released directly into surface waters (although mechanical treatment has some effect on eliminating organic matter, this is neglected because on the other hand stormwater overflows usually result in direct discharges to surface water even in the case of biological treatment. It is assumed that these two adverse effects compensate each other more or less with regard to the pollution of the environment).

The degree of removal in a wastewater treatment plant is determined by the physico-chemical and biological properties of the substance (biodegradation, adsorption onto sludge, sedimentation of insoluble material, volatilisation) and the operating conditions of the plant. As the type and amount of data available on degree of removal may vary, the following order of preference should be considered:

R.16.5.5.2 Measured data in full scale STP

The percentage removal should preferably be based upon measured influent and effluent concentrations. As with measured data from the environment, the measured data from STPs should be assessed with respect to their adequacy and representativeness.

Consideration must be given to the fact that the effectiveness of elimination in treatment plants is quite variable and depends on operational conditions, such as retention time in the aeration tank, aeration intensity, influent concentration, age and adaptation of sludge, extent of utilisation, rainwater retention capacity, etc. The data may be used provided that certain minimum criteria have been met, e.g. the measurements have been carried out over a longer period of time. Furthermore, consideration should be given to the fact that removal may be due to stripping or adsorption (not degradation). In case no mass balance study has been performed, the percentage of transport to air or sludge should be estimated, e.g. by scaling the fractions to air and sludge from the tables in [Appendix R.16-3](#) to the measured removal.

Data from dedicated STPs should be used with caution. For example, when measured data are available for highly adapted STPs on sites producing high volume site-limited intermediates, these data should only be used for the assessment of this specific use category of the substance.

R.16.5.5.3 Simulation test data

Simulation testing is the examination of the potential of a substance to biodegrade in a laboratory system designated to represent either the activated sludge-based aerobic treatment stage of a wastewater treatment plant or other environmental situations, for example a river. For information on simulation testing, see Section R.7.9.

There is insufficient information available on the applicability of elimination data from the laboratory test to the processes of a real sewage plant. The results can be extrapolated to degradation in the real environment only if the concentrations that were used in the test are in the same order of magnitude as the concentrations that are to be expected in the real environment. If this is not the case, extrapolation can seriously overestimate the degradation rates especially when the extrapolation goes from high to low concentrations. If concentrations are in the same order of magnitude then the results of these tests can be used quantitatively to estimate the degree of removal of substances in a mechanical-biological STP.

If a complete mass balance is determined, the fraction removed by adsorption and stripping should be used for the calculation of sludge and air concentrations. In case no mass balance study has been performed, the percentage of transport to air or sludge should be estimated for example by using the tables in [Appendix R.16-3](#).

R.16.5.5.4 Modelling STP

If there are no measured data available, the degree of removal can be estimated by means of a wastewater treatment plant model using $\log K_{ow}$ (K_{oc} or more specific partition coefficients can also be used; see Section [R.16.4.3.2](#)), Henry's Law constant and the results of biodegradation tests as input parameters. However, it should be remembered that the distribution behaviour of transformation products is not considered by this approach. It is proposed to use in the screening phase of exposure estimation a revised version of the sewage treatment plant model SimpleTreat (Struijs et al., 1991). This model is a multi-compartment box model, calculating steady-state concentrations in a sewage treatment plant, consisting of a primary settler, an aeration tank and a liquid-solid separator. With SimpleTreat, the sewage treatment plant is modelled for an average size treatment plant based on aerobic degradation by active sludge, and consisting of 9 compartments (see [Figure R.16-5](#)). Depending on the test results for ready and/or inherent biodegradability of a substance, specific first order biodegradation rate constants are assigned to the compound. An improved process formulation for volatilisation from the aeration tank, which is also applicable to semi-volatile substances (Mikkelsen, 1995), has been incorporated in the revised version.

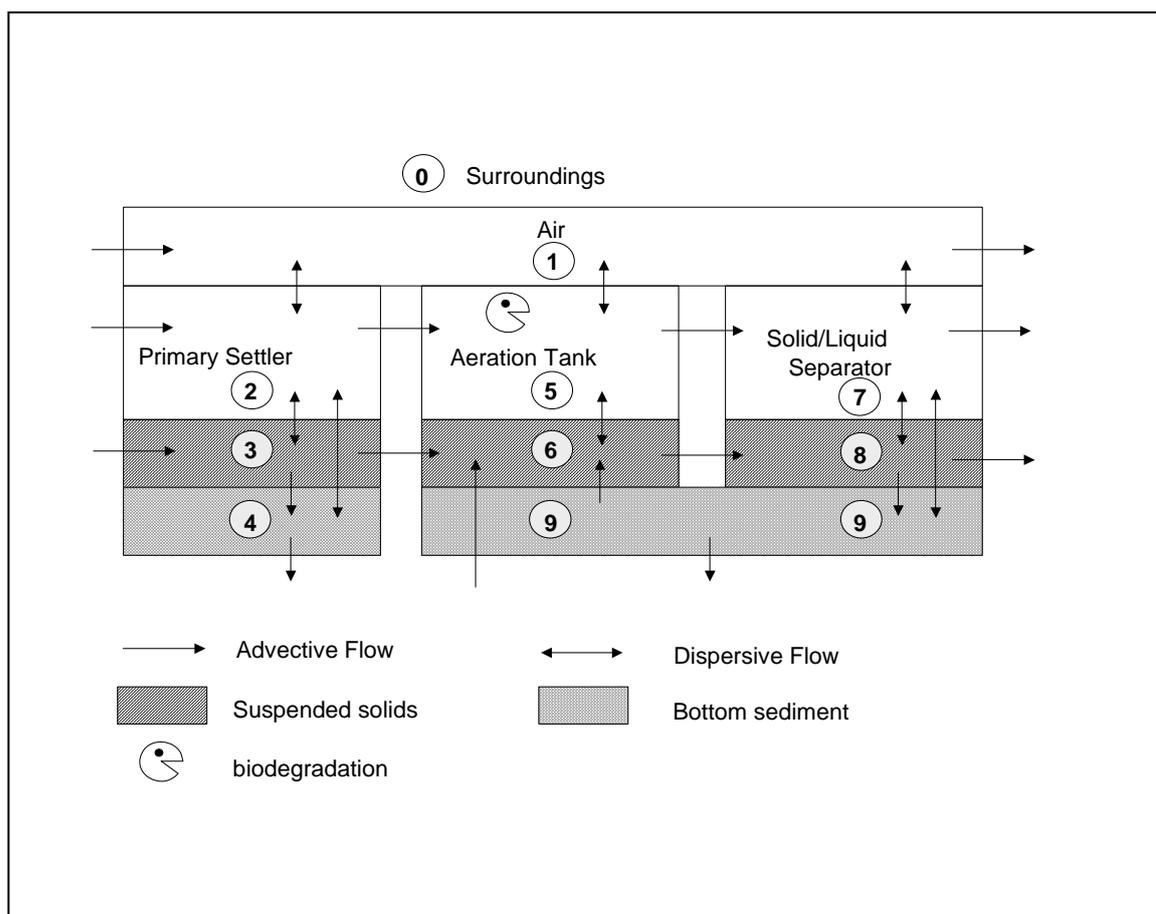


Figure R.16-5: Schematic design of the sewage treatment plant model SimpleTreat

For the purpose of modelling a STP, the rate constants presented in [Table R.16-6](#) have been derived from the biodegradation screening tests. The modelling results from SimpleTreat using these first-order rate constants of 0, 0.1, 0.3 and 1 h⁻¹ are tabulated in [Appendix R.16-3](#). It contains relative emission data pertaining to air, water, and sludge as a function of Henry's Law constant and log K_{ow} for the different biodegradation categories. If no specific measured biodegradation rate data are available for a particular substance, the tabulated values from [Table R.16-6](#) and [Appendix R.16-3](#) should be used.

Typical characteristics of the standard sewage treatment plant are given in [Table R.16-12](#). The amount of surplus sludge per person equivalent and the concentration of suspended matter in influent are taken from SimpleTreat (run at low loading rate). At a higher tier in the risk assessment process more specific information on the biodegradation behaviour of a substance may be available. In order to take this information into account a modified version of the SimpleTreat model may be used. In this version the following scenarios are optional:

- temperature dependence of the biodegradation process;
- degradation kinetics according to the Monod equation;
- degradation of the substance in the adsorbed phase;
- variation in the sludge retention time;

- not considering a primary settler.

Table R.16-12: Standard characteristics of a municipal sewage treatment plant

Parameter	Symbol	Unit	Value
Capacity of the local STP	CAPACITY _{stp}	[eq]	10,000
Amount of wastewater per inhabitant	WASTEWinhab	[l · d ⁻¹ · eq ⁻¹]	200
Surplus sludge per inhabitant	SURPLUSsludge	[kg · d ⁻¹ · eq ⁻¹]	0.011
Concentration susp. matter in influent	SUSPCONC _{inf}	[kg · m ⁻³]	0.45

The input-output parameters are (See [Appendix R.16-3](#)):

Input			
HENRY	Henry's law constant	[Pa · m ³ · mol ⁻¹]	Equation R.16-10
Kow	octanol-water partitioning coefficient	[-]	data set
k _{bio_{stp}}	first-order rate constant for biodegradation in STP	[d ⁻¹]	Table R.16-6
Output			
F _{stp_{air}}	fraction of emission directed to air by STP	[-]	
F _{stp_{water}}	fraction of emission directed to effluent by STP	[-]	
F _{stp_{sludge}}	fraction of emission directed to sludge by STP	[-]	

Calculation of the STP influent concentration

For local scale assessments, it is assumed that one point source is releasing its wastewater to one STP. The concentration in the influent of the STP, i.e. the untreated wastewater, can be calculated from the local emission to wastewater and the influent flow to the STP. The influent flow equals the effluent discharge.

$$C_{local\ inf} = \frac{E_{local\ water} \cdot 10^6}{EFFLUENT_{stp}} \quad \text{EQUATION R.16-23}$$

Explanation of symbols

E _{local_{water}}	local emission rate to (waste) water during episode	[kg · d ⁻¹]	Equation R. 16-1.
EFFLUENT _{stp}	effluent discharge rate of STP	[l · d ⁻¹]	Equation R.16-25
C _{local_{inf}}	concentration in untreated wastewater	[mg · l ⁻¹]	

R.16.5.5.5 Calculation of the STP-effluent concentration

The fraction of the substance reaching the effluent of the STP is tabulated in the Guidance Document ([Appendix R.16-3](#)). The concentration of the effluent of the STP is given by the fraction directed to effluent and the concentration in untreated wastewater as follows:

$$C_{local\,eff} = C_{local\,inf} \cdot F_{stp\,water} \quad \text{EQUATION R.16-24}$$

Explanation of symbols

$C_{local\,inf}$	concentration in untreated wastewater	[mg · l ⁻¹]	Equation R.16-23
$F_{stp\,water}$	fraction of emission directed to water by STP	[-]	Appendix R.16-3
$C_{local\,eff}$	concentration of substance in the STP effluent	[mg · l ⁻¹]	

If no specific data are known, EFFLUENT_{stp} should be based on an averaged wastewater flow of 200 l per capita per day for a population of 10,000 inhabitants (see [Table R.16-12](#)):

$$EFFLUENT_{stp} = CAPACITY_{stp} \cdot WASTEWinhab \quad \text{EQUATION R.16-25}$$

Explanation of symbols

$CAPACITY_{stp}$	capacity of the STP	[eq]	Table R.16-12
$WASTEWinhab$	sewage flow per inhabitant	[l · d ⁻¹ · eq ⁻¹]	Table R.16-12
$EFFLUENT_{stp}$	effluent discharge rate of STP	[l · d ⁻¹]	

For calculating the PEC in surface water without sewage treatment, the fraction of the emission to wastewater, directed to effluent ($F_{stp\,water}$) should be set to 1. The fractions to air and sludge ($F_{stp\,air}$ and $F_{stp\,sludge}$ resp.) should be set to zero.

Calculation of the emission to air from the STP

The indirect emission from the STP to air is given by the fraction of the emission to wastewater, which is directed to air:

$$E_{stp\,air} = F_{stp\,air} \cdot E_{local\,water} \quad \text{EQUATION R.16-26}$$

Explanation of symbols

$F_{stp_{air}}$	fraction of the emission to air from STP	[-]	Appendix R.16-3
$E_{local_{water}}$	local emission rate to water during emission episode	[kg · d ⁻¹]	Equation R. 16-1
$E_{stp_{air}}$	local emission to air from STP during emission episode	[kg · d ⁻¹]	

Calculation of the STP sludge concentration

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

$$C_{sludge} = \frac{F_{stp_{sludge}} \cdot E_{local_{water}} \cdot 10^6}{SLUDGERATE} \quad \text{EQUATION R.16-27}$$

Explanation of symbols

$E_{local_{water}}$	local emission rate to water during episode	[kg · d ⁻¹]	Equation R. 16-1
$F_{stp_{sludge}}$	fraction of emission directed to sludge by STP	[-]	Appendix R.16-3
SLUDGERATE	rate of sewage sludge production	[kg · d ⁻¹]	Equat R.16-28
C_{sludge}	Concentration in dry sewage sludge	[mg · kg ⁻¹]	

The rate of sewage sludge production can be estimated from the outflows of primary and secondary sludge as follows:

$$SLUDGERATE = \frac{2}{3} \cdot SUSPCONC_{inf} \cdot EFFLUENT_{stp} + SURPLUS_{sludge} \cdot CAPACITY_{stp} \quad \text{EQUAT R.16-28}$$

Explanation of symbols

$SUSPCONC_{inf}$	concentration of suspended matter in STP influent	[kg · m ⁻³]	Table R.16-12
$EFFLUENT_{stp}$	effluent discharge rate of STP	[m ³ · d ⁻¹]	Equation R.16-25
$SURPLUS_{sludge}$	surplus sludge per inhabitant equivalent	[kg · d ⁻¹ · eq ⁻¹]	Table R.16-12
$CAPACITY_{stp}$	capacity of the STP	[eq]	Table R.16-12
SLUDGERATE	rate of sewage sludge production	[kg · d ⁻¹]	

Anaerobic degradation may lead to a reduction of the substance concentration in sewage sludge during digestion. This is not yet taken into account.

R.16.5.5.6 Calculation of the STP concentration for evaluation of inhibition to microorganisms

As explained above in the section on STP modeling, the removal of a chemical in the STP is computed from a simple mass balance. For the aeration tank this implies that the inflow of sewage (raw or settled, depending on the equipment with a primary sedimentation tank) is balanced by the following removal processes: degradation, volatilization and outflow of activated sludge into the

secondary settler. Activated sludge flowing out of the aeration tank contains the chemical at a concentration similar to the aeration tank, which is the consequence of complete mixing. It consists of two phases: water, which is virtually equal to effluent flowing out of the solids-liquid separator (this is called the effluent of the STP), and suspended particles, which largely settle to be recycled into the aeration tank. Assuming steady state and complete mixing in all tanks (also the aeration tank), the effluent concentration approximates the really dissolved concentration in activated sludge. It is assumed that only the dissolved concentration is bioavailable, i.e. the actual concentration to which the microorganisms in activated sludge are exposed. For the risk characterisation of a substance upon microorganisms in the STP, it can therefore be assumed that homogeneous mixing in the aeration tank occurs which implies that the dissolved concentration of a substance is equal to the effluent concentration:

$$PEC_{STP} = CLOCAL_{EFF} \quad \text{EQUATION R.16-29}$$

Explanation of symbols

$Clocal_{eff}$	total concentration of substance in STP effluent	$[mg \cdot l^{-1}]$	Equation R.16-24
PEC_{stp}	PEC for microorganisms in the STP	$[mg \cdot l^{-1}]$	

In the case of intermittent release the situation is much more complex. During an interval shorter than several sludge retention times (SRT), presumably a small portion of the competent microorganisms will remain in the system. If the interval between two releases is shorter than one month (three times an average SRT), adaptation of the activated sludge is maintained resulting in rapid biodegradation when a next discharge enters the STP. Such a situation is not considered as an intermittent release and the PEC_{STP} can still be considered equal to $Clocal_{eff}$. After longer intervals the specific bacteria that are capable to biodegrade the compound, may be completely lost.

If the activated sludge is de-adapted, the concentration in the aeration tank may increase during the discharge period. In that case the concentration in influent of the STP is more representative for the PEC for microorganisms:

$$PEC_{STP} = CLOCAL_{INF} \quad \text{EQUATION R.16-30}$$

Explanation of symbols

$Clocal_{inf}$	total concentration of substance in STP influent	$[mg \cdot l^{-1}]$	Equation R.16-23
PEC_{stp}	PEC for microorganisms in the STP	$[mg \cdot l^{-1}]$	

However, it needs to be noted that when the discharge period is shorter than the hydraulic retention time of the aeration tank (7-8 h), the maximum concentration in the effluent will be lower than the initial concentration at the discharge, due to peak dispersion, dilution and sorption in the sewer system, the primary settler and the activated sludge process. It is estimated that this maximum concentration will be at least a factor of three lower than the initial concentration. Whether or not this correction factor must be applied needs to be decided on a case-by-case basis. For such short emission periods care must be taken that the emission rates are in fact calculated over the actual emission period (as $kg \cdot h^{-1}$) and not averaged out over one day.

The choice of using the effluent concentration is also reflected in the choice of the assessment factors used for deriving a PNEC for the STP microorganisms. In modern wastewater treatment plants with a denitrification stage, an additional tank is normally placed at the inlet of the biological stage. As the main biological degradation processes are taking place in the second stage, the microbial population in the denitrification tank is clearly exposed to higher concentrations of the substance as compared to the effluent concentration. As the technical standard of the STPs improves, this will have to be addressed in this assessment scheme in the near future.

Example R.16-1 Removal in the STP continued from **Example R.16-2**

The substance A is characterized as being readily biodegradable. It is furthermore non-volatile and has a logKow of 3.

From the lookup-tables in this Guidance Document ([Appendix R.16-3](#)) the fraction discharged to water can be found at F_{stp_water} 0.12.

d) pass levels within 28 days in a test on “ready biodegradability”, 10-day window criterion is fulfilled

Fate of chemicals that are “readily biodegradable” in an OECD/EU test: $k_{bio_stp} = 1 \text{ hr}^{-1}$ in the aqueous phase of activated sludge.

		log H										
		% to air	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	3	19	55	66	68	
	1	0	0	0	0	0	3	19	55	66	68	
	2	0	0	0	0	0	3	19	54	66	67	
	3	0	0	0	0	0	3	18	53	64	66	
	4	0	0	0	0	0	3	16	46	56	57	
	5	0	0	0	0	0	1	9	29	36	37	
	6	0	0	0	0	0	1	4	15	20	20	

		log H										
		% to water	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	13	13	13	13	13	12	9	5	4	3	
	1	13	13	13	13	13	12	9	5	4	3	
	2	13	13	13	13	12	12	9	5	4	3	
	3	12	12	12	12	12	11	9	5	4	3	
	4	11	11	11	11	11	10	8	4	3	3	
	5	8	8	8	8	8	7	6	4	3	3	
	6	7	7	7	7	7	7	6	4	3	3	

The emission of substance A from the STP can be estimated to:

$$E_{local_water} = F_{stp_water} \cdot E_{local_wastewater} = 0.12 \cdot 0.0625 \frac{kg}{d} = 0.0075 \frac{kg}{d}$$

R.16.5.6 Derivation of PEC

In the following sections guidance is given for the calculation of the PEC_{local} for each compartment and Section [R.16.5.6.8](#) presents the calculation of regional steady-state concentrations ($PEC_{regional}$).

In defining the standard environments a number of assumptions have to be made with respect to scale and time. These are summarised briefly here. More detail is given in the relevant sections.

- the concentration in surface water (PEC_{localwater}) is in principle calculated after complete mixing of the effluent outfall. Because of the short time between effluent discharge and exposure location, dilution will usually be the dominant “removal” process. Therefore, degradation in surface waters, volatilisation from the water body, and sedimentation are not normally taken into account as removal processes. A standard dilution factor is used. To allow for sorption, a correction is made to take account of the fraction of substance that is adsorbed to suspended matter. The resulting dissolved concentration is used for comparison with PNEC_{water}. The concentration in sediment is calculated at the same location. For exposure of aquatic organisms, having a relatively short lifespan, the concentration during an emission episode is calculated. For indirect exposure of humans and predatory birds and mammals, annual averages are used, being more appropriate with respect to chronic exposure;
- the concentration in soil (PEC_{localsoil}) is calculated as an average concentration over a certain time-period in agricultural soil, fertilised with sludge from a STP and receiving continuous aerial deposition from a nearby point source (Section [R.16.5.6.6](#)) (production/processing site and STP aeration tank). Two different soil types are distinguished: arable land and grassland, which differ in the amount of sludge applied, and the mixing depth. For the terrestrial ecosystem, the concentration is averaged over 30 days, for human indirect exposure a period of 180 days is used. The concentration in groundwater is calculated below this agricultural area;
- the concentration in air (PEC_{localair}) is calculated as an average concentration at 100 meters from the source. This distance is assumed to be representative for the average size of an industrial site. The concentration in air is used for exposure of humans, therefore, an annual average concentration is calculated. Deposition is calculated as an average for a circle around the source with a radius of 1000 m, which is supposed to represent the local agricultural area (Section [R.16.5.6.1](#)). Deposition is used as input for the soil module, annual average deposition fluxes are used.

R.16.5.6.1 Calculation of PEC_{local} for the atmosphere

In this section, the following parameters are derived:

- local concentration in air during emission episode;
- annual average local concentration in air;
- total deposition flux (annual average).

The air compartment receives its input from direct emission to air, and volatilisation from the sewage treatment plant. The most important fate processes in air, are schematically drawn in [Figure R.16-6](#).

PEC_{local} for air cannot be compared with the PNEC for air because the latter is usually not available. The PEC_{local} for air is used as input for the calculation of the intake of substances through inhalation in the indirect exposure of humans. Deposition fluxes are used as input for the calculation of PEC_{local} in soil. Therefore, both deposition flux and concentration are calculated as annual average values.

Many air models are available that are highly flexible and can be adjusted to take specific information on scale, emission sources, weather conditions etc. into account. For new substances, as well as very often for existing substances, this type of information is normally not available. Hence a standardised exposure estimation is carried out making a number of explicit assumptions and using a number of fixed default parameters. The gaussian plume model OPS, as described by Van Jaarsveld (1990) is proposed using the standard parameters as described by Toet and de Leeuw (1992). These authors used the OPS model and carried out a number of default calculations in order to describe a relationship between the basic characteristics of substances (vapour pressure and Henry's Law constant) and the concentration in air and deposition flux to soil near to a point source. The following assumptions/model settings are made:

- realistic average atmospheric conditions are used, obtained from a 10-year data set of weather conditions for The Netherlands;
- transport of vaporised and aerosol-bound substances is calculated separately. The partitioning between gas and aerosol is determined by means of the equation of Junge (see Equation R.16-8);
- the atmospheric reaction rate is set at a fixed value of 5% per hour. However, on the spatial scale that is regarded (i.e. a distance of 100 m from the source), atmospheric reactions do not play any role in the removal of the substance (even at very high reaction rates) (Toet and De Leeuw, 1992);
- losses due to deposition are neglected for estimation of the concentration and deposition fluxes at this short distance from the source;
- assumed source characteristics are:
 - source height: 10 meters, representing the height of buildings in which production, processing or use take place;
 - heat content of emitted gases: 0; this assumes there is no extra plume rise caused by excess heat of vapours compared to the outdoor temperature;

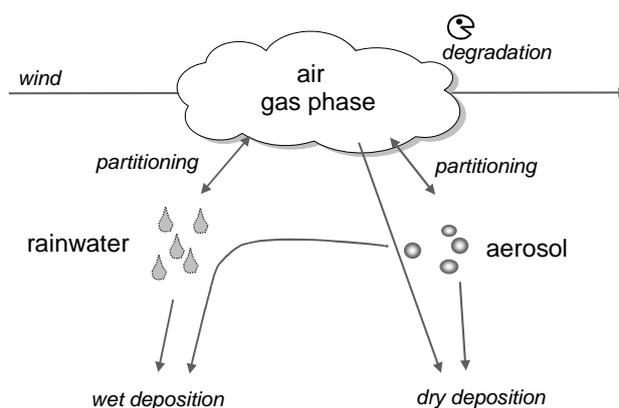


Figure R.16-6 Fate processes in the air compartment

- source area: 0 meter; representing an ideal point source which is obviously not always correct but which is an acceptable choice;
- calculated concentrations are long-term averages.

The concentration in air at a distance of 100 meters from the point source is estimated. This distance is chosen to represent the average distance between the emission source and the border of the industrial site. The deposition flux of gaseous and aerosol-bound substances is estimated analogous to the estimation of atmospheric concentrations by means of an estimation scheme and with help of the OPS model. The deposition flux to soil is averaged over a circular area around the source, with a radius of 1000 m to represent the local agricultural area. Deposition velocities are used for three different categories:

- dry deposition of gas/vapour: estimated at 0.01 cm/s;
- wet deposition of gas/vapour: determined with the OPS model;
- dry and wet deposition of aerosol particles; determined within the OPS model using an average particle size distribution.

Based on the assumptions and model settings as listed above, calculations with the original OPS-model were performed for both gaseous and aerosol substances (Toet and de Leeuw, 1992). These calculations were only carried out for a source strength of 1 g/s, as it was proven that concentrations and deposition fluxes are proportional to the source strength. From these calculations it was concluded that local atmospheric concentrations are largely independent of the physical-chemical properties of the compounds. Hence, once the emission from a point source is known, the concentration at 100 meter from the source can be estimated from a simple linear relationship.

In the calculation of PEC_{local} for air both emission from a point source as well as the emission from a STP is taken into account. The concentration on the regional scale ($PEC_{regional}$) is used as background concentration and therefore, summed to the local concentration. The STP is assumed as a point source and the concentration of the chemical is calculated at a 100 m distance from it. The maximum from the two concentrations (direct and via STP) is used as the PEC_{local} :

$$C_{local\ air} = \max (E_{local\ air} , E_{stp\ air}) \cdot C_{std\ air} \quad \text{EQUATION R.16-31}$$

$$C_{local\ air, ann} = C_{local\ air} \cdot \frac{T_{emission}}{365} \quad \text{EQUATION R.16-32}$$

Explanation of symbols

$E_{local,air}$	local direct emission rate to air during episode	$[kg \cdot d^{-1}]$	eq. (5)
$E_{stp,air}$	local indirect emission to air from STP during episode	$[kg \cdot d^{-1}]$	Equation R.16-26
$C_{std,air}$	concentration in air at source strength of $1 kg \cdot d^{-1}$	$[mg \cdot m^{-3}]$	$2.78 \cdot 10^{-4}$
$T_{emission}$	number of days per year that the emission takes place	$[d \cdot year^{-1}]$	Appendix R.16-1
$C_{local,air}$	local concentration in air during emission episode	$[mg \cdot m^{-3}]$	
$C_{local,air,ann}$	annual average concentration in air, 100 m from point source	$[mg \cdot m^{-3}]$	

$$PEC_{local,air,ann} = C_{local,air,ann} + PEC_{regional,air} \quad \text{EQUATION R.16-33}$$

Explanation of symbols

$C_{local,air,ann}$	annual average local concentration in air	$[mg \cdot m^{-3}]$	Equation R.16-31
$PEC_{regional,air}$	regional concentration in air	$[mg \cdot m^{-3}]$	Section R.16.5.6.8
$PEC_{local,air,ann}$	annual average predicted environmental conc. in air	$[mg \cdot m^{-3}]$	

The calculation of deposition flux is slightly more complex because of the dependence of the deposition flux on the fraction of the substance that is associated with the aerosols. In calculating the deposition flux, the emissions from the two sources (direct and STP) are summed:

$$DEP_{total} = (E_{local,air} + E_{stp,air}) \cdot (F_{ass,aer} \cdot DEP_{std,aer} + (1 - F_{ass,aer}) \cdot DEP_{std,gas}) \quad \text{EQUATION R.16-34}$$

$$DEP_{total,ann} = DEP_{total} \cdot \frac{T_{emission}}{365} \quad \text{EQUATION R.16-35}$$

Explanation of symbols			
$E_{local,air}$	local direct emission rate to air during emission episode	$[kg \cdot d^{-1}]$	Equation R. 16-1.
$E_{stp,air}$	local indirect emission to air from STP during episode	$[kg \cdot d^{-1}]$	Equation R.16-26
$F_{ass,aer}$	fraction of the substance bound to aerosol	$[-]$	Equation R.16-8
$DEP_{std,aer}$	standard deposition flux of aerosol-bound compounds at a source strength of $1 kg \cdot d^{-1}$	$[mg \cdot m^{-2} \cdot d^{-1}]$	$1 \cdot 10^{-2}$
$DEP_{std,gas}$	deposition flux of gaseous compounds as a function of Henry's Law constant, at a source strength of $1 kg \cdot d^{-1}$	$[mg \cdot m^{-2} \cdot d^{-1}]$	
	$^{10}\log HENRY \leq -2$:		$5 \cdot 10^{-4}$
	$-2 < ^{10}\log HENRY \leq 2$:		$4 \cdot 10^{-4}$
	$^{10}\log HENRY > 2$:		$3 \cdot 10^{-4}$
$T_{emission}$	number of days per year that the emission takes place	$[d \cdot yr^{-1}]$	Section R.16.2
DEP_{total}	total deposition flux during emission episode	$[mg \cdot m^{-2} \cdot d^{-1}]$	
$DEP_{total,ann}$	annual average total deposition flux	$[mg \cdot m^{-2} \cdot d^{-1}]$	

R.16.5.6.2 Calculation of PEC_{local} for the aquatic compartment

In this section, the following parameters are derived:

- local concentration in surface water during emission episode;
- annual average local concentration in surface water.

The effluent of the sewage treatment plant is diluted into the surface water. [Figure R.16-7](#) shows the most important fate processes of the aquatic compartment. For the calculations, the following assumptions are made:

- complete mixing of the effluent in surface water is assumed as a representative exposure situation for the aquatic eco-system;
- for the first approach in the local assessments, volatilisation, degradation, and sedimentation are ignored because of the short distance between the point of effluent discharge and the exposure location.

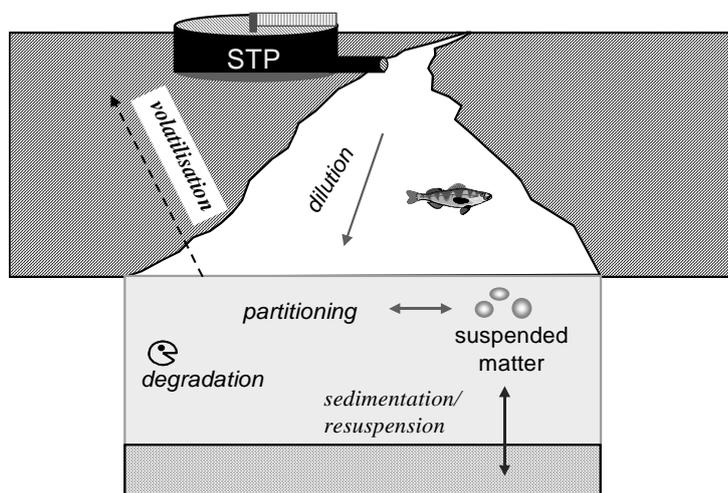


Figure R.16-7 Fate processes in the surface water

The calculation of the PEC_{local} for the aquatic compartment involves several sequential steps (see also [Figure R.16-7](#)). It includes the calculation of the discharge concentration of a STP to a water body, dilution effects and removal from the aqueous medium by adsorption to suspended matter.

Dilution in the receiving surface water and adsorption to suspended matter

The distance from the point of discharge where complete mixing may be assumed will vary between different locations. A fixed dilution factor may be applied. Dilution factors are dependent on flow rates and the industry specific discharge flow. Due to the different seasonal, climatic and geographical conditions in the Member States, those dilution factors may vary over wide ranges. They have been reported in a range from 1 (e.g. dry riverbeds in summer) up to 100,000 (de Greef and de Nijs, 1990). The dilution factor is generally linked to the release scenario of the use category. For example, for consumer products an average dilution factor for sewage from municipal treatment plants of 10 is recommended. This is also regarded as a default dilution value for other types of substances if no specific data are available.

When a substance is released to surface water predominately as particles (e.g. as precipitates or incorporated in small material pieces) this may lead to overestimation of PEC surface water and underestimation of PEC sediment. If this is expected to occur it should be considered in the further evaluation (e.g. when comparing PEC with monitoring data and in the risk characterisation).

In certain circumstances, it may be possible to identify specific emission points which would allow the use of more precise information regarding the available distribution and fate processes. Such site-specific assessments should only be used when it is known that all the emissions emanating from the particular point in the life-cycle e.g. manufacture, arise from a limited number of specific and identifiable sites. In these circumstances each specific point of release will need to be assessed individually. If it is not possible to make this judgement, then the default assumptions should be applied. In site-specific assessments, due account can be taken of the true dilution available to the given emission as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC. Normally, only dilution and adsorption to suspended sediment need to be considered but site-specific conditions may indicate that local distribution models can be used.

It must be noted that with the assumption of complete mixing of the effluent in the surface water no account is taken of the fact that in reality in the mixing zone higher concentrations will occur. For situations with relatively low dilution factors this mixing-zone effect can be accepted. For situations with very high dilution factors, however, the mixing zones may be very long and the overall area that is impacted by the effluent before it is completely mixed can be very substantial. Therefore, in case of site-specific assessments the dilution factor that is applied for calculation of the local concentration in surface water should not be greater than 1000.

If no measured data are available on the partition coefficient between suspended matter and water, K_{psusp} , it can be estimated from the K_{oc} of the substance, determined for other sorbents like soil or sediments (Section [R.16.4.3.3](#)) by taking into account different organic carbon contents of the media.

For some substances it may be possible that PECs are calculated in water which are in excess of the water solubility. These results need to be interpreted carefully on a case-by-case basis. The concentration in surface water will not be corrected, but the result needs to be flagged. The PEC has to be interpreted based on the effects found in the aquatic toxicity tests.

In a situation where a substance is released through several point sources into the same river, the resulting cumulative concentration may in a first approach be estimated by assuming it to be released from one point source. If this PEC leads to “concern” then refined approaches may be used, such as river flow models, e.g. OECD (1992) which address the specific emission pattern as well as river parameters.

The local concentration in surface water is calculated as follows:

$$C_{local\ water} = \frac{C_{local\ eff}}{(1 + K_{p\ susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION} \quad \text{EQUATION R.16-36}$$

Explanation of symbols			
$C_{local\ eff}$	concentration of the substance in the STP effluent	[mg · l ⁻¹]	Equation R.16-24
$K_{p\ susp}$	solids-water partitioning coefficient of suspended matter	[l · kg ⁻¹]	Equation R.16-12
$SUSP_{water}$	concentration of suspended matter in the river	[mg · l ⁻¹]	15
DILUTION	dilution factor	[-]	10
$C_{local\ water}$	local concentration in surface water during emission episode	[mg · l ⁻¹]	

When considering the available dilution, account should be taken of the fluctuating flow-rates of typical receiving waters. The low-flow rate (or 10th percentile) should always be used. Where only average flows are available, the flow for dilution purposes should be estimated as one third of this average. When a site-specific assessment is appropriate, the actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate (this approach should only be used for rivers, not for estuaries or lakes):

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}} \quad \text{EQUATION R.16-37}$$

Explanation of symbols			
$EFFLUENT_{stp}$	effluent discharge rate of stp	[l · d ⁻¹]	Equation R.16-25
FLOW	flow rate of the river	[l · d ⁻¹]	data set
DILUTION	dilution factor at the point of complete mixing	[-]	(max. = 1000)

For indirect human exposure and secondary poisoning, an annual average concentration in surface water is calculated:

$$C_{local\ water, ann} = C_{local\ water} \cdot \frac{T_{emission}}{365} \quad \text{EQUATION R.16-38}$$

Explanation of symbols

$C_{local,water}$	local concentration in surface water during emission episode	$[mg \cdot l^{-1}]$	Equation R.16-36
$T_{emission}$	number of days per year that the emission takes place	$[d \cdot yr^{-1}]$	Appendix R.16-1
$C_{local,water,ann}$	annual average local concentration in surface water	$[mg \cdot l^{-1}]$	

The concentration at the regional scale ($PEC_{regional,water}$) is used as background concentration for the local scale. Therefore, these concentrations are summed:

$$PEC_{local,water} = C_{local,water} + PEC_{regional,water} \quad \text{EQUATION R.16-39}$$

$$PEC_{local,water,ann} = C_{local,water,ann} + PEC_{regional,water} \quad \text{EQUATION R.16-40}$$

Explanation of symbols

$C_{local,water}$	local concentration in surface water during episode	$[mg \cdot l^{-1}]$	Equation R.16-36
$C_{local,water,ann}$	annual average concentration in surface water	$[mg \cdot l^{-1}]$	Equation R.16-38
$PEC_{regional,water}$	regional concentration in surface water	$[mg \cdot l^{-1}]$	Section R.16.5.6.8
$PEC_{local,water}$	predicted environmental concentration during episode	$[mg \cdot l^{-1}]$	
$PEC_{local,water,ann}$	annual average predicted environmental concentration	$[mg \cdot l^{-1}]$	

Example R.16-2 Concentration in surface water

See [Section R.16.5.6.2](#) for detailed description of the model.

Only the manufacturer M is discharging substance A to the STP. The substance A is incorporated in an article matrix and is not expected to be released from the article.

For the assessment the background concentration is neglected. The local concentration in the surface water in the vicinity of the outlet of the STP, which is discharging to a river, can be estimated at:

$$PEC_{local,water} = \frac{E_{local,water}}{Q_{stp} \cdot DILUTION} = \frac{0.0075kg/d}{2,000m^3/d \cdot 10} = 0.375 \mu g / L$$

The $PNEC_{water}$ of substance A has been determined to 0.5 ug/L. As the PNEC value is higher than the $PEC_{local,water}$, it is concluded that the substance A does not exhibit a risk to the surface water.

R.16.5.6.3 Calculation of PEC_{local} for the sediment compartment

In this section, the following parameter is derived:

- local concentration in sediment during the emission episode.

PEC_{local} for sediment can be compared to the PNEC for sediment dwelling organisms. The concentration in freshly deposited sediment is taken as the PEC for sediment, therefore, the properties of suspended matter are used. The concentration in bulk sediment can be derived from the corresponding water body concentration, assuming a thermodynamic partitioning equilibrium (see also Di Toro et al., 1991):

$$PEC_{local_{sed}} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PEC_{local_{water}} \cdot 1000 \quad \text{EQUATION R.16-41}$$

Explanation of symbols

PEC _{local_{water}}	concentration in surface water during emission episode	[mg.l ⁻¹]	Equation R.16-39
K _{susp-water}	suspended matter-water partitioning coefficient	[m ³ .m ⁻³]	Equation R.16-13
RHO _{susp}	bulk density of suspended matter	[kg.m ⁻³]	Equation R.16-22
PEC _{local_{sed}}	predicted environmental concentration in sediment	[mg.kg ⁻¹]	

Highly adsorptive substances may not be considered adequately with the approach described above, as they are often not in equilibrium distribution between water and suspended matter because of their cohesion to the suspended matter; however they may be desorbed after ingestion by benthic or soil organisms.

In the case when release to the surface water predominately occurs as particles this calculation may underestimate the sediment concentration. If this is expected to occur it should be considered in the further evaluation (e.g. when comparing PEC with monitoring data and in the risk characterisation).

R.16.5.6.4 Calculation of PEC_{local} for the marine aquatic compartment

The use of local marine exposure scenarios can be necessary for specific sites releasing directly into the sea. In such cases, potential local releases to the marine environment can occur and, hence, it is necessary to perform a local exposure estimation for the local marine environment.

Dilution and the presence (or absence) of a STP parameters have large influences on the local concentration in seawater (C_{local_{seawater}}). The calculation needs to consider whether effluents are treated in an STP or not.

For discharges to a coastal zone, local dilution will be greater than in a freshwater river. First, initial dilution may occur if the density between the effluent and the saline receiving medium differs (Lewis, 1997). The initial dilution factor is usually around 10. Further dilution due to currents can also be assumed, particularly if the point of release is subject to tidal influences. In the Baltic or the Mediterranean sea, where there are almost no tidal influences compared to the Atlantic Ocean or the North Sea, only initial dilution may occur on calm days, but normally, further dilution due to currents is probable. Dilution factors of more than 500 have been determined from model simulations (based on current measurements) in the North Sea, 200 m away from the discharge point (e.g. Pedersen et al., 1994).

In “site-specific” assessments, due account can be taken of the true dilution available to the given emission as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC. Normally, only dilution and adsorption to suspended sediment need be considered but site-specific

conditions may indicate that valid local distribution models can be used. A realistic worst case dilution factor for discharges to a coastal zone of 100 may be assumed if no further information is available. The same estimation method as for inland exposure estimation can then be used to obtain the local concentration in seawater ($C_{local_seawater}$).

For estuaries, which are influenced by currents and tidal movements, it is assumed as a first approach that they are covered by either the inland or the marine risk assessment. Specific approaches (using higher tier models) can be used if needed.

Then, the local concentration in seawater can be obtained with:

$$C_{local_seawater} = \frac{C_{local_eff}}{(1 + K_{p_susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION} \quad \text{EQUATION R.16-42}$$

Explanation of symbols

C_{local_eff}	concentration of the substance in the STP effluent	[mg · l ⁻¹]	Equation R.16-24
K_{p_susp}	solids-water partitioning coefficient of suspended matter	[l · kg ⁻¹]	Equation R.16-13
$SUSP_{water}$	concentration of suspended matter in the seawater	[mg · l ⁻¹]	15
DILUTION	dilution factor	[-]	100
$C_{local_seawater}$	local concentration in seawater during emission episode	[mg · l ⁻¹]	

K_{p_susp} is derived as for inland risk assessment. For a specific estimation of the partitioning behaviour of substances in saltwater environments see Section [R.16.4.3.4](#)

It is recognised that the dilution available to a discharge will also be related to the actual volume of that discharge. In the freshwater scenario, this discharge volume is standardised to a volume of 2,000 m³/day ie. the outflow from a standard STP. It is therefore proposed that the discharge volume to the marine environment is also normalised at 2,000 m³/day such that the quantity of the substance discharged (in kg/day) is assumed, for modelling purposes, to be diluted into this volume prior to discharge.

For indirect human exposure and secondary poisoning, an annual average concentration in surface water is calculated:

$$C_{local_seawater,ann} = C_{local_seawater} \cdot \frac{T_{emission}}{365} \quad \text{EQUATION R.16-43}$$

Explanation of symbols			
$C_{local,seawater}$	local concentration in seawater during emission episode	$[mg \cdot l^{-1}]$	Equation R.16-42
$T_{emission}$	number of days per year that the emission takes place	$[d \cdot yr^{-1}]$	Appendix R.16-1
$C_{local,seawater,ann}$	annual average local concentration in seawater	$[mg \cdot l^{-1}]$	

The concentration at the regional scale ($PEC_{regional,seawater}$) is used as background concentration for the local scale. Therefore, these concentrations are summed:

$$PEC_{local,seawater} = C_{local,seawater} + PEC_{regional,seawater} \quad \text{EQUATION R.16-44}$$

$$PEC_{local,seawater,ann} = C_{local,seawater,ann} + PEC_{regional,seawater} \quad \text{EQUATION R.16-45}$$

Explanation of symbols			
$C_{local,seawater}$	local concentration in seawater during episode	$[mg \cdot l^{-1}]$	Equation R.16-42
$C_{local,seawater,ann}$	annual average concentration in seawater	$[mg \cdot l^{-1}]$	Equation R.16-43
$PEC_{regional,seawater}$	regional concentration in seawater	$[mg \cdot l^{-1}]$	Section R.16.5.6.8
$PEC_{local,seawater}$	predicted environmental concentration during episode	$[mg \cdot l^{-1}]$	
$PEC_{local,seawater,ann}$	annual average predicted environmental concentration	$[mg \cdot l^{-1}]$	

If relevant site-specific information is available, it can be used to improve the assessment. Some significantly different exposure situations need to be reviewed though:

substances released from offshore platforms. A harmonised mandatory control system for the use and reduction of the discharge of offshore chemicals is already agreed within OSPAR (OSPAR [Figure R.16-7](#) Fate processes in the surface water

- 2000a;2000b). For this specific exposure situation within the EU legislation, the methodology proposed by OSPAR can be taken into consideration⁷;
- substances released from harbours, marinas, fish farms and dry-docks. Specific scenarios will have to be developed for these situations, which are most relevant for biocides.

R.16.5.6.5 Calculation of PEC_{local} for the marine sediment compartment

The concentration in freshly deposited sediment is taken as the PEC for sediment; therefore the properties of suspended matter are used. The concentration in bulk sediment can be derived from the corresponding water body concentration, assuming a thermo-dynamic partitioning equilibrium (Di Toro et al., 1991):

⁷ The methodology for assessing releases from platforms (e.g. CHARM-model) that has been developed in the context of these OSPAR decisions was not re-discussed in the context of the development of the present guidance document for marine risk assessment.

$$PEC_{local\ sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PEC_{local\ seawater} \cdot 1000 \quad \text{EQUATION R.16-46}$$

Explanation of symbols

$PEC_{local\ seawater}$	Concentration in seawater during emission episode	$[mg \cdot l^{-1}]$	
$K_{susp-water}$	suspended matter-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	Equation R.16-13
RHO_{susp}	bulk density of suspended matter	$[kg \cdot m^{-3}]$	Equation R.16-22
$PEC_{local\ sed}$	predicted environmental concentration in sediment	$[mg \cdot kg^{-1}]$	

Highly adsorptive substances may not be considered adequately with the approach described above, as they are often not in equilibrium distribution between water and suspended matter because of their cohesion to suspended matter; however they may be desorbed after ingestion by benthic organisms.

Suspended matter exposed to local releases can subsequently be transported over long distances and deposited to sediment in distant areas. Therefore, it is possible that areas unrelated to local settings are exposed to the same sediment concentrations as would be expected only in the immediate vicinity of the releases. This has especially to be taken into account when comparing measured concentrations to estimated concentrations.

R.16.5.6.6 Calculation of PEC_{local} for the soil compartment

In this section, the following parameters are derived:

- local concentration in agricultural soil (averaged over a certain time period);
- local concentration in grassland (averaged over a certain time period);
- percentage of steady-state situation (to indicate persistency).

Exposure estimation for the soil compartment is important with respect to exposure of terrestrial organisms. Furthermore, crops are grown on agricultural soils for human consumption, and cattle, producing meat and milk, are grazing on grasslands. [Figure R.16-8](#) shows the most important fate processes in the soil compartment.

Guidance for calculating PEC_{local} in soil is given for the following exposure routes:

- application of sewage sludge in agriculture;
- dry and wet deposition from the atmosphere.

Direct application of substances (on the basis of the maximum recommended application rate; e.g. pesticide adjuvants or fertilisers) is

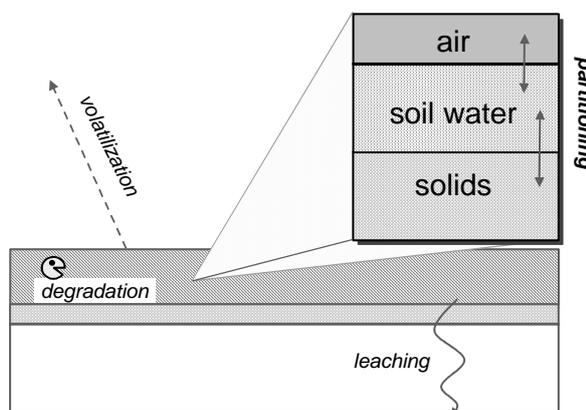


Figure R.16-8 Calculation of PEC_{soil}

not taken into account. Guidance may need to be developed in the future.

For sludge application to agricultural soil an application rate of 5,000 kg/ha dry weight per year is assumed while for grassland a rate of 1000 kg/ha/yr should be used. Sludge application is treated as a single event once a year. The contribution to the overall impact from wet and dry deposition is based on the emission calculation of a point source (Section [R.16.5.6.1](#)) and is related to a surrounding area within 1000 m from that source. The deposition is averaged over the whole area.

Atmospheric deposition is assumed to be a continuous flux throughout the year. It should be noted that the deposition flux is averaged over a year. This is obviously not fully realistic, since the deposition flux is linked to the emission episode. Averaging is done to facilitate calculation of a steady-state level. Furthermore, it is impossible to indicate when the emission episode takes place within a year: in the beginning of the growing season, any impact on exposure levels will be large, after the growing season, the impact may well be insignificant. Therefore, averaging represents an appropriate scenario choice.

The PEC in agricultural soil is used for two purposes:

- for risk characterisation of terrestrial ecosystems
- as a starting point for the calculation of indirect human exposure via crops and cattle products (see Section [R.16.5.8](#) and Chapter R.17).

There are several extensive numerical soil and groundwater models available (mainly for pesticides). These models, however, require a detailed definition of soil and environmental characteristics. This makes this type of models less appropriate for a generic risk assessment at EU-level. For the initial assessment, a simplified model is used. The top layer of the soil compartment is described as one compartment, with an average influx through aerial deposition and sludge application, and a removal from the box by degradation, volatilisation, leaching, and other processes if relevant. The concentration in this soil box can now be described with a simple differential equation.

The initial concentration, $C_{soil}(0)$, is governed by the input of the substance through sludge application.

$$\frac{dC_{soil}}{dt} = -k \cdot C_{soil} + D_{air} \quad \text{EQUATION R.16-47}$$

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	$[\text{mg} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]$	Equation R.16-48
t	Time	[d]	
k	first order rate constant for removal from top soil	$[\text{d}^{-1}]$	Equation R.16-52
C_{soil}	concentration in soil	$[\text{mg} \cdot \text{kg}^{-1}]$	

In the formula above, the aerial deposition flux is used in mg substance per kg of soil per day. D_{air} can be derived by converting the total deposition flux ($DE_{total,ann}$) as follows:

$$D_{air} = \frac{DEP_{total_{ann}}}{DEPTH_{soil} \cdot RHO_{soil}} \quad \text{EQUATION R.16-48}$$

Explanation of symbols

DEP _{total_{ann}}	annual average total deposition flux	[mg · m ⁻² · d ⁻¹]	Equation R.16-35
DEPTH _{soil}	mixing depth of soil	[m]	Table R.16-13
RHO _{soil}	bulk density of soil	[kg · m ⁻³]	Equation R.16-22
D _{air}	aerial deposition flux per kg of soil	[mg · kg ⁻¹ · d ⁻¹]	

The differential [Equation R.16-47](#) has an analytical solution, given by:

$$C_{soil}(t) = \frac{D_{air}}{k} - \left[\frac{D_{air}}{k} - C_{soil}(0) \right] \cdot e^{-kt} \quad \text{EQUATION R.16-49}$$

With this equation, the concentration can be calculated at each moment in time, when the initial concentration in that year is known.

Accumulation of the substance may occur when sludge is applied over consecutive years. This is illustrated in. As a realistic worst-case exposure scenario, it is assumed that sludge is applied for 10 consecutive years. To indicate for potential persistency of the substance, the percentage of the steady-state situation is calculated. As shown in [Figure R.16-9](#), the concentration in soil is not constant in time.

The concentration will be high just after sludge application (in the beginning of the growth season), and lower at the end of the year due to removal processes. Therefore, for exposure of the endpoints, the concentration needs to be averaged over a certain time period. Different averaging times should be considered for these endpoints: for the ecosystem a period of 30 days after application of sludge is used. In order to determine biomagnification effects and indirect human exposure, it is more appropriate to use an extended period of 180 days.

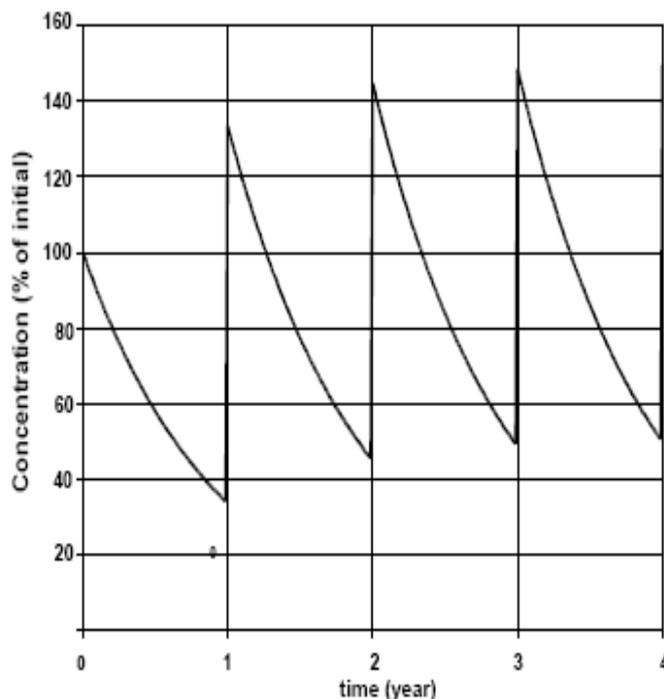


Figure R.16-9 Accumulation in soil due to several years of sludge application.

This averaging procedure is illustrated in [Figure R.16-10](#) where the average concentration is given by the area of the shaded surface, divided by the number of days.

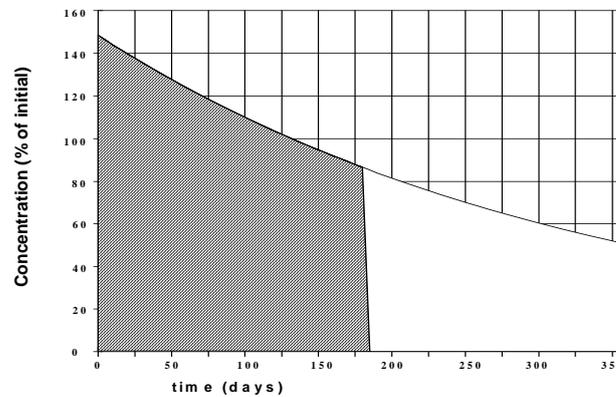


Figure R.16-10 The concentration in soil after 10 years.

The shaded area is the integrated concentration over a period of 180

The local concentration in soil is defined as the average concentration over a certain time period T. The average concentration over T days is given by:

$$C_{local\,soil} = \frac{1}{T} \cdot \int_0^T C_{soil}(t) dt \quad \text{EQUATION R.16-50}$$

Solving this equation for the range 0 to T gives the final equation for the average concentration in this period:

$$C_{local\,soil} = \frac{D_{air}}{k} + \frac{1}{kT} \left[C_{soil}(0) - \frac{D_{air}}{k} \right] \cdot [1 - e^{-kT}] \quad \text{EQUATION R.16-51}$$

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	$[mg \cdot kg^{-1} \cdot d^{-1}]$	Equation R.16-48
T	averaging time	[d]	Table R.16-14
k	first order rate constant for removal from top soil	$[d^{-1}]$	Equation R.16-52
$C_{soil}(0)$	initial concentration (after sludge application)	$[mg \cdot kg^{-1}]$	Equation R.16-59
$C_{local\,soil}$	average concentration in soil over T days	$[mg \cdot kg^{-1}]$	

Derivation of the removal rate constants

The total rate constant for removal is made up of several parts:

- biodegradation rate constant;
- volatilisation of substance from soil;
- leaching to deeper soil layers.

Other removal processes may be important in some cases (e.g. uptake by plants). If rate constants are known for these processes, they may be added to the total removal. The overall removal rate constant is given by:

$$k = k_{volat} + k_{leach} + k_{bio_{soil}} \quad \text{EQUATION R.16-52}$$

Explanation of symbols

k_{volat}	pseudo-first order rate constant for volatilisation from soil	[d ⁻¹]	Equation R.16-53
k_{leach}	pseudo-first order rate constant for leaching from top soil	[d ⁻¹]	Equation R.16-54
$k_{bio_{soil}}$	pseudo-first order rate constant for biodegradation in soil	[d ⁻¹]	Table R.16-8
k	first order rate constant for removal from top soil	[d ⁻¹]	

The rate constant for diffusive transfer from soil to air is estimated as the reciprocal of the sum of mass transfer resistances at the air- and soil sides of the soil/air interface. Given a substance-independent air-side partial mass transfer coefficient, $kasl_{air}$, and the soil-referenced overall mass transfer coefficient, $kasl_{soil}$, the rate constant for volatilization, k_{volat} , becomes:

$$\frac{1}{k_{volat}} = \left(\frac{1}{kasl_{air} * K_{air-water} / K_{soil-water}} + \frac{1}{kasl_{soil}} \right) * DEPTH_{soil} \quad \text{EQUATION R.16-53}$$

Explanation of symbols

$kasl_{air}$	partial mass transfer coeff. at air-side of the air-soil interface	[m.d-1]	120
$kasl_{soil}$	partial mass transfer coeff. at soilair-side of the air-soil int.	[m.d-1]	Equation R.16-66
$K_{air-water}$	air-water equilibrium distribution constant	[m3.m-3]	Equation R.16-11
$K_{soil-water}$	soil-water partitioning coefficient	[m3.m-3]	Equation R.16-13
$DEPTH_{soil}$	mixing depth of soil	[m]	
k_{volat}	pseudo first-order rate constant for volatilisation from soil	[d-1]	

A pseudo first-order rate constant for leaching can be calculated from the amount of rain flushing the liquid-phase of the soil compartment:

$$k_{leach} = \frac{Finf_{soil} \cdot RAINrate}{K_{soil-water} \cdot DEPTH_{soil}} \quad \text{EQUATION R.16-54}$$

Explanation of symbols

$Finf_{soil}$	fraction of rain water that infiltrates into soil	[-]	0.25
$RAINrate$	rate of wet precipitation (700 mm/year)	[m.d ⁻¹]	$1.92 \cdot 10^{-3}$
$K_{soil-water}$	soil-water partitioning coefficient	[m ³ · m ⁻³]	Equation R.16-13
$DEPTH_{soil}$	mixing depth of soil	[m]	Table R.16-3
k_{leach}	pseudo first-order rate constant for leaching from soil layer	[d ⁻¹]	

Derivation of the initial concentration after 10 years of sludge application

As a realistic worst-case assumption for exposure, it is assumed that sludge application takes place for 10 consecutive years. To be able to calculate the concentration in this year averaged over the time period T (Equation R.16-51), an initial concentration in this year needs to be derived. For this purpose, the contributions of deposition and sludge applications are considered separately.

The concentration due to 10 years of continuous deposition only, is given by applying Equation R.16-49 with an initial concentration of zero and 10 years of input:

$$Cdep_{soil10}(0) = \frac{D_{air}}{k} - \frac{D_{air}}{k} \cdot e^{-365 \cdot 10 \cdot k} \quad \text{EQUATION R.16-55}$$

For sludge application, the situation is more complicated as this is not a continuous process. The concentration just after the first year of sludge application is given by:

$$Csludge_{soil1}(0) = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO_{soil}} \quad \text{EQUATION R.16-56}$$

Explanation of symbols

C_{sludge}	concentration in dry sewage sludge	[mg · kg ⁻¹]	Equation R.16-27
$APPL_{sludge}$	dry sludge application rate	[kg · m ⁻² · yr ⁻¹]	Table R.16-13
$DEPTH_{soil}$	mixing depth of soil	[m]	Table R.16-13
RHO_{soil}	bulk density of soil	[kg · m ⁻³]	Equation R.16-22
$Csludge_{soil1}(0)$	concentration in soil due to sludge in first year at t=0	[mg · kg ⁻¹]	

The fraction of the substance that remains in the top soil layer at the end of a year is given by:

$$F_{acc} = e^{-365 k} \quad \text{EQUATION R.16-57}$$

Explanation of symbols

k	first order rate constant for removal from top soil	[d ⁻¹]	Equation R.16-52
F _{acc}	fraction accumulation in one year	[-]	

At the end of each year, a fraction F_{acc} of the initial concentration remains in the top-soil layer. The initial concentration after 10 applications of sludge is given by:

$$C_{sludge_{soil\ 10}}(0) = C_{sludge_{soil\ 1}}(0) \cdot \left[1 + \sum_{n=1}^9 F_{acc}^n \right] \quad \text{EQUATION R.16-58}$$

The sum of both the concentration due to deposition and sludge is the initial concentration in year 10:

$$C_{soil\ 10}(0) = C_{dep_{soil\ 10}}(0) + C_{sludge_{soil\ 10}}(0) \quad \text{EQUATION R.16-59}$$

This initial concentration can be used in Equation R.16-50 to calculate the average concentration in soil over a certain time period.

Indicating persistency of the substance in soil

Ten consecutive years of accumulation may not be sufficient for some substances to reach a steady-state situation. These substances may accumulate for hundreds of years. To indicate potential problems of persistency in soil, the fraction of the steady-state concentration can be derived:

$$F_{st-st} = \frac{C_{soil\ 10}(0)}{C_{soil\ \infty}(0)} \quad \text{EQUATION R.16-60}$$

Explanation of symbols

C _{soil 10} (0)	initial concentration after 10 years	[mg · kg ⁻¹]	Equation R.16-59
C _{soil ∞} (0)	initial concentration in steady-state situation	[mg · kg ⁻¹]	Equation R.16-61
F _{st-st}	fraction of steady-state in soil achieved	[-]	

The initial concentration in the steady-state year is given by:

$$C_{soil\infty}(0) = \frac{D_{air}}{k} + C_{sludge_{soil\ 1}}(0) \cdot \frac{1}{1 - Facc} \quad \text{EQUATION R.16-61}$$

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	$[mg \cdot kg^{-1} \cdot d^{-1}]$	Equation R.16-48
k	first order rate constant for removal from top soil	$[d^{-1}]$	Equation R.16-52
$Facc$	fraction accumulation in one year	$[-]$	Equation R.16-57
$C_{sludge_{soil\ 1}}(0)$	concentration in soil due to sludge in first year at $t=0$	$[mg \cdot kg^{-1}]$	Equation R.16-56
$C_{soil\infty}(0)$	initial concentration in steady-state situation	$[mg \cdot kg^{-1}]$	

Calculation of $PEC_{local_{soil}}$

For soil, three different PECs are calculated, for different endpoints ([Table R.16-13](#)).

Table R.16-13 Characteristics of soil and soil-use for the three different endpoints

	Depth of soil compartment [m]	Averaging time [days]	Rate of sludge application [$kg_{dwt} \cdot m^{-2} \cdot year^{-1}$]	Endpoint
$PEC_{local_{soil}}$	0.20	30	0.5	terrestrial ecosystem
$PEC_{local_{agr. soil}}$	0.20	180	0.5	crops for human consumption
$PEC_{local_{grassland}}$	0.10	180	0.1	grass for cattle

The “depth of soil” represents the depth range for the top soil layer which is of interest. The depth of 20 cm is taken because this range usually has a high root density of crops, and represents the ploughing depth. For grassland, the depth is less since grasslands are not ploughed. The averaging period of 180 days for crops is chosen as a representative growing period for crops. For grassland this period represents a reasonable assumption for the period that cattle is grazing on the field. For the ecosystem a period of 30 days is taken as a relevant time period with respect to chronic exposure of soil organisms.

The concentration at the regional scale is used as background concentration for the local scale. For this purpose, the concentration in unpolluted soil needs to be applied (“natural soil”, only input through deposition). Otherwise, sludge application is taken into account twice.

$$PEC_{local_{soil}} = C_{local_{soil}} + PEC_{regional_{natural\ soil}} \quad \text{EQUATION R.16-62}$$

Explanation of symbols

$C_{local,soil}$	Local concentration in soil	$[mg \cdot kg^{-1}]$	Equation R.16-50
$PEC_{regional,natural\ soil}$	regional concentration in natural soil	$[mg \cdot kg^{-1}]$	Section R.16.5.6.8
$PEC_{local,soil}$	predicted environmental conc. in soil	$[mg \cdot kg^{-1}]$	

The equation for deriving the concentration in the pore water is:

$$PEC_{local,soil,porew} = \frac{PEC_{local,soil} \cdot RHO_{soil}}{K_{soil-water} \cdot 1000} \quad \text{EQUATION R.16-63}$$

Explanation of symbols

$PEC_{local,soil}$	predicted environmental conc. in soil	$[mg \cdot kg^{-1}]$	Equation R.16-62
$K_{soil-water}$	soil-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	Equation R.16-13
RHO_{soil}	bulk density of wet soil	$[kg \cdot m^{-3}]$	Equation R.16-22
$PEC_{local,soil,porew}$	predicted environmental conc. in porewater	$[mg \cdot l^{-1}]$	

R.16.5.6.7 Calculation of concentration in groundwater

In this section, the following parameter is derived:

- local concentration in groundwater.

The concentration in groundwater is calculated for indirect exposure of humans through drinking water. For the calculation of groundwater levels, several numerical models are available (mainly for pesticides). These models, however, require a characterisation of the soil on a high level of detail. This makes these models less appropriate for the initial standard assessment. Therefore, as an indication for potential groundwater levels, the concentration in porewater of agricultural soil is taken. It should be noted that this is a worst-case assumption, neglecting transformation and dilution in deeper soil layers.

$$PEC_{local,grw} = PEC_{local,agr.soil,porew} \quad \text{EQUATION R.16-64}$$

Explanation of symbols

$PEC_{local,agr.soil,porew}$	predicted environmental conc. in porewater	$[mg \cdot l^{-1}]$	Equation R.16-63
$PEC_{local,grw}$	predicted environmental conc. in groundwater	$[mg \cdot l^{-1}]$	

In order to illustrate the calculation methodology, an example on the calculations is given below (continued from the previous example).

Example R.16-3 Concentration in agricultural soil

When estimating the concentration in agricultural soil, the deposition from air (D_{air}) should also be considered. However, as the substance A is involatile this is not relevant for this situation.

From the lookup-tables in this Guidance Document ([Appendix R.16-3](#)) the fraction discharged to sludge can be found at $F_{\text{stp}_{\text{sludge}}}$ 0.03. The same release fraction can be estimated using the model SimpleTreat.

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	0	0	0	0	0	0	0	0	0	0
	3	3	3	3	3	3	3	3	3	3	3
	4	16	16	16	16	16	16	16	15	15	15
	5	47	47	47	47	47	47	46	45	45	45
	6	72	72	72	72	72	72	71	69	67	67

The concentration in sludge is calculated to:

$$C_{\text{sludge}} = \frac{F_{\text{stp}_{\text{sludge}}} \cdot E_{\text{local}_{\text{wastewater}}} \cdot 10^6}{\text{SLUDGERATE}}$$

SLUDGERATE is the rate of sewage sludge production. SLUDGERATE = 710 kg/d for the standard sewage treatment plant,

The concentration in sludge is calculated to:

$$C_{\text{sludge}} = \frac{0.03 \cdot 0.0625 \frac{\text{kg}}{\text{d}} \cdot 10^6 \frac{\text{mg}}{\text{kg}}}{710 \frac{\text{kg}}{\text{d}}} = 2.64 \frac{\text{mg}}{\text{kg}}$$

The concentration contribution to the soil concentration for one sludge application is calculated by:

$$\Delta C_{\text{sludge}_{\text{soil}}}(0) = \frac{C_{\text{sludge}} \cdot \text{APPL}_{\text{sludge}}}{\text{DEPTH}_{\text{soil}} \cdot \text{RHO}_{\text{soil}}}$$

APPL_{sludge} is the dry sludge application rate. Default value is 0.5 kg/m²/yr (when assessing the terrestrial ecosystem)

DEPTH_{soil} is the mixing depth of soil. Default value is 0.2 m.

RHO_{soil} is the bulk density of soil. Default value is 1700 kg/m³

$$\Delta C_{sludge_{soil}}(0) = \frac{2.64 \frac{mg}{kg} \cdot 0.5 \frac{kg}{m^2 \cdot yr} \cdot 1 yr}{0.2m \cdot 1700 \frac{kg}{m^3}} = 0.004 \frac{mg}{kg}$$

The substance will be removed from the soil by leaching (k_{leach}), degradation ($k_{bio_{soil}}$) and volatilization (k_{volat}). The total rate constant (k) is calculated from

$$k = k_{leach} + k_{bio_{soil}} + k_{volat}$$

$$k_{leach} = \frac{F_{inf_{soil}} \cdot RAINrate}{K_{soil-water} \cdot DEPTH_{soil}}$$

$F_{inf_{soil}}$: fraction of rain water that infiltrates into soil. Default value is 0.25

$RAINrate$: the rate of wet precipitation. Default value is $1.92 \cdot 10^{-3}$ m/d

$K_{soil-water}$: soil-water partitioning coefficient. For this substance, having calculated the K_{oc} from the QSAR assuming that the substance belongs to the group “Predominantly hydrophobics”, K_{psoil} is estimated at $K_{soil-water}$ is calculated at $10.4 \text{ m}^3/\text{m}^3$

$$k_{leach} = \frac{0.25 \cdot 1.92 \cdot 10^{-3} \frac{m}{d}}{10.4 \frac{m^3}{m^3} \cdot 0.2m} = 0.0002 \text{ d}^{-1}$$

$k_{bio_{soil}}$ is found from the half-life in soil ($DT50_{bio_{soil}}$), which is 30 days in Table R.16-8 (readily biodegradable substance, $K_{psoil} < 100 \text{ l/kg}$):

$$k_{bio_{soil}} = \frac{\ln(2)}{DT50_{bio_{soil}}} = \frac{\ln(2)}{30} \text{ d}^{-1} = 0.023 \text{ d}^{-1}$$

As the substance is involatile: $k_{volat} = 0 \text{ d}^{-1}$

The total rate of removal is thus: $k = 0.023 \text{ d}^{-1} + 0.0002 \text{ d}^{-1} + 0 \text{ d}^{-1} = 0.023 \text{ d}^{-1}$

The fraction of the substance that remains in the top soil layer at the end of a year is:

$$F_{acc} = e^{-365 \cdot k} = e^{-365 \cdot 0.023} = 0.0002$$

The initial concentration after 10 applications of sludge is calculated at:

$$C_{soil,10} = \Delta C_{sludge_{soil}}(0) \cdot \left[1 + \sum_{n=1}^9 F_{acc}^n \right] = 0.003 \frac{mg}{kg} \cdot \left[1 + \sum_{n=1}^9 0.0002^n \right] = 0.003 \frac{mg}{kg}$$

The average concentration in soil during the first 30 days after the sludge application at year 10 is calculated at:

$$C_{local_{soil}} = \frac{D_{air}}{k} + \frac{1}{k \cdot T} \left[\Delta C_{sludge_{soil}}(0) - \frac{D_{air}}{k} \right] \cdot [1 - e^{-k \cdot T}]$$

$$= 0 + \frac{1}{0.023 \cdot 30} \left[0.003 \frac{mg}{kg} - 0 \right] \cdot [1 - e^{-0.023 \cdot 30}] = 0.002 \frac{mg}{kg}$$

The $PEC_{local_{soil}}$ is calculated by adding $C_{local_{soil}}$ to the regional concentration in natural soil, which is set to 0 mg/kg in this example. The $PEC_{local_{soil}} = 0.002$ mg/kg.

$PNEC_{soil}$ of substance A has been determined to 0.10 mg/kg. As the $PNEC$ value is higher than the $PEC_{local_{soil}}$, it is concluded that the substance A does not exhibit a risk to the soil ecosystem.

R.16.5.6.8 Calculation of $PEC_{regional}$

In this section, the following parameters are derived:

- Regional exposure concentrations in all environmental compartments.

Regional computations are done by means of multimedia fate models based on the fugacity concept. Models have been described by Mackay et al. (1992), Van de Meent (1993) and Brandes et al., (1996) (SimpleBox). These models are box models, consisting of a number of compartments (see [Figure R.16-11](#)) which are considered homogeneous and well mixed. A substance released into the model scenario is distributed between the compartments according to the properties of both the substance and the model environment. Several types of fate processes are distinguished in the regional assessment, as drawn in [Figure R.16-11](#):

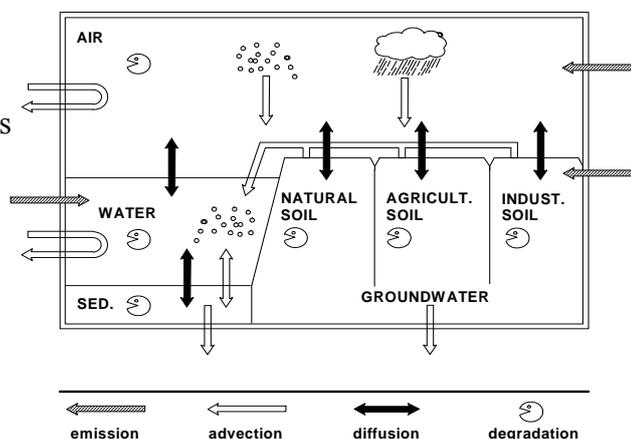


Figure R.16-11 Regional calculations

- emission, direct and indirect (via STP) to the compartments air, water, industrial soil, and agricultural soil;
- degradation, biotic and abiotic degradation processes in all compartments;
- diffusive transport, as e.g. gas absorption and volatilisation. Diffusive mass transfer between two compartments goes both ways, the net flow may be either way, depending on the concentration in both compartments;
- advective transport, as e.g. deposition, run-off, erosion. In the case of advective transport, a substance is carried from one compartment into another by a carrier that physically flows from one compartment into the other. Therefore, advective transport is strictly one-way.

Substance input to the model is regarded as continuous and equivalent to continuous diffuse emission. The results from the model are steady-state concentrations, which can be regarded as estimates of long-term average exposure levels. The fact that a steady state between the compartments is calculated, does not imply that the compartment to which the emission takes place is of no importance.

In a Mackay-type level III model, the distribution and absolute concentrations may highly depend upon the compartment of entry.

Advective import and export (defined as inflow from outside the model or outflow from the model environment) can be very important for the outcome of both regional and local model calculations. Therefore, the concentration of a substance at the “border” of the region must be taken into account. This is defined as the background concentration of a substance. The background concentration in a local model can be obtained from the outcome of the regional model. For substances with many relatively small point sources, this background concentration may represent a significant addition to the concentration from a local source. The background concentration in the regional model has to be calculated using a similar box model of a larger scale, e.g. with the size of the European continent. In this continental model, however, it is assumed that no inflow of air and water across the boundaries occurs. Furthermore it is assumed that all substance releases enter into this continental environment. The resulting steady-state concentrations are then used as transboundary or background concentrations in the regional model. The continental and regional computations should thus be done in sequence.

For the PEC_{regional} calculation, in contrast to PEC_{local}, an average percentage connection rate to STPs should be included in the calculation. This leads to a more realistic estimation of the likely background concentration on a regional scale. For the purposes of the generic regional model, a STP connection rate of 80% (the EU average according to [Appendix R.16-4](#)) will be assumed.

The results from the regional model should be interpreted with caution. The environmental concentrations are averages for the entire regional compartments (which were assumed well mixed). Locally, concentrations may be much higher than these average values. Furthermore, there is a considerable degree of uncertainty due to the uncertainty in the determination of input parameters (e.g. degradation rates, partitioning coefficients).

Model parameters for PEC_{regional}

When calculating the PEC_{regional} it is important which modelling parameters are chosen and what fraction of the total emissions is used as emission for the region. There are two different possibilities:

calculation of a PEC_{regional} on the basis of a standardised regional environment with agreed model parameters;

- calculation of a PEC_{regional} on the basis of country specific model parameters.

A standardised regional environment should be used for the first approach in the calculation of PEC_{regional}. When more specific information is available on the location of production /emission sites, this information can be applied to refine the regional assessment. The second approach may sometimes result in a better estimation of the concentrations for a specific country. However, depending on the information on production site location, it will lead to a number of different PEC values which makes a risk characterisation at EU level more complicated.

Calculations are performed for a densely populated area of 200 · 200 km with 20 million inhabitants. Unless specific information on use or emission per capita is available, it is assumed that 10% of the European production and use takes place within this area, i.e. 10% of the estimated emission is used as input for the region. The model parameters proposed for this standard region are given in [Table R.16-14](#). It should be noted that it is extremely difficult to select typical or representative values for a standard European region. Therefore, the rationale behind the values of [Table R.16-14](#) is limited. Nevertheless, these values present a starting point for the regional scale assessments. Characterisation of the environmental compartments for the regional model should be done according to the values in [Table R.16-14](#).

Table R.16-14 Proposed model parameters for regional model

Parameter	Value in regional model
area of the regional system	4.104 km ²
area fraction of water	0.03
area fraction of natural soil	0.60
area fraction of agricultural soil	0.27
area fraction of industrial/urban soil	0.10
mixing depth of natural soil	0.05 m
mixing depth of agricultural soil	0.2 m
mixing depth of industrial/urban soil	0.05 m
atmospheric mixing height	1000 m
depth of water	3 m
depth of sediment	0.03 m
fraction of the sediment compartment that is aerobic	0.10
average annual precipitation	700 mm · yr ⁻¹
wind speed	3 m · s ⁻¹
residence time of air	0.7 d
residence time of water	40 d
fraction of rain water infiltrating soil	0.25
fraction of rain water running off soil	0.25
EU average connection percentage to STP	80%

The area fractions for water and for natural, agricultural and industrial/urban soils, are average values obtained from ECETOC (1994), supplemented with data received from Sweden and Finland. Data for Norway and Austria are obtained from the FAO statistical databases (<http://apps.fao.org/>). The residence time for air (defined as the time between air entering and leaving the region) of 0.7 days is derived from the wind speed of 3 m/s and the area of the region. The residence time of water of 40 days is selected as a reasonable average for the European situation.

The amount of wastewater discharged, is the product of the amount of wastewater discharged per person equivalent and the number of inhabitants of the system. Using a flow per capita of $200 \text{ l} \cdot \text{d}^{-1}$ (equivalent to the value used in the SimpleTreat model, see [Figure R.16-12](#)) and a population of 20 million, this results in an additional water flow through the model environment of $4.0 \cdot 10^6 \text{ m}^3 \cdot \text{d}^{-1}$. The inflow caused by inflowing riverwater, is $6.5 \cdot 10^7 \text{ m}^3 \cdot \text{d}^{-1}$.

In addition to the environmental characteristics of the region, selected intermedia mass transfer coefficients are required in the multimedia fugacity model to ensure comparability of the outcome with other models. These transfer coefficients are summarised in [Table R.16-15](#).

Table R.16-15 Intermedia mass transfer coefficients

Parameter	Value
air-water interface: air side partial mass transfer coefficient	Equation R.16-75
air-water interface: water side partial mass transfer coefficient	Equation R.16-76
Aerosol deposition rate	0.001 m.s-1
air-soil interface: air side partial mass transfer coefficient	$1.39 \cdot 10^{-3} \text{ m.s}^{-1}$
air-soil interface: soil side partial mass transfer coefficient	Equation R.16-66
sediment-water interface: water side partial mass transfer coefficient	$2.78 \cdot 10^{-6} \text{ m.s}^{-1}$
sediment-water interface: pore water side partial mass transfer coefficient	$2.78 \cdot 10^{-8} \text{ m.s}^{-1}$
net sedimentation rate	3 mm.yr-1

Mass transfer at air-soil and air-water interface on the regional and continental scale

Soil-air interface

A substance-dependent soil-side partial mass transfer coefficient (PMTC) at the soil-air interface $kasl_{soil}$ ($\text{m} \cdot \text{d}^{-1}$) is deduced from the exponential concentration profile in an undisturbed soil:

$$kasl_{soil} = \left(V_{eff,soil} + \frac{D_{eff,soil}}{d_p} \right) \quad \text{EQUATION R.16-65}$$

In undisturbed soil, processes of downward advection (pore water + small particles), diffusion (air, water, solids), and degradation take place simultaneously. These processes are included in Simplebox 3.0 (Den Hollander et al., 2004). The result is an exponential decrease of the

concentration with depth, characterised by a substance-dependent penetration depth (d_p) (Hollander, 2004 and 2006).

$$d_p = \frac{V_{eff\ soil} + \sqrt{V_{eff\ soil}^2 + D_{eff\ soil} \cdot 4 \cdot k\ deg_{soil}}}{2 \cdot k\ deg_{soil}} \quad \text{EQUATION R.16-66}$$

In which:

$$V_{eff\ soil} = FR_{w.soil} \frac{RAINRATE \cdot F_{inf\ soil}}{F_{water\ soil}} + FR_{s.soil} \cdot \frac{SOLID_{adv.soil}}{F_{solid\ soil}} \quad \text{EQUATION R.16-67}$$

$$D_{eff\ soil} = FR_{a.soil} \frac{DIFF_{gas} \cdot Fair_{soil}^{1.5}}{Fair_{soil}} + FR_{w.soil} \cdot \frac{DIFF_{water} \cdot F_{water\ soil}^{1.5}}{F_{water\ soil}} + FR_{s.soil} \cdot \frac{SOLID_{diff.soil}}{F_{solid\ soil}} \quad \text{EQUATION R.16-68}$$

$$FR_{w.soil} = \frac{F_{water\ soil}}{Fair_{soil} \cdot K_{air-water} + F_{water\ soil} + F_{solid\ soil} \cdot K_{soil-water}} \quad \text{EQUATION R.16-69}$$

$$FR_{s.soil} = \frac{F_{solid\ soil}}{Fair_{soil} \cdot K_{air-water} / K_{soil-water} + F_{water\ soil} / K_{soil-water} + F_{solid\ soil}} \quad \text{EQUATION R.16-70}$$

$$FR_{a.soil} = 1 - FR_{w.soil} - FR_{s.soil} \quad \text{EQUATION R.16-71}$$

$$DIFF_{gas} = 2.57 \cdot 10^{-5} \sqrt{\frac{18}{MOLW}} \quad \text{EQUATION R.16-72}$$

$$DIFF_{water} = 2.0 \cdot 10^{-9} \sqrt{\frac{32}{MOLW}} \quad \text{EQUATION R.16-73}$$

Explanation of symbols

MOLW	molecular weight of the substance	[kg·mol ⁻¹]	
kdeg _{soil}	rate constant for degradation in bulk soil	[d ⁻¹]	
RAINRATE	average daily rate of wet precipitation	[m·d ⁻¹]	Table R.16-14
F _{inf} _{soil}	fraction of precipitation that penetrates into the soil	[-]	Table R.16-14
d _p	substance-dependent penetration depth	[m]	Equation R.16-67
V _{eff} _{soil}	effective advection (with penetrating porewater)	[m]	Equation R.16-68
D _{eff} _{soil}	effective diffusion coefficient	[m ² ·d ⁻¹]	Equation R.16-69
FR _a .soil	mass fraction of the substance in the air phase of soil	[-]	Equation R.16-72
FR _w .soil	mass fraction of the substance in the water phase of soil	[-]	Equation R.16-70
FR _s .soil	mass fraction of the substance in the solid phase of soil	[-]	Equation R.16-71
F _{air} _{soil}	volume fraction of air in the soil compartment	[m _{air} ³ ·m _{soil} ⁻³]	Table R.16-11
F _{water} _{soil}	volume fraction of water in the soil compartment	[m _{water} ³ ·m _{soil} ⁻³]	Table R.16-11
F _{solid} _{soil}	volume fraction of solids in the soil compartment	[m _{solid} ³ ·m _{soil} ⁻³]	Table R.16-11
K _{air-water}	air-water partitioning coefficient	[m ³ ·m ⁻³]	Equation R.16-12
K _{soil-water}	soil-water partitioning coefficient	[m ³ ·m ⁻³]	Equation R.16-13
DIFF _{gas}	molecular diffusivity of the substance in the gas phase	[m ² ·d ⁻¹]	Equation R.16-73
DIFF _{water}	molecular diffusivity of the substance in the water phase	[m ² ·d ⁻¹]	Equation R.16-74
SOLID _{adv} .soil	rate of advective downward transport of soil particles	[m·d ⁻¹]	6.34·10 ⁻¹²
SOLID _{diff} .soil	solid phase diffusion coefficient in the soil compartment	[m ² ·d ⁻¹]	6.37·10 ⁻¹²
kas _{soil}	partial mass-transfer coefficient at soil side at the air-soil interface	[m·d ⁻¹]	

The maximum value for the penetration depth (*dp*) is set to 1 metre for all the three soil types on the regional scale. The minimum depth is set to the default soil depth ([Table R.16-14](#)).

Water-air interface

The partial mass transfer coefficients of the air-water interface depend on the windspeed of the system and the molecular weight of the substance:

$$kaw_{air} = 0.01 \cdot (0.3 + 0.2 \cdot WINDSPEED) \cdot \left(\frac{0.018}{MOLW}\right)^{0.335} \quad \text{EQUATION R.16-74}$$

$$kaw_{water} = 0.01 \cdot (0.0004 + 0.0004 \cdot WINDSPEED^2) \cdot \left(\frac{0.032}{MOLW}\right)^{0.25} \quad \text{EQUATION R.16-75}$$

Explanation of symbols		
MOLW	molecular weight of the substance	[kg·mol ⁻¹]
WINDSPEED	average windspeed	[m·d ⁻¹]
kaw _{air}	partial mass-transfer coefficient at the air side of the air-water interface	[m·d ⁻¹]
kaw _{water}	partial mass-transfer coefficient at the water side of the air-water interface	[m·d ⁻¹]

[Table R.16-14](#)

PEC regional for the marine environment

The impact of substances on the marine situation that are released from point and diffuse sources over a wider area can be assessed in a similar way as for the freshwater environment.

To assess the potential impacts of multiple point and diffuse sources of substances on the marine environment a river plume in coastal sea water is considered as a marine regional generic environment as follows:

An area of coastal sea that receives all the water from the rivers from the regional system. This seawater compartment is exchanging chemical with the continental seawater compartment by dispersion and advection (a current of seawater flowing in a certain direction). The size of the coastal compartment is 40 km long, 10 km wide and 10 m deep. In addition to the input from the regional river water it receives 1% of the direct emissions from the inland sources which is supposed to represent a relevant fraction of the sources that are located near the sea and also have direct emissions into the sea compartment. Most of the relevant characteristics of the coastal compartment are similar to the freshwater compartment apart from the suspended matter concentration that is set to 5 mg/l. In the absence of specific information (e.g. from marine simulation tests) it is assumed that the biodegradation rate in the water column is approximately three times lower than in freshwater.

This scenario can be modelled with a multi-media fate model that is used for the freshwater PEC calculations, modified to allow dispersive exchange between the coastal zone to the continental sea water. By default, mixing of river water into the coastal sea gives a dilution factor of approximately 10. As a result concentrations in coastal seawater are expected to be a factor of 10 (for conservative chemicals) or more (for chemicals that react, volatilize or sediment) lower than in river water. The extent of degradation, volatilization, etc. in this coastal sea scenario is also incorporated in the multi-media model.

The calculation of PEC_{regional,marine} according to this standard scenario may be sufficient for generic risk assessment. If additional information is available on sources and emissions and site-specific information on the suspended matter concentration, the flow rate and the dispersion velocity, the generic assessment can be made more site-specific by overriding some of the default parameters or can even be replaced by site-specific models. The dispersion velocity greatly affects all calculated concentrations, while in addition the suspended matter content further affects the dissolved concentration in seawater for chemicals with a high log K_{ow}. For the marine environment, models are available that can be used to assess the concentrations in certain specific compartments (bays, estuaries, regions) of the marine environment to which specific industrial sites discharge wastewater.

Model parameters for the continental concentration

The continental box covers all 15 EU countries and Norway and similar percentages for water and natural, agricultural and industrial/urban soils as given in [Table R.16-14](#). All other parameters are similar to the ones given in the preceding tables. Emission estimation to this continental box should be based on the EU-wide production volume of the substance. The resulting concentrations in water and air must be used as background concentrations (i.e. concentrations in water or air that enter the system) in the regional model. When the model is built according to [Figure R.16-11](#) it is assumed that no inflow of the substance into the continental system takes place. More recent versions of multimedia models do also contain so-called global scales for different temperature regions, for instance moderate, tropic and arctic (see e.g. Brandes et al., 1996). In this case the continent is embedded in the moderate scale just like the region is embedded in the continent. The size of the total global scale is that of the northern hemisphere. The global scales allow for a more accurate estimation of continental concentrations although this effect tends to be marginal. However, the global scales provide more insight in the ultimate persistence of the chemical.

Table R.16-16 Parameters for continental model

Parameter	Value in continental model
area of the continental system	3.56.10 ⁶ km ²
area fraction of water	0.03
area fraction of natural soil	0.60
area fraction of agricultural soil	0.27
area fraction of industrial/urban soil	0.10

R.16.5.6.9 Decision on the environmental concentrations used for exposure estimation

When PECs have been derived from both measured data and calculation, they are compared. If they are not of the same order of magnitude, analysis and critical discussion of divergences are important steps for developing an environmental risk assessment of existing substances. The following cases can be distinguished:

- Calculated PEC ≈ PEC based on measured concentrations

The result indicates that the most relevant sources of exposure were taken into account. For risk characterisation, the value with the highest confidence should be used;

- Calculated PEC > PEC based on measured concentrations

This result might indicate that relevant elimination processes were not considered in the PEC calculation or that the employed model was not suitable to simulate the real environmental conditions for the regarded substance. On the other hand measured data may not be reliable or represent only the background concentration or PEC_{regional} in the regarded environmental compartment. If the PEC based on measured data has been derived from a sufficient number of representative samples then they should override the model predictions. However if it cannot be

demonstrated for the calculated PEC that the scenario is not unrealistically worst-case, the calculated PEC should be preferred.

- Calculated PEC < PEC based on measured concentrations

This relation between calculated PEC and PEC based on measured concentrations can be caused by the fact that relevant sources of emission were not taken into account when calculating the PEC, or that the used models were not suitable. Similarly, an overestimation of degradation of the compound may be the explanation. Alternative causes may be spillage, a recent change in use pattern or emission reducing measures that are not yet reflected in the samples.

If it is confirmed that the PEC based on measured concentrations is still representative for the exposure situation of the substance further work is needed to elucidate the exposure situation. Other reasons might cause the described divergence:

- there is a transboundary influx;
- a natural source exists;
- the compound represents a metabolite of another substance;
- a retarded remobilisation results from a pool present in other environmental compartments (e.g. from scrap or waste materials or former applications).

If the measured values have passed the procedure of critical statistical and geographical evaluation, a high degree of confidence can be attributed to those data and they shall overwrite the calculated PECs. It is necessary to consider all environmental compartments when the measurements and predictions are made otherwise the possibility of chance agreement may be overlooked.

R.16.5.7 Predators (secondary poisoning)

R.16.5.7.1 Output

The output of the calculations are predicted concentration in the food for the predators, i.e. the concentration in worms and fish.

R.16.5.7.2 Input

For fish-eating predators, the local and regional PECs for surface water (Sections [R.16.5.6.2](#) and [R.16.5.6.4](#)), BCF for fish and BMF₁/BMF₂ (Section [R.16.4.3.5](#)) are needed.

For worm-eating predators, the PEC for soil (Section [R.16.5.6.6](#)) and BCF for worms (Section [R.16.4.3.5](#)) are needed.

Assessment whether exposure route is relevant

The first step in the assessment strategy is to consider whether there are indications for bioaccumulation potential. These indications have been discussed in Section [R.16.4.3.5](#).

Subsequently, it is necessary to consider whether the substance has a potential to cause toxic effects if accumulated in higher organisms. This assessment is based on classifications on the basis of mammalian toxicity data, i.e. the classification Very Toxic (T+) or Toxic (T) or harmful (Xn) with at least one of the risk phrases R48 “Danger of serious damage to health by prolonged exposure”, R60 “May impair fertility”, R61 “May cause harm to the unborn child”, R62 “Possible risk of

impaired fertility”, R63 “Possible risk of harm to the unborn child”, R64 “May cause harm to breastfed babies”. Here it is assumed that the available mammalian toxicity data can give an indication on the possible risks of the chemical to higher organisms in the environment.

The current, either qualitative or quantitative, approach in the human health risk assessment for genotoxic carcinogens is not practicable in the environmental part. Tumor incidence rates for a genotoxic carcinogen and subsequent cancer risks are related to individual risks in man and it is in most cases difficult to link those effects to populations. Endangered species might be an exception, particularly those characterized by long-life-cycles where individuals may need to be protected to support survival of the species.

It is not unlikely, however, that the conservative approach followed in the risk assessment for man indirectly exposed via the environment for genotoxic substances, will also be protective for individual top predators.

If a substance is classified accordingly or if there are other indications (e.g. endocrine disruption), an assessment of secondary poisoning should be performed.

Fish-eating predators

A schematic view of the assessment scheme for the exposure route water → aquatic organisms → fish → fish-eating mammal or fish-eating bird described above is given in [Figure R.16-12](#).

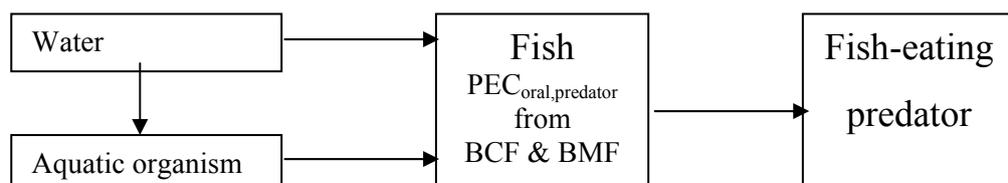


Figure R.16-12 Assessment of secondary poisoning

No specific assessment of the risk to fish as a result of the combined intake of contaminants from water and contaminated food (aquatic organism) is considered necessary as this is assumed to be covered by the aquatic risk assessment and the risk assessment for secondary poisoning of fish-eating predators.

The risk to the fish-eating predators (mammals and/or birds) is calculated as the ratio between the concentration in their food ($PEC_{oral,predator}$) and the no-effect-concentration for oral intake ($PNEC_{oral}$). The concentration in fish is a result of uptake from the aqueous phase and intake of contaminated food (aquatic organisms). Thus, $PEC_{oral,predator}$ is calculated from the bioconcentration factor (BCF) and a biomagnification factor (BMF). Note that $PEC_{oral,predator}$ could also be calculated for other relevant species that are part of the food of predators.

The details of the individual assessment steps are described in the following sections.

Calculation of a predicted environmental concentration in food

The concentration of contaminant in food (fish) of fish-eating predators ($PEC_{oral,predator}$) is calculated from the PEC for surface water, the measured or estimated BCF for fish and the biomagnification factor (BMF):

$$PEC_{oral,predator} = PEC_{water} \cdot BCF_{fish} \cdot BMF \quad \text{EQUATION R.16-76}$$

Explanation of symbols		
$PEC_{oral,predator}$	Predicted Environmental Concentration in food	$[\text{mg} \cdot \text{kg}_{\text{wet fish}}^{-1}]$
PEC_{water}	Predicted Environmental Concentration in water	$[\text{mg} \cdot \text{l}^{-1}]$
BCF_{fish}	bioconcentration factor for fish on wet weight basis	$[\text{l} \cdot \text{kg}_{\text{wet fish}}^{-1}]$
BMF	biomagnification factor in fish	$[-]$

The BMF is defined as the relative concentration in a predatory animal compared to the concentration in its prey ($BMF = C_{predator}/C_{prey}$). The concentrations used to derive and report BMF values should, where possible, be lipid normalised.

An appropriate PEC_{water} reflecting the foraging area of fish-eating mammals and birds should be used for the estimate. The foraging area will of course differ between different predators, which makes it difficult to decide on an appropriate scale. For example use of PEC_{local} may lead to an overestimation of the risk as fish-eating birds or mammals do also forage on fish from other sites than the area around the point of discharge. Also, biodegradation in surface water is not taken into account using PEC_{local} . However, using $PEC_{regional}$ may have the opposite effect, as there may be large areas in the region with higher concentrations. It has therefore been decided that a scenario where 50% of the diet comes from a local area (represented by the annual average PEC_{local}) and 50% of the diet comes from a regional area (represented by the annual average $PEC_{regional}$) is the most appropriate for the assessment.

Marine fish-eating predators and marine top-predators

The principal endpoints for the secondary poisoning assessment are the predators and top predators that prey on organisms that are in direct contact with the marine aqueous phase and receive the substances from this source. A relatively simple food chain is modelled which consists of the marine water phase, marine food, marine fish and two separate levels of predators. This food chain is visualised in [Figure R.16-13](#). As can be seen from this scheme risks for three different trophic levels need to be assessed:

1. *risks to marine fish:* No specific calculation needs to be performed for estimating the risk to marine fish as this is covered by the risk assessment for aquatic organisms.
2. *risks to marine predators:* The risk to marine predators is calculated as the ratio between the concentration in their food (marine fish) and the no-effect concentration for oral intake ($PNEC_{oral,predator}$). The concentration in the marine fish (C_{fish}) is obtained from bioconcentration of the substance from the aqueous phase and (for very hydrophobic substances) as a result of bioaccumulation from the food the fish consumes (which consists of different types of aquatic organisms). Therefore, both a bioconcentration factor (BCF) and a biomagnification factor (BMF_1) are used to calculate C_{fish} . Note that for the BCF_{fish} also information for other organisms such as mussels may be considered.
3. *risks to marine top predators:* The risk to marine top-predators is calculated as the ratio between the concentration in their food (marine predators) and the no-effect concentration for oral intake ($PNEC_{oral,top predator}$). Since very hydrophobic substances may biomagnify in the

tissue and organs of the predator, for the calculation of the internal concentration of the predator an additional biomagnification factor (BMF_2) must be applied. Note that no additional BMF factor for the top predator itself is required since the comparison between PEC_{oral} and PNEC_{oral} is not based on internal concentrations but on intake rates.

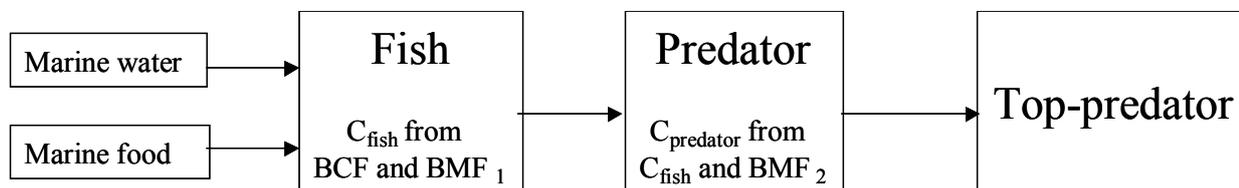


Figure R.16-13 Secondary poisoning food chain

Assessment of secondary poisoning via the aquatic food chain

It should be recognised that the schematic aquatic food chain water → aquatic organism → fish → fish-eating bird or mammal is a very simplistic scenario as well as the assessment of risks for secondary poisoning based on it. Any other information that may improve the input data or the assessment should therefore be considered as well. For substances where this assessment leads to the conclusion that there is a risk of secondary poisoning, it may be considered to conduct additional laboratory tests (e.g. tests of bioaccumulation in fish or feeding studies with laboratory mammals or birds) in order to obtain better data.

The simplified food chain is only one example of a secondary poisoning pathway. Safe levels for fish-eating animals do not exclude risks for other birds or mammals feeding on other aquatic organisms (e.g. mussels and worms). Therefore it is emphasised that the proposed methodology gives only an indication that secondary poisoning is a critical process in the aquatic risk characterisation of a chemical.

For a more detailed analysis of secondary poisoning, several factors have to be taken into account (US EPA, 1993; Jongbloed et al., 1994):

- differences in metabolic rates between animals in the laboratory and animals in the field;
- normal versus extreme environmental conditions: differences in metabolic rate under normal field conditions and more extreme ones, e.g. breeding period, migration, winter;
- differences in caloric content of different types of food: cereals versus fish, worms or mussels. As the caloric content of fish is lower than cereals birds or mammals in the field must consume more fish compared to cereals for the same amount of energy needed leading to a higher body burden of the pollutant;
- pollutant assimilation efficiency: differences in bioavailability in test animals (surface application of a test compound) and in the field (compound incorporated in food) and/or;
- relative sensitivity of animals for certain chemicals: differences in biotransformation of certain compounds between taxonomic groups of birds or mammals. The US EPA uses a species sensitivity factor (SSF) which ranges from 1 to 0.01.

Whether these factors should be used is still under debate.

Assessment of secondary poisoning via the terrestrial food chain

Biomagnification may also occur via the terrestrial food chain. A similar approach as for the aquatic route can be used here. The food-chain soil → earthworm → worm-eating birds or mammals is used as has been described by Romijn et al. (1994).

Since birds and mammals consume worms with their gut contents and the gut of earthworms can contain substantial amounts of soil, the exposure of the predators may be affected by the amount of substance that is in this soil. The $PEC_{oral, predator}$ is calculated as:

$$PEC_{oral, predator} = C_{earthworm} \quad \text{EQUATION R.16-77}$$

where $C_{earthworm}$ is the total concentration of the substance in the worm as a result of bioaccumulation in worm tissues and the adsorption of the substance to the soil present in the gut.

For PEC_{soil} the PEC_{local} is used in which with respect to sludge application the concentration is averaged over a period of 180 days (see Section [R.16.5.6.6](#)). The same scenario is used as for the aquatic food chain, i.e. 50% of the diet comes from PEC_{local} and 50% from $PEC_{regional}$.

Gut loading of earthworms depends heavily on soil conditions and available food (lower when high quality food like dung is available). Reported values range from 2-20 % (kg dwt gut/kg wwt voided worm), 10% can therefore be taken as a reasonable value. The total concentration in a full worm can be calculated as the weighted average of the worm's tissues (through BCF and porewater) and gut contents (through soil concentration):

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} \cdot W_{earthworm} + C_{soil} \cdot W_{gut}}{W_{earthworm} + W_{gut}} \quad \text{EQUATION R.16-78}$$

Explanation of symbols

$PEC_{oral, predator}$	Predicted Environmental Concentration in food	$[\text{mg} \cdot \text{kg}_{\text{wet earthworm}}^{-1}]$
$BCF_{earthworm}$	bioconcentration factor for earthworms on wet weight basis	$[\text{L} \cdot \text{kg}_{\text{wet earthworm}}^{-1}]$
$C_{earthworm}$	concentration in earthworm on wet weight basis	$[\text{mg} \cdot \text{kg}_{\text{wet earthworm}}^{-1}]$
$C_{porewater}$	concentration in porewater	$[\text{mg} \cdot \text{L}^{-1}]$
C_{soil}	concentration in soil	$[\text{mg} \cdot \text{kg}_{\text{wwt}}^{-1}]$
$W_{earthworm}$	weight of earthworm tissue	$[\text{kg}_{\text{wwt tissue}}]$
W_{gut}	weight of gut contents	$[\text{kg}_{\text{wwt}}]$

The weight of the gut contents can be rewritten using the fraction of gut contents in the total worm:

$$W_{gut} = W_{earthworm} \cdot F_{gut} \cdot CONV_{soil} \quad \text{EQUATION R.16-79}$$

where:

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid} \cdot RHO_{solid}} \quad \text{EQUATION R.16-80}$$

Explanation of symbols

CONV _{soil}	conversion factor for soil concentration wet-dry weight soil	[kg _{wwt} · kg _{dwt} ⁻¹]	
F _{solid}	volume fraction of solids in soil	[m ³ · m ⁻³]	Table R.16-11
F _{gut}	fraction of gut loading in worm	kg _{dwt} · kg _{wwt} ⁻¹	0.1
RHO _{soil}	bulk density of wet soil	[kg _{wwt} · m ⁻³]	Equation R.16-22
RHO _{solid}	density of solid phase	[kg _{dwt} · m ⁻³]	Table R.16-11

Using this equation, the concentration in a full worm can be written as:

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} + C_{soil} \cdot F_{gut} \cdot CONV_{soil}}{1 + F_{gut} \cdot CONV_{soil}} \quad \text{EQUATION R.16-81}$$

When measured data on bioconcentration in worms is available the BCF factors can be inserted in the above equation. For most substances, however, these data will not be present and BCF will have to be estimated. For organic chemicals, the main route of uptake into earthworms will be via the interstitial water. Bioconcentration can be described as a hydrophobic partitioning between the pore water and the phases inside the organism and can be modelled according to the following equation as described by Jager (1998):

$$BCF_{earthworm} = (0.84 + 0.012K_{ow}) / RHO_{earthworm} \quad \text{EQUATION R.16-82}$$

where for RHO_{earthworm} by default a value of 1 (kg_{wwt} · L⁻¹) can be assumed.

Jager (1998) has demonstrated that this approach performed very well in describing uptake in experiment with earthworms kept in water. For soil exposure, the scatter is larger and the experimental BCFs are generally somewhat lower than the predictions by the model. The reasons for this discrepancy are unclear but may include experimental difficulties (a lack of equilibrium or purging method) or an underestimated sorption.⁸

Earthworms are also able to take up chemicals from food and it has been hypothesized that this process may affect accumulation at $\log Kow > 5$ (Belfroid et al., 1995). The data collected by Jager (1998), however, do not indicate that this exposure route actually leads to higher body residues than expected on the basis of simple partitioning. Care must be taken in situations where the food of earthworms is specifically contaminated (e.g. in case of high concentrations in leaf litter) although reliable models to estimate this route are currently lacking.

The model was supported by data with neutral organic chemicals in soil within the range $\log Kow$ 3-8 and in water-only experiments from 1-6. An application range of 1-8 is advised and it is reasonable to assume that extrapolation to lower Kow values is possible. The model could also be used for chlorophenols when the fraction in the neutral form was at least 5% and when both sorption and BCF are derived from the Kow of the neutral species. The underlying data are however too limited to propose this approach in general for ionised chemicals.

R.16.5.8 Humans exposed indirectly via the environment

R.16.5.8.1 Introduction

Indirect exposure of humans via the environment may occur by consumption of food (fish, crops, meat and milk) and drinking water, inhalation of air and ingestion of soil. The different routes of exposure are illustrated in [Figure R.16-14](#).

Exposure via soil ingestion and dermal contact is not addressed in this guidance because they represent significant exposure routes only for specific situations of soil pollution. The indirect exposure is assessed by estimating the total daily intake of a substance based on the predicted environmental concentrations for (surface) water, groundwater, soil and air.

⁸ According to certain studies some soil ingesting organisms may accumulate chemical substances not only from the soil pore water but also directly (possibly by extraction in the digestive tract) from the fraction of the substance adsorbed onto soil particles. This may become important for strongly adsorbing chemicals, e.g. those with a $\log Kow > 3$. For these compounds the total uptake may be underestimated. In other studies however it has been shown that soil digesters virtually only bioaccumulate the substance via the pore water, i.e. bioconcentrate chemical substances from the soil pore water. At present the latter process can be modelled by use of the equilibrium partitioning theory

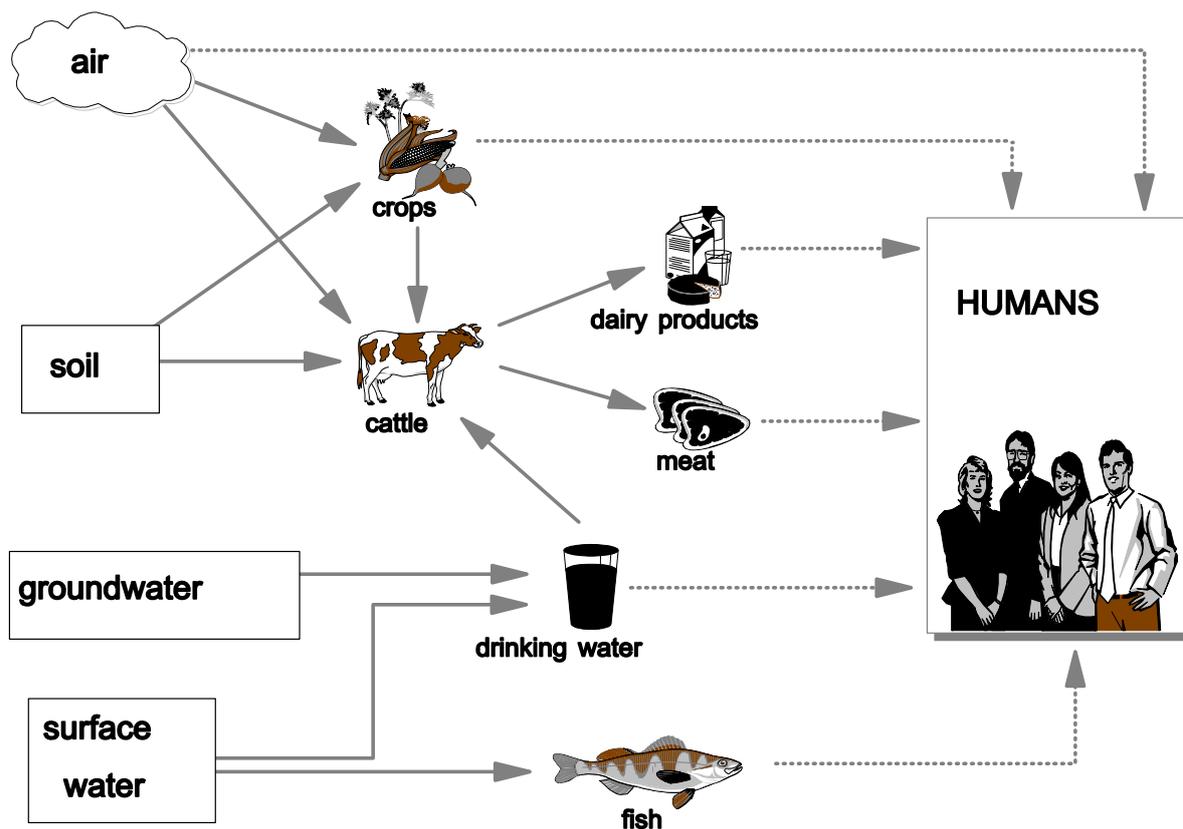


Figure R.16-14 Schematic representation of the exposure routes considered in human exposure

The calculation methods described serve primarily for screening purposes. The concentrations in the environmental compartments which are required as input data in the models for the calculation of the total daily intake via the different exposure routes should be derived on the basis of monitoring data and/or modelling by applying the approaches described in [Section R.16.5](#). The concentration of a substance in food is related to its concentration in water, soil and air and to its potential for bioaccumulation and its biotransfer behaviour. The models for the estimation of daily intake allow the use of local or regional environmental concentrations, as appropriate. The methods require the use of a limited number of input parameters and can, if required, be adapted for specific human populations for which it may be necessary to assess the exposure separately. Standard default values for the input parameters are presented.

Human behaviour shows an appreciable amount of variation between the different EU countries. But also within countries, large deviations occur between individuals. As a consequence, indirect exposure will vary greatly over the population we seek to protect. The choice of the exposure scenario will have a major influence on the result of the assessment. This choice will always be a compromise as a scientifically sound solution is extremely difficult to obtain (this would involve elaborate statistical evaluation of human sourcing and mobility behaviour, as well as the distribution and intensity of all local sources).

Indirect exposure is principally assessed on two spatial scales: locally near a point source of the substance, and regionally using averaged concentrations over a larger area. In the local assessment, all food products are derived from the vicinity of one point source, in the regional assessment, all food products are taken from the regional model environment. It should be noted that the local and

regional environments are not actual sites or regions, but standardised environments as defined in Section [R.16.5.4](#) and Section [16.5.6.8](#). Clearly, the local scale represents a worst-case situation. People do not consume 100% of their food products from the immediate vicinity of a point source.

Therefore, the local assessment represents a situation which does not exist in reality. However usually, one or two routes dominate the total exposure and local exposure through these routes may not be unrealistic. In contrast, the regional assessment represents a highly averaged exposure situation which cannot insure protection of individuals who consume food products from the vicinity of point sources. A regional assessment gives an indication of potential average exposure of the inhabitants of the region. In light of the above mentioned limitations, it is clear that a generic indirect exposure estimation, as required in this framework, can only be used to indicate potential problems. The assessment should be seen as a helpful tool for decision making and not as a prediction of human exposure actually occurring at some place or time.

For an indirect exposure estimation on EU-level, a standard consumption pattern needs to be defined. Food consumption rates and patterns differ between EU Member States so it is impossible to select an average or worst-case EU country. To account for the fact that intake rates vary between countries, for each food product, the highest country-average consumption rate of all member states will be used. This will of course lead to a total food basket which is an unrealistic, worst-case scenario. In practice however, usually only one or two routes form the bulk of the indirect exposure. The fact that in the exposure scenario worst-case intake through other routes also occurs is therefore negligible. This makes this scenario appropriate as a first approach to indicate possible concern. The outcome of this assessment is comparable to assessing all countries separately (using average intakes), and taking the highest exposure level of all countries.

It should be noted that extreme consumers of certain food products are not accounted for. Taking extreme consumption into account would lead to more severe worst-case local assessments since the entire food basket is already derived for 100% from the local standard environment.

In a case where the regional assessment indicates reason for concern, there is a clear need for refinement of the assessment. In cases where the local assessment does not indicate a potential risk, there is no reason for concern. The situation is less clear in the grey area where a regional assessment does not give reason for concern, but the local assessment does. It should be noted that there is no testing strategy triggered by the indirect exposure estimation. Instead, when there is reason for concern in the local assessment only, a further analysis of the major exposure routes is required to investigate the realism of the local exposure scenario. As the most important routes are indicated by the assessment, this provides a clear starting point for refinement.

R.16.5.8.2 Output

The output of the calculations is regional and local total human doses via the environment of the substance. These values are to be compared with the DNEL values for external exposure.

R.16.5.8.3 Input

The data needed for the calculations are PEC-values derived in the distribution calculation (section 8.3-8.4). The needed PEC-values are given in [Table R.16-17](#).

In addition to the data required for the environmental exposure estimation (see [Section R.16.5](#)), the bioconcentration factor (BCF), soil accumulation factors (BSAFs), human intake rates of crops, milk and meat are required. Default values for the latter (from EUSES) are given in [Table R.16-18](#).

Table R.16-17 Environmental concentrations used as input for indirect exposure calculations

Compartment	Local assessment	Regional assessment
surface water	annual average concentration after complete mixing of STP-effluent	steady-state concentration in surface water
air	annual average concentration at 100 m from source or STP (maximum)	steady-state concentration in air
agricultural soil	concentration averaged over 180 days after 10 years of sludge application and aerial deposition	steady-state concentration in agricultural soil
porewater	concentration in porewater of agricultural soil as defined above	steady-state concentration in porewater of agricultural soil
groundwater	concentration in porewater of agricultural soil as defined above	steady-state concentration in porewater of agricultural soil

Table R.16-18 Human daily intake of food and water (from EUSES)

Food	Intake
Drinking water	2 l/d
Fish	0.115 kg/d
Leaf crops (incl. Fruit and cereals)	1.2 kg/d
Root crops	0.384 kg/d
Meat	0.301 kg/d
Dairy products	0.561 kg/d

Assessment whether indirect exposure route is relevant

Assessment of indirect exposure is generally only conducted if:

- the tonnage >1,000 t/y or
- the tonnage >100 t/Y and the substance is classified
 - as “Toxic” with a risk phrase “R48”; or
 - as a carcinogen or mutagen (of any category); or
 - as toxic to reproduction (category 1 or 2).

Assessment of the concentrations in intake media (food, water, air and soil)

Currently, the scenario for indirect human exposure cannot take into account exposure from aquatic organisms apart from fish, because to date an internationally validated bioaccumulation standard test is only available for fish and consumption data on aquatic organisms other than fish are scarce.

A general description of the different relevant exposure routes and guidance for the assessment of the resulting indirect exposure is given in the following sections.

R.16.5.8.4 Exposure via the environmental compartmentsExposure via inhalation of air

This exposure route can contribute significantly to the total exposure for volatile compounds.

The concentration in the intake medium (air) can be calculated with distribution models of Section [R.16.5.6.1](#).

Only the intake scenario chosen has important consequences on exposure through this route. It is proposed to follow a worst case, but transparent, scenario: continuous, chronic exposure of humans to the air concentration (which is assumed constant). Exposure through inhalation will be summed with exposure through oral routes.

Exposure via soil ingestion and dermal contact

These exposure routes will not be handled in this context while exposure through these routes is usually very unlikely. Only in cases of extremely polluted soils (e.g. in dump sites or through calamities) can these routes provide significant contributions to the total exposure.

Exposure via drinking water

Drinking water can be prepared from surface water or from groundwater. Groundwater can be contaminated through leaching from the soil surface, surface water can be polluted through direct or indirect emission. Hrubec and Toet (1992) evaluated the predictability of the fate of organic substances during drinking water treatment. One of their conclusions was that groundwater treatment, which is generally not intended for removal of organic substances, can be neglected. The accuracy of the predicted removal efficiencies for surface water treatment is rather low. This is mainly due to uncertainties in the most effective treatment processes (such as activated carbon filtration).

R.16.5.8.5 Exposure via food consumption

Assessing concentrations in food products (in this context fish, leaf crops, root crops, meat and dairy products) in initial or intermediate screening stages usually involves calculation of bioconcentration (BCF) or biotransfer factors (BTF). These are defined as the external exposure (as a concentration or a dose) divided by the internal concentration in the organisms. The use of fixed factors implies that these factors describe a steady-state situation in which the exposure period is assumed long enough to reach a steady-state.

It should be noted that reliable (and relevant) experimental bioconcentration factors are always preferred above estimated factors.

Bioconcentration in fish

Fish, residing in contaminated surface water, are able to take up appreciable amounts of (especially lipophilic) substances through the gills or through their food. The concentration in fish may be orders of magnitude greater than the concentration in water. The bioconcentration factor in fish is found to be well correlated with the octanol-water partitioning coefficient (K_{ow}), indicating that lipid or fat is the main dissolving medium. The estimation of fish-water bioconcentration is more specifically discussed in Section [R.16.4.3.5](#).

Biotransfer from soil and air to plants

Plant products form a major part of the food products for humans and cattle. Contamination of plants will therefore have significant influence on the exposure of humans. When trying to predict concentrations in plant tissues, one will immediately encounter several important conceptual problems:

- there are hundreds of different plant species forming the heterogenous group of food crops. Furthermore, varietal differences can also account for large differences;
- different tissues from plants are consumed (roots, tubers, fruit, leaves);
- crops differ in contaminant exposure, many crops are for instance grown in greenhouses;
- crops can be exposed through uptake from the soil, but also through gas uptake and aerial deposition.

From the above it may be clear that a modelling approach can only give a rough approximation of the concentrations in plants. To account for the predicted variety in plant products, it is proposed to distinguish between tuberous plants and leaf crops. Furthermore, the exposure of plants should include the soil route, as well as the air route.

Uptake from soil is, in general, a passive process governed by the transpiration stream of the plant (in case of accumulation in leaves) or physical sorption (in case of roots). Uptake into the leaves from the gaseous phase can be viewed as a passive process, in which the leaves components (air, water, lipids) equilibrate with the air concentration. A general form of steady state partitioning, coefficient) between these compartments is given by Riederer (1990). K_{ow} and K_{aw} (the air-water partitioning coefficient) are used to assess the distribution between the air and the plant. It is proposed to use the modelling approach of Trapp and Matthies (1995) to estimate levels in leaves and roots due to uptake from soil and air.

Biotransfer to meat and milk

Lipophilic substances are known to accumulate in meat, and can be subsequently transferred to milk. Cattle can be exposed to substances in grass (or other feed) with adhering soil, drinking water, and through inhalation of air. Biotransfer factors can be defined as the steady-state concentration in meat, divided by the daily intake of the substance. Travis and Arms (1988) calculated biotransfer factors for cow's meat and milk by log-linear regression on a number of substances (28 for milk and 36 for beef).

Even though the theoretical background is limited, these factors provide a useful tool in risk assessment. It is proposed to use the same exposure estimates for air and crops which have been derived for human exposure for cattle, and the same soil concentration as for plants.

It should be noted that no distinction is made between different milk products like cheese or yoghurt. For all dairy products, the concentration in milk is used.

R.16.5.8.6 Total daily intake for humans

If concentrations in the intake media are calculated, the total daily intake of humans can be estimated from the daily intake rate of each medium by summing the contribution of each medium.

R.16.6 Tools based on models presented in section R.16.5**R.16.6.1 EUSES**

EUSES (2.0.3) and a manual to the program can freely be downloaded from the internet (<http://ecb.jrc.it/euses>) and can be run on a normal PC. EUSES can be used for the environmental exposure estimation with the release estimation from Section [R.16.2](#). Besides the release estimation, only a few data on substance properties are needed to calculate PECs at Tier 1. If the use of default exposure estimates do not lead to a conclusion of safe use in the first tentative ES, a higher Tier assessment is possible by including more specific information on releases (Section [R.16.2](#)) and improved data on substance properties.

The parameters used for the emission estimates using **ERC** are available as standard files (in excel) for each ERC, to be loaded into EUSES for PEC derivation.

Input (Tier 1 assessment)

For Tier 1 assessments of environmental distribution, the information described in [Table R.16-19](#) should be collected (more information on fate may be needed for inorganic substances).

Table R.16-19 Information requirements for Tier 1 assessment of environmental distribution

Parameter	Description	Source
MOLW	Molecular weight	Technical dossier – chapter 2
MP	Melting point of substance	Technical dossier– chapter 7
BP	Boiling point of substance	Technical dossier– chapter 7
VP	Vapour pressure of substance	Technical dossier– chapter 7
SOL	Water solubility of substance	Technical dossier– chapter 7
KOW	Octanol water partition coefficient of substance	Technical dossier– chapter 7 (not inorganics)
Kpsoil	Soil-water partition coefficient. As a default, EUSES calculates the parameter on the basis of KOW. For inorganic substances however, Kpsoil should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role.	Technical dossier –adsorption-desorption screening – chapter 9 See also Section R.16.4.3.3
Kpsed	Sediment-water partition coefficient. As a default, EUSES calculates the parameter on the basis of KOW. For inorganic substances however, Kpsed should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role.	Technical dossier –adsorption-desorption screening– chapter 9 See also Section R.16.4.3.3
Kpsusp	Solids-water partition coefficient in suspended matter. As a default, EUSES calculates the parameter on the basis of KOW. For inorganic substances however, Kpsusp should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role.	Technical dossier –adsorption-desorption screening– chapter 9 See also Section R.16.4.3.3
Biodegradability	Results of screening test on biodegradability. Not relevant for inorganic substances.	Technical dossier– chapter 9 See also Sections R.16.4.4.4 , R.16.4.4.5 , R.16.4.4.7
Ej,local	Local emission to compartment j (j: water, air, soil). May be based on fraction of main source ($F_{\text{mainsource}}$) and number of emission days (T_{emission}), M/I_volume, and release fractions	Release estimation based on use scenario See Section R.16.2
Eij,regional	Regional emission from source i to compartment j (j: water, air, soil)}	Release estimation based on exposure scenario See Section R.16.2

Output

The output of the Tier 1 consists of the predicted environmental concentrations (PECs) for environmental risk assessment (see [Table R.16-20](#)). EUSES can prepare an electronic report of all the input and output data in a Word or Excel format. It is not possible to print a report in a selected format, e.g., where only data for the Tier 1 assessment are shown.

Nevertheless, it is possible to program a macro in Word or Excel that can select the lines containing the information needed for the safety assessment

Table R.16-20 EUSES – output: Predicted environmental concentrations, PECs

	Parameter	Destination
PECstp	Concentration in the aeration tank of the sewage treatment plant	Assessment of whether the substance may inhibit processes in the STP
PEClocal.air,ann	Annual average local PEC in air (total)	
PEClocal.water	PEC in surface water during episode	Risk assessment fresh water
PEClocal.water,ann	Annual average local PEC (dissolved)	Secondary poisoning
PEClocal.water,marine	PEC in marine water during episode	Risk assessment marine water
PEClocal.water,ann,marine	Annual average local PEC in marine surface water (dissolved)	Secondary poisoning
PEClocal.sed	PEC in sediment	Risk assessment fresh water Secondary poisoning
PEClocal.sed,marine	PEC in marine sediment	Risk assessment marine water
PEClocal.agric,30	Local PEC in agricultural soil (total) averaged over 30 days	Risk assessment terrestrial environment
PEClocal.agric,180	Local PEC in agricultural soil (total) averaged over 180 days (to calculate concentration in crops)	Secondary poisoning Indirect exposure of humans
PEClocal.grass,180	Local PEC in grassland (total) averaged over 180 days	Secondary poisoning Indirect exposure of humans
PECreg.water,tot	Regional PEC in surface water (total)	Risk assessment fresh water Secondary poisoning Indirect exposure of humans
PECreg.seawater,tot	Regional PEC in seawater (total)	Risk assessment marine water Secondary poisoning Indirect exposure of humans
PECreg.air	Regional PEC in air (total)	
PECreg.agric	Regional PEC in agricultural soil (total)	Risk assessment terrestrial environment Secondary poisoning Indirect exposure to man
PECreg.natural	Regional PEC in natural soil (total)	Risk assessment terrestrial environment Secondary poisoning
PECreg.ind	Regional PEC in industrial soil (total)	
PECreg.sed	Regional PEC in sediment (total)	Risk assessment fresh water
PECreg.seased	Regional PEC in seawater sediment (total)	Risk assessment marine water

How to run EUSES

A Tier 1 assessment of environmental exposure using EUSES is discussed in Part D.5.5.

R.16.6.2 Tier 1 and higher Tiers: TGD excel sheet

The TGD excel sheet (EU TGD 2003 Risk Assessment Spreadsheet Model) can be obtained free of charge from the Radboud University Nijmegen (<http://www.envsci.science.ru.nl/cem-nl/products.html>) and can be run on a normal PC.

The TGD excel sheet may be an alternative of using EUSES, which was described in the previous section. The tool can only be used for environmental exposure estimation and the assessment of Man exposed via the environment. The TGD excel sheet and EUSES are based on the models and equations provided in [Section R.16.5](#).

How to use the TGD excel model

A Tier 1 environmental exposure assessment using the TGD excel sheet is explained in the accessory files that can be downloaded from the link indicated in [Section R.16.6.3](#).

R.16.6.3 EUSES and TGD excel sheet - Refinement options

EUSES or TGD excel sheet calculations may be improved by refining some of the input data. [Table R.16-21](#) gives an overview of some of the possible improvements.

Table R.16-21 Determinants and input information for refined assessment

Determinant	Description
Koc	Organic carbon water partition coefficient In Tier 1 estimated from log Kow Used for estimation of 1 Kpsusp (solids-water partition coefficient in suspended matter) 2 Kpsed (solids-water partition coefficient in sediment) 3 Kpsoil (solids-water partition coefficient in soil) 4 Kpsludge (solids-water partition coefficient in sewage sludge)
HENRY	Henrys law constant. In Tier 1 estimated from VP, SOL and MOLW. For highly water soluble substances this may give wrong estimates of HENRY
k _{bio} _{stp}	Rate constant for biodegradation in STP. In Tier 1 estimated from Biodegradability
k _{bio} _{water}	Rate constant for biodegradation in bulk surface water. In Tier 1 estimated from Biodegradability
k _{deg} _{soil} k _{deg} _{sed}	Total rate constant for biodegradation in bulk soil and sediment. In Tier 1 estimated from Biodegradability
DT50 _{hydr} _{water}	Half-life for hydrolysis in water at the temperature of the data set
DT50 _{photo} _{water}	Half-life for photolysis in water at the temperature of the data set
DT50 _{air}	Half life for degradation in air at the temperature of the data set
STP defaults	In Tier 1, the predicted removal of the substance in the sewage treatment plant is based on a number of parameters describing the STP. For local assessments, these predictions may be improved by using actual settings for the local STP.
DILUTION	Dilution factor. A default dilution factor for discharges to a coastal zone (marine environment) of 100 and 10 for fresh water is assumed. Higher dilution factor can be applied if this can be founded by site-specific information (better dilution capacity of receiving water, lower discharge rate).

R.16.7 Other tools for environmental exposure estimation

R.16.7.1 FOCUS-models (surface water, agricultural soil)

If your substance is applied in a way similar to a pesticide, for example as a fertilizer, the modelling suite proposed by FOCUS can be an alternative to EUSES/TGD excel for this specific use.

FOCUS is an abbreviation for FORum for the Co-ordination of pesticide fate models and their USE. The organisation is an initiative of the European Commission to harmonise the calculation of predicted environmental concentrations (PEC) of active substances of plant protection products (PPP) in the framework of the EU Directive 91/414/EEC.

FOCUS has recommend a number of models to be used for

Soil and ground water exposure estimation: MACRO, PEARL, PELMO, PRZM_GW

Surface water exposure estimation

- STEP1-2, which is a screening tool to assess whether there is a risk to fresh water living organism)
- SWASH, which is a higher tier tool combining tools for leaching, drift, run-off, and fate in surface water

All tools together with documentation and manuals can be downloaded for free from: <http://viso.jrc.it/focus/index.html>.

R.16.7.2 CHARM

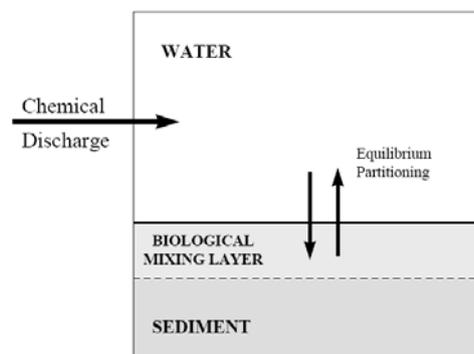
If your substance is applied in an offshore installation, the CHARM model can be an alternative to EUSES/TGD excel for this specific use.

CHARM has been developed for risk assessment at a screening level of offshore chemicals, e.g. “drilling” and “production” chemicals. or “completion/workover”.

Since offshore drilling and production of oil and gas may result in environmental effects, it was decided to control the use and discharge of chemicals in the North Sea OSPAR area. Some of the participating countries within the framework of the Oslo and Paris Conventions agreed upon the development of a Harmonised Mandatory Control System (PARCOM Decision 96/3, now OSPAR Decision 2000/2). In this Control System, CHARM is referred to as a model for calculations leading to a ranking of chemicals on the basis of the PEC/PNEC ratios.

Long term exposure of persistent and bioaccumulative substances cannot be assessed by CHARM, neither inorganic substances.

Most of the calculations within CHARM are concerned with the estimation of the concentration of a chemical in the waste stream, and different models are used in dependence of the process in which it is used, the dosage of the chemical, its partitioning characteristics, the oil (or condensate) and water production at the platform, the in-process degradation mechanisms and the residence time before release. Within CHARM the offshore environment is divided into two compartments: water and sediment. This is done in order to acknowledge the fact that a chemical present in the environment will partition between the water and organic matrix in the sediment. This is illustrated in Figure xx. The concentration of a chemical may, therefore vary greatly from one compartment to another. Consequently, two PEC values are calculated: PEC_{water} and PEC_{sediment}.



For further details see for example <https://www.ogp.org.uk/pubs/CHARMManualFeb05.pdf>

R.16.7.3 Emission scenario documents for biocides

If your substance is applied in a way similar to a specific type of biocide, for example in liquid cooling systems (product type 11) or as protection coating (e.g. product type 8 or 10), the release estimation may be based on the information from the emission scenario documents for biocidal active substances.

A complete list of currently available ESDs is available under: <http://ecb.jrc.it/biocides/>

REFERENCES

- Belfroid A, Seinen W, van Gestel K, Hermens J and van Leeuwen K (1995). Modelling the accumulation of hydrophobic organic chemicals in earthworms. Application of the equilibrium partitioning theory. *Environ. Sci. Pollut. Res.* **2**, 5-15.
- Brandes LJ, den Hollander H, van de Meent D (1996). SimpleBox 2.0: a Nested Multimedia Fate Model for Evaluating the Environmental Fate of Chemicals. National Institute of Public Health and Environmental Protection (RIVM), RIVM Report 719101 029, Bilthoven, The Netherlands.
- BUA (1992). OH Radicals in the Troposphere. GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance, BUA Report 100, April 1992.
- De Greef J and de Nijs ACM (1990). Risk Assessment of New Chemical Substances. Dilution of effluents in the Netherlands. National Institute of Public Health and Environmental Protection (RIVM), RIVM Report 670208001, Bilthoven, The Netherlands.
- Den Hollander HA, van de Meent D (2004). Model parameters and equations used in SimpleBox 3.0. National Institute for Public Health and the Environment. Report No. 601200 003, RIVM Bilthoven, The Netherlands.
- Di Toro DM, Zarba CS, Hansen DJ, Berry WJ, Schwarz RC, Cowan CE, Pavlou SP, Allen HE, Thomas NA, Paquin PR (1991). Technical basis of establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. *Environ. Toxicol. Chem.* **10**, 1541-1583.
- EC (1999). Study on the Prioritisation of Substances Dangerous to the Aquatic Environment: II Assessment of Options of the Statistical Treatment and Evaluation of Monitoring Data within the COMMPS Procedure. Office for Official Publications of the EC, Luxembourg.
- ECETOC (1994). Environmental Exposure Assessment. European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Technical Report No. 61, Brussels.
- EU (2003). Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market.
- Esser HO and Mosser P (1982). An appraisal of problems related to the measurement and evaluation of bioaccumulation. *Ecotox. Env. Saf.* **6**, 131-148..
- Finizio A, Mackay D, Bidleman T and Hamer T (1997). Octanol-air partition coefficient as a predictor of partitioning of semi-volatile organic chemicals to aerosol. *Atmospheric Environment* **30**, 2289-2296.
- Heijna-Merkus E and Hof M (1993). Harmonisation of Model Parameters. National Institute of Public Health and
- Hollander A, Hessels L, De Voogt P, Van de Meent D (2004).. Implementation of depth-dependent soil concentrations in multimedia mass balance models. *SAR and QSAR in Environmental Research* **15**, 457-468.
- Hollander A, Baijens I, Ragas A, Huijbregts M, Van de Meent D (2006). Validation of predicted exponential concentration profiles of chemicals in soils. *Environmental Pollution* **147**, 757-763.
- Hrubeč, J. and C. Toet, 1992. Predictability of the removal of organic compounds by drinking water treatment. RIVM report 714301007. National Institute for Public Health and the Environment, Bilthoven, Netherlands.
- Jager T (1998). Mechanistic approach for estimating bioconcentration of organic chemicals in earthworms (Oligochaeta). *Environmental Toxicology and Chemistry* **17**(10), 2080-2090.
- Jongbloed RH, Pijnenburg J, Mensink BJWG, Traas TP and Luttik R (1994). A Model for Environmental Risk Assessment and Standard Setting Based on Biomagnification. Top Predators in Terrestrial Ecosystems. National Institute of Public Health and Environmental Protection (RIVM). RIVM Report 71901012, Bilthoven, The Netherlands.
- Junge CE (1977). **In:** Fate of Pollutants in the Air and Water Environment. Suffet IH (ed), Wiley Interscience, New York, NY, 7-25.
- Lewis R (1997). Dispersion in Estuaries and Coastal Waters. John Wiley & Sons Publishers, Chichester, UK, p. 312.
- Mackay D (1991). Multimedia Environmental Models. Lewis Publishers, Chelsea, MI, USA.

Mackay D, Paterson S, Shiu WY (1992). Generic models for evaluating the regional fate of chemicals; *Chemosphere* **24**(6), 695-717.

Mikkelsen J (1995). Fate Model for Organic Chemicals in an Activated Sludge Wastewater Treatment Plant - Modification of SimpleTreat. National Environmental Research Institute, Denmark. Prepared for the Danish EPA.

OECD (1992). Screening Assessment Model System (SAMS), Version 1.1. Organisation for Economic Cooperation and Development (OECD), Paris.

OECD (2000). Report of the OECD Workshop on Improving the Use of Monitoring Data in the Exposure Assessment of Industrial Chemicals. Organisation for Economic Cooperation and Development (OECD), OECD Environmental Health and Safety Publications, Series on Testing and Assessment No. 18, Paris.

OECD (2001). Guidance Document on the Use of the Harmonized System for the Classification of Chemicals which are Hazardous for the Aquatic Environment. Organisation for Economic Cooperation and Development (OECD), OECD Environmental Health and Safety Publications, Series on Testing and Assessment, No. 27.

OSPAR (2000a). Decision 2000/2 on a Harmonised Mandatory Control System for the Use and Reduction of the Discharge of Offshore Chemicals, OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic.

OSPAR (2000b). Decision 2000/3 on the Use of Organic Phase Drilling Fluids and the Discharge of OPF-Contaminated Cuttings. OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic.

Pedersen F, Kristensen P, Damborg A and Christensen HW (1994). Ecotoxicological Evaluation of Industrial Wastewater. Ministry of the Environment, Danish Environmental Protection Agency, Miljøprojekt Nr. 254, pp. 80-81.

Riederer (1990). Estimating partitioning and transport of organic chemicals in foliage/atmosphere system: discussion of a fugacity-based model. *Environ. Sci. Technol.* **24** (1990), pp. 829–837.

Romijn CFAM, Luttk R, Canton JH (1994). Presentation of a general algorithm to include effect assessment on secondary poisoning in the derivation of environmental quality criteria. Part 2. Terrestrial food chains. *Ecotox. Environ. Saf.* **27**, 107-127.

Schwarzenbach RP, Gschwend PM and Imboden DM (1993). *Environmental Organic Chemistry*. Wiley-Interscience, New York, NY.

Struijs J, Stoltenkamp J, Van De Meent D (1991). A Spreadsheet-based Model to Predict the Fate of Xenobiotics in a Municipal Wastewater Treatment Plant. *Wat. Res.* **25**(7), 91-900.

Toet C and de Leeuw FAAM (1992). Risk Assessment System for New Chemical Substances: Implementation of atmospheric transport of organic compounds. National Institute of Public Health and Environmental Protection (RIVM), RIVM Report No. 679102 008, Bilthoven, The Netherlands.

Trapp, S., Matthies, M. (1995). Generic One-Compartment Model for the Uptake of Organic Chemicals by Foliar Vegetation. *Environ. Sci. Technol.* **29**(9) 2333-2338. Generic One-Compartment Model and Erratum (1996), **30**, 360.

Travis C.C. & D.D. Arms (1988): Bioconcentration of Organics in beef, milk and vegetation. *Environ. Sci. Technol.*, **22**(3), 271-274.

Van de Meent D (1993). Simplebox: a Generic Multimedia Fate Evaluation Model. National Institute of Public Health and the Environment (RIVM), RIVM Report No. 672720 001, Bilthoven, The Netherlands.

Van Jaarsveld JA (1990). An operational atmospheric transport model for Priority Substances; specifications and instructions for use. National Institute of Public Health and the Environment (RIVM), RIVM Report No. 222501002, Bilthoven, The Netherlands.

Xie WH, Shiu WY and Mackay D (1997). A review of the effects of salts on the solubility of organic compounds in seawater. *Marine Env. Res.* **44**, 429-444.

Appendix R.16-1- Environmental Release Categories
Table R.16-22 Name, description and background of Environmental Release Categories

ERC NUMBER	Name	Description	NOTES
ERC1	Production of chemicals	Production of organic and inorganic substances in chemical, petrochemical, primary metals and minerals industry including intermediates, monomers using continuous processes or batch processes applying dedicated or multi-purpose equipment, either technically controlled or operated by manual interventions	1
ERC2	Formulation of preparations	Mixing and blending of substances in (chemical) preparations in all types of industries such as paints and do-it-yourself products, pigment paste, fuels, household products (cleaning products), lubricants etc.	2
ERC3	Formulation in materials	Mixing or blending of substances, which will be physically or chemically bound into or onto a matrix (material) such as plastics additives in master batches or plastic products. For instance a plasticizers or stabilizers in pvc-master batches or products, crystal growth regulator in photographic films etc.	2
ERC4	Industrial use of processing aids	Industrial use of processing aids in continuous processes or batch processes applying dedicated or multi-purpose equipment, either technically controlled or operated by manual interventions. For example, solvents used in chemical reactions or the ‘use’ of solvents during the application of paints, lubricants in metal working fluids, anti-set off agents in polymer moulding/casting	3,4
ERC5	Industrial use resulting in inclusion into or onto a matrix	Industrial use of substances (non-processing aids), which will be physically or chemically bound into or onto a matrix (material) such as binding agent in paints and coatings or adhesives, dyeing of textile fabrics and leather products, metal plating and galvanizing.	3
ERC6A	Industrial use of intermediates	Use of intermediates in primarily the chemical industry using continuous processes or batch processes applying dedicated or multi-purpose equipment, either technically controlled or operated by manual interventions, for the synthesis (manufacture) of other substances. For instance the use of chemical building blocks (feedstock) in the synthesis of agrochemicals, pharmaceuticals, monomers etc.	4

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ERC NUMBER	Name	Description	NOTES
ERC6B	Industrial use of reactive processing aids	Industrial use of reactive processing aids in continuous processes or batch processes applying dedicated or multi-purpose equipment, either technically controlled or operated by manual interventions. For example the use of bleaching agents in the paper industry.	4
ERC6C	Production of plastics	Industrial use of monomers in the production of plastics (thermoplastics), polymerization processes. For example the use of vinyl chloride monomer in the production of pvc	4
ERC6D	Production of resins/rubbers	Industrial use of chemicals (cross-linking agents, curing agents) in the production of thermosets and rubbers, polymerization processes. For instance the use of styrene in polyester production or vulcanization agents in the production of rubbers	4
ERC 7	Industrial use of substances in closed systems	Industrial use of substances in closed systems. Use in closed equipment, such as the use of liquids in hydraulic systems, cooling liquids in refrigerators and lubricants in engines and dielectric fluids in electric transformers and oil in heat exchangers.	5
ERC8A	Wide dispersive indoor use of processing aids in open systems	Indoor use of processing aids by the public at large or professional use. Use (usually) results in direct release into the environment, for example, detergents in fabric washing, machine wash liquids and lavatory cleaners, automotive and bicycle care products (polishes, lubricants, de-icers), solvents in paints and adhesives or fragrances and aerosol propellants in air fresheners.	3,5,6
ERC8B	Wide dispersive indoor use of reactive substances in open systems	Indoor use of reactive substances by the public at large or professional use. Use (usually) results in direct release into the environment, for example, sodium hypochlorite in lavatory cleaners, bleaching agents in fabric washing products, hydrogen peroxide in dental care products	4,6

ERC NUMBER	Name	Description	NOTES
ERC8C	Wide dispersive indoor use resulting in inclusion into or onto a matrix	Indoor use of substances (non-processing aids) by the public at large or professional use, which will be physically or chemically bound into or onto a matrix (material) such as binding agent in paints and coatings or adhesives, dyeing of textile fabrics.	3,6
ERC8D	Wide dispersive outdoor use of processing aids in open systems	Outdoor use of processing aids by the public at large or professional use. Use (usually) results in direct release into the environment, for example, automotive and bicycle care products (polishes, lubricants, de-icers, detergents), solvents in paints and adhesives.	3,6,7
ERC8E	Wide dispersive outdoor use of reactive substances in open systems	Outdoor use of reactive substances by the public at large or professional use. Use (usually) results in direct release into the environment, for example, the use of sodium hypochlorite or hydrogen peroxide for surface cleaning (building materials)	4,6
ERC8F	Wide dispersive outdoor use resulting in inclusion into or onto a matrix	Outdoor use of substances (non-processing aids) by the public at large or professional use, which will be physically or chemically bound into or onto a matrix (material) such as binding agent in paints and coatings or adhesives.	3,6
ERC9A	Wide dispersive indoor use of substances in closed systems	Indoor use of substances by the public at large or professional (small scale) use in closed systems. Use in closed equipment, such as the use of cooling liquids in refrigerators, oil-based electric heaters.	5,6
ERC9B	Wide dispersive outdoor use of substances in closed systems	Outdoor use of substances by the public at large or professional (small scale) use in closed systems. Use in closed equipment, such as the use of hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids in automotive brake systems.	5,6

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ERC NUMBER	Name	Description	NOTES
ERC10A	Wide dispersive outdoor use of long-life articles and materials with low release	Low release of substances included into or onto articles and materials during their service life from outdoor use, such as metal, wooden and plastic construction and building materials (gutters, drains, frames etc.)	6,8
ERC10B	Wide dispersive outdoor use of long-life articles and materials with high or intended release	Substances included into or onto articles and materials with high or intended release during their service life from outdoor use. Such as tires, treated wooden products, treated textile and fabric like sun blinds and parasols and furniture, zinc anodes in commercial shipping and pleasure craft, and brake pads in trucks or cars.	6,7,9
ERC11A	Wide dispersive indoor use of long-life articles and materials with low release	Low release of substances included into or onto articles and materials during their service life from indoor use. For example, flooring, furniture, toys, construction materials, curtains, footwear, leather products, paper and cardboard products (magazines, books, news paper and packaging paper), electronic equipment (casing)	6,8
ERC11B	Wide dispersive indoor use of long-life articles and materials with high or intended release	Substances included into or onto articles and materials with high or intended release during their service life from indoor use. For example: release from fabrics, textiles (clothing, floor rugs) during washing	6,7,8

Notes

General note on Emission factors

For each environmental release class the emission factors are based on the highest emission factors available for representative use patterns. A use pattern represents the use of a chemical that has its specific function during a process within a certain type of industry or sector or has a specific function in a material or article. The highest emission factors have been selected from general release information from EC (2003) for selected representative cases. In the design of the ERCs it is assumed that no risk management measures are included.

General note on regional and local scale

For industrial production, formulation and use only the local scale is considered. The highest emissions and concentrations are to be expected at the local scale for these applications. In addition to the compartments air and water, soil is also taken into account on the regional scale for the scenarios that refer to wide dispersive and outdoor use (ERC 8d-f, 9b, 10a and 10b).

For wide dispersive use (large number of small point sources) to the contrary the regional scale is the most relevant as emissions result from the use by the public at large, i.e. households or small scale professional use. For local release to waste water ('the standard town' scenario), the sewage treatment plant (STP) has to be considered as well. Therefore a general local release is defined, which should be applied to all release classes covering wide dispersive use and emissions to waste water (ERC 8-11).

1) Production of chemicals

The emission factors are based on the information for the production of basic chemicals and chemicals used in synthesis (including monomers and catalysts). Besides basic (organic) chemicals both the production of chemicals in petrochemical industry and metal extraction and refining industry are included. Emission factors are derived from the general emission factors for the production of chemicals provided by (EC, 2003).

2) Formulation

For the life cycle stage formulation a distinction is made between mixing en blending of substances (processing aids) in preparations like liquids, pastes or (compressed) gases for instance in aerosol cans, and on the other hand processes of mixing, which result into inclusion on a matrix, for instance in the plastics industry. To meet the requirements of specific applications for plastics materials the polymers are blended or mixed with various types of additives, including fillers, pigments, plasticizers etc. In the polymers industry this process of compounding takes place before conversion of the plastic material into finished arte facts. Often the process of compounding and conversion are performed as successive process steps at the same facility. Also the production of master batches, which are made up to contain high concentrations of specific additives, are also considered as a process of mixing and blending resulting in inclusion into or onto a matrix. The production of photographic films is also considered as formulation into a matrix. Emission factors are derived from the general emission factors for formulation from the (EC, 2003). The highest emissions factors for formulation resulting in inclusion into or onto a matrix have been selected for mixing of plastic additives, pigments, fillers and plasticizers with the polymer matrix (compounding) and the production of photographic films (EC, 2003).

3) Processing aids

Processing aids are substance facilitating a process and will usually not be consumed (reacted) or included into or onto a matrix. It should be stressed though that processing aids might be converted at high temperature processes like metal cutting and combustion of fuels (fuel additives). Processing aids are for instance detergents in fabric washing products, which facilitate the washing process and will be directly released to waste streams after use. Pigments or fillers in paints on the other hand will be included in the paint layer (matrix) after the painting process. Emission factors for industrial use of processing aids have been derived from the emission factor tables for industrial use of processing aids (processing). For each compartment the highest emission factors for this specific use pattern are taken from EC (2003) Besides the specific use of chemicals as processing aids, chemicals are also processed with the specific goal to be included into or onto a matrix (filler in paint or a dye of colouring textile). The highest emission factors for air and water for this specific type of use have been taken from EC (2003). In addition to industrial use emission factors have been derived for the use by the public at large (households) Emission factors for wide dispersive use of processing aids have been derived from EC (2003) for the sector personal or domestic use. For air the emission factor is set at 100% for instance to represent the use of propellants in aerosol cans and for water the emission factor is also set a 100% for instance for the use of cleaning and washing agents and surface-active agents in all kinds of cleaning products. The emission of these type of chemicals is assumed to be complete to either air or water.

4) Substances reacting on use

Substances reacting on use have been categorized into intermediates, reactive processing aids and monomers used in the polymers industry.

Reactive processing aids so far have not been covered in the default emission factors from the Guidance Document (EC, 2003). Several assumptions have been made to provide emission rates for air and water. Generally this type of substances are highly soluble in water and therefore release to air has been considered to be negligible and an emission factor of 0.1% has been assumed. A default halve life of 10 minutes has been assumed. For industrial use a residence time of 4 hours in a recirculation system has been assumed. For wide dispersive use a residence time of 1 hour has been assumed in the sewer (once-through system). Furthermore a distinction has been made between polymerization processes for the production of thermoplastics and thermosetting resins and polymer processing of rubbers and thermosetting resins (prepolymers) for the polymers industry. The emission factors for intermediates have been taken from available emission factors for the chemical industry and the specific use of intermediates in the synthesis of other chemicals. Emission factors for the use of monomers in the polymers industry have also been taken from EC (2003) for this specific type of use (polymerization processes). Emissions to air and water from the processing of rubbers and thermosetting resins are provided by EC (2003) (polymer processing) for the following type of chemicals; curing agents and cross-linking agents.

5) Release from closed systems

The emission factors have been based on leakage of cooling liquids from refrigerators and leakage of engine oil from cars. A leakage rate of 5% percent per year to air is assumed based on Matthijsen and Kroeze (1996) and Folkert and Peek (2001). The leakage rates include losses from recharging or filling of machinery but in general this is negligible compared to the annual losses (about 0.2% to air and 0,1% to water). Emission to soil and water is based on leakage rates for engine oil as this is thought to be a representative case for this type of use. Based on an average leakage rate, annual number of kilometres travelled per vehicle and the amount of engine oil per vehicle the emission factor can be calculated:

A leakage rate of 10 mg/km and a mileage of 20,000 km per year and 4 litres of engine oil per vehicle results in an emission factor of about 5% per year. The figures have been taken from Klein et al. (2004) and are in line with the figures provided by OECD (2004a). For hydraulic fluids leakage rates are very similar, they vary from 1% up to about 15% per year (two applications) for soil. For water leakage rates are somewhat lower about 0,5 up to 7 percent (OECD, 2004a). Because of the possible spills during use to (waste) water also for indoor use the emission to water has been accounted for.

6) Indoor and outdoor use

Industrial activities are primarily considered to be indoor processes, though many processes also may be executed outdoors. Therefore direct release to soil has not been considered for industrial use. Another reason for not considering soil for industrial activities is that industrial soil is not directly a protection goal in the risk assessment of chemicals. For the regional scale though besides the compartments air and water, soil is also taken into account for the scenarios that refer to wide dispersive and outdoor use in order to perform a proper estimation of the back ground concentration. Emission factors for the soil compartment for outdoor use of reactive processing aids refer to use by the public at large of cleaning products. For outdoor use of processing aids the emission factor for soil refers to private use (consumers) of solvents. For the outdoor use of substances, which results in inclusion into or onto a matrix, the emission factors have been taken for the private use of paints and specifically refers to substances like fillers and pigments

7) Complete release to air and water

As substance properties have not been accounted for in the environmental release classes, complete release for both the air and water compartment has been assumed. At two extremes a substance might either be highly soluble in water or very volatile to air. In case of highly soluble substance 100% release to water might be assumed, the same holds for non-water soluble and non-volatile compounds discharged to waste water. For very volatile substances 100% release to air might be assumed. Very volatile substances have a vapour pressure ≥ 1000 Pa. Without taking into account substance properties and disposal routes, the distribution between air and water can not be substantiated and therefore the highest values for release to both air and water have been taken. This does not only hold for the release classes with 100% release to both air and water but for all environmental release classes.

8) Release from articles/materials during service life, low release

Emission factors are taken from the OECD emission scenario document on plastic additives. The service life time has already been accounted for in the emission factors assuming a steady-state situation. For new substances recently placed on the market, there is no steady-state situation. Also the annual tonnage will change in the future depending on the growth-curve, before steady-state will be finally reached. For outdoor use the emission factor to air is 0.05% over the service life period, for water the emission factor is $0.16\% * T_{service\ life}$ over the service life time period. Thus for air the release does not depend on the service life time period but for soil the service life time period has to be taken into account. For the soil compartment the same emission factor as for water is used for outdoor use. The reasoning behind this assumption is that release might either occur to water or to soil for outdoor applications. For indoor use the emission factors are also taken from the OECD emission scenario document on plastic additives (OECD, 2004b).

9) Release from articles/materials during service life, high release

Emission factors are taken from the emission scenario document for textile processing industry, industrial category (IC) 13. The service life time has to be accounted for in determining the emission factors for soil and water. For outdoor use the emission factor to air is set at 100% per year (steady state situation), for water and soil the emission factor is also set at 100% assuming steady state and total release to the environment during the service life time period following the emission scenario document for the textile processing industry, IC 13 (EC, 2003). For the soil compartment the same emission factor as for water is used for outdoor use. The reasoning behind this assumption is that release might either occur to water or to soil for outdoor applications. For indoor use the same emission factors can be used for air and water. The soil compartment is considered not to be relevant.

Table R.16-23 Specification of the parameters for environmental release categories.

LCS = life cycle stage, STP = sewage treatment plant, PEC = predicted environmental concentration.

ERC	Lifecycle Stage	level of containment	type of use in LCS	Dispersion of emission sources	indoor/ outdoor	release promotion during service life	Amount of substance used as input to emission calculation ²	Fraction used by largest customer (main source)	Release time in days per year ³	With STP/Yes no	Default release to air	Default release to water from process	Default release to soil	Dilution to be applied for PEC derivation ¹⁰
1	Production	open-closed	na	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	5%	6%	n.a.	:10 (20.000 m ³ /d)
2	Formulation	open-closed	not included into matrix	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	2.5%	2%	n.a.	:10 (20.000 m ³ /d)
3	Formulation	open-closed	inclusion into/onto matrix	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	30%	0.2%	n.a.	:10 (20.000 m ³ /d)
4	Use	open-closed	processing aid	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	95% ⁴	100% ⁴	n.a.	:10 (20.000 m ³ /d)
5	Use	open-closed	inclusion into/onto matrix	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	50%	50%	n.a.	:10 (20.000 m ³ /d)
6a	Use	open-closed	intermediate	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	5%	2%	n.a.	:10 (20.000 m ³ /d)
6b	Use	open-closed	reactive processing aid	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	0.10%	5%	n.a.	:10 (20.000 m ³ /d)
6c	Use	open-closed	monomers for polymers	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	5%	5%	n.a.	:10 (20.000 m ³ /d)
6d	Use	open-closed	monomers for thermosets/rubbers	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	35%	0.005 %	n.a.	:10 (20.000 m ³ /d)
7	Use	closed system	processing aid	Industrial	indoor	na	100% M/I volume ¹	1	20	Yes/no	5% ⁵	5% ⁵	n.a.	:10 (20.000 m ³ /d)
8a	Use	open	processing aid	wide disperse	indoor	na	10% M/I volume	n.a.	365	80% with STP	100% ⁴	100% ⁴	n.a.	25x10 ⁹ (m ³ /year)
8b	Use	open	reaction on use	wide disperse	indoor	na	10% M/I volume	n.a.	365	80% with STP	0.10% ⁶	2% ⁷	n.a.	25x10 ⁹ (m ³ /year)
8c	Use	open	inclusion into/onto matrix	wide disperse	indoor	na	10% M/I volume	n.a.	365	80% with STP	15%	1%	n.a.	25x10 ⁹ (m ³ /year)

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8d	Use	open	processing aid	wide disperse	outdoor	na	10% M/I volume	n.a.	365	80% with STP	100% ⁴	100% ⁴	1%	25x10 ⁹ (m ³ /year)
8e	Use	open	reaction on use	wide disperse	outdoor	na	10% M/I volume	n.a.	365	80% with STP	0.10% ⁶	2% ⁸	1%	25x10 ⁹ (m ³ /year)
8f	Use	open	inclusion into/onto matrix	wide disperse	outdoor	na	10% M/I volume	n.a.	365	80% with STP	15%	1%	0.5%	25x10 ⁹ (m ³ /year)
9a	Use	closed systems	processing aid	wide disperse	indoor	na	10% M/I volume	n.a.	365	80% with STP	5% ⁵	n.a.	n.a.	25x10 ⁹ (m ³ /year)
9b	Use	closed systems	processing aid	wide disperse	outdoor	na	10% M/I volume	n.a.	365	80% with STP	5% ⁵	5% ⁵	5%	25x10 ⁹ (m ³ /year)
10a	Service life	open	inclusion into/onto matrix	wide disperse	outdoor	low	10% M/I volume	n.a.	365	80% with STP	0.05%	0.16% *Tservice%	0.16% *Tservice%	25x10 ⁹ (m ³ /year)
10b	Service life	open	inclusion into/onto matrix	wide disperse	outdoor	high or intended	10% M/I volume	n.a.	365	80% with STP	100% ⁹	100% ⁹	100%	25x10 ⁹ (m ³ /year)
11a	Service life	open	inclusion into/onto matrix	wide disperse	indoor	low	10% M/I volume	n.a.	365	80% with STP	0.05%	0.05%	n.a.	25x10 ⁹ (m ³ /year)
11b	Service life	open	inclusion into/onto matrix	wide disperse	indoor	high or intended	10% M/I volume	n.a.	365	80% with STP	100% ⁹	100% ⁹	n.a.	25x10 ⁹ (m ³ /year)
8-11	Use and service life; local wide dispersive			local STP for wide dispersive use	indoor/outdoor		10% M/I volume	0.2%	365	Yes	n.a.	see specific ERC 8-11		:10 (20.000 m ³ /d)

¹ If information on number of production sites, size distribution and geographic distribution is available the 10 % rule may be applied.

² If information on the market distribution is available the amount per use or process can be further specified.

³ Adjustment is possible when applied substance volume of the largest customer is known (see [Table R.16-24](#)). The default number of 20 emission days is only representative for the lower tonnages. At higher tonnages the calculated capacities in tonnage per day may be too high. For a more realistic estimate of the tonnage per day, [Table R.16-24](#) in this Appendix can be applied for the life cycle stages production, formulation and industrial use (ERCs 1-7). The default (fixed) number of emission days is 365 days per year for wide dispersive use (ERCs 8-11). For the life cycle stage formulation the relevant tonnage should be based on the fraction of the substance in the formulation (TONNAGE_{local} = TONNAGE/F_{formulation}).

⁴ Because a substance might be either highly soluble in water or highly volatile to air, releases are set to a maximum value for water and air.

⁵ includes losses from recharging or filling of machinery, otherwise it would be much lower (about 0.2% to air and 0,1% to water).

⁶ Because of high water solubility, emission is assumed to be negligible.

⁷ Based on DT50 = 10 min and a residence time of 4 hrs (recirculation)

⁸ Based on $DT50 = 10$ min and a residence time of 1 hrs for sewer.

⁹ Complete release during the service life time period has been assumed following the emission scenario document for the textile processing industry. Release might be to air, water or soil depending on the volatility of the substance and whether the article is used indoors or outdoors.

¹⁰ For a default local release to waste water, the average wastewater flow of 200 Liter per capita per day for a population of 10,000 inhabitants leads to a dilution volume of 20.000 m³/d. The default regional dilution volume is the sum of regional waste water flow and inflowing river water, see section R.16.5.6.8.

Table R.16-24 Number of emission days depending on tonnage and life cycle stages

Life cycle stage	Tonnage (local)	No. Of days
Production	< 1,000	20
	1,000-10,000	100
	>10,000	300
Formulation	<100	10
	100-2,000	100
	>2,000	300
Use	< 1,000	20
	1,000-5,000	100
	>5,000	300

REFERENCES

EC (2003). Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market.

OECD (2004a). Emission Scenario Document on lubricants and lubricant additives. OECD series on Emission Scenario Documents number 10

OECD (2004b). Emission Scenario Document on plastics additives. OECD series on Emission Scenario Documents number 3

R.J.M. Folkert and C.J. Peek (2001). Onderbouwing emissieprognose van de niet CO₂-broeikasgassen in de MV5. National Institute for Public Health and the Environment (RIVM), Bilthoven, The Netherlands. RIVM report no. 773001018 (in Dutch)

A.J.C.M. Matthijsen and C. Kroeze (1996). Emissies van HFK's, PFK's, FIK's en SF₆ in Nederland in 1990, 1994, 2000, 2005, 2010 en 2020. National Institute for Public Health and the Environment (RIVM), Bilthoven, The Netherlands. RIVM report no. 773001008 (in Dutch)

J. Klein et al. (2004). Methode voor de berekening van de emissies door mobiele bronnen in Nederland t.b.v. Emissiemonitor, jaarcijfers 2001 en ramingen 2002. Rapportagereeks Milieumonitor Nr. 13, februari 2004

Appendix R.16-2: Overview of OECD exposure scenario documents (ESDs).

ESD TITLE	NACE	IC	PT	REFERENCE	REMARKS
<i>Industrial manufacturing process/preparation type</i>					
Wood preservatives, part 1 , part 2 , part 3, part 4	16	15/0	8	OECD_1	BIOCIDAL PRODUCTS
Plastic additives	20.6/22.2	11	9	OECD_2	
Water treatment chemicals	20	2/3/6/12/15/0	2/5/11/12	OECD_3	
Photographic industry	20.5	10		OECD_4	
Rubber additives	22.1	11	9	OECD_5	
Textile finishing	13	13	9	OECD_6	
Leather processing	15	7	9	OECD_7	
Photoresist use in semiconductor manufacturing	26/27	4		OECD_8	
Lubricants and lubricant additives	24 E.O	8E.O	13E.O	OECD_9	
Automotive spray application	29/30	14	6/7	OECD_10	
Metal finishing	!	4/8/16/15/0		OECD_11	

ESD TITLE	NACE	IC	PT	REFERENCE	REMARKS
Antifoulants		15/0	21	OECD_12	BIOCIDAL PRODUCTS
Insecticides for stables and manure storage systems		15/0	18	OECD_13	BIOCIDAL PRODUCTS
Kraft pulp mills	17	12	12	OECD_14	
Non-integrated paper mills	17	12	12	OECD_15	
Recovered paper mills	17	12	12	OECD_16	
Chemical industry: chemicals used in synthesis	20.2/20.4/20.5/21	3		EU_1	
Personal/domestic and public domain		5/6		EU_1	
Leather processing industry		7	9	EU_1	
Metal extraction, refining and processing industry	24	8	13	EU_1	
Photographic industry		10		EU_1	
Pulp, paper and board industry		12	9	EU_1	
Textile processing industry		13	9	EU_1	
Paint, lacquers and varnishes industry		14	6/7	EU_1	

ESD TITLE	NACE	IC	PT	REFERENCE	REMARKS
Rubber industry		11	9	EU_1	
<i>Biocidal products</i>					
Human hygiene		5	1	EUB_1	
Private area and public health area disinfectants		5/6	2	EUB_2	
Drinking water disinfectants		6/15/0	5	EUB_3	
In-can preservatives		5/6/7/8/12/13/14	6	EUB_4	
Paper coating and finishing		12	6/7/9	EUB_5	
Film preservatives		14/11	7	EUB_6	
Wood preservatives		15/0	8	EUB_7	
Leather industry		7	9	EUB_8	
Textile processing industry		13	9	EUB_9	
Rubber polymerised materials preservatives		11	9	EUB_10	
Masonry preservatives	23.5/23.6	15/0	10	EUB_11	

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ESD TITLE	NACE	IC	PT	REFERENCE	REMARKS
Preservatives for liquid-cooling and processing systems		2/3/9	11	EUB_12	
Slimicides		12	12	EUB_13	
Metalworking fluid	25	8	13	EUB_14	
Rodenticides		1/5/6/15/0	14	EUB_15	
Avicides		1/6/15/0	15	EUB_16	
Insecticides for stables and manure		1	18	EUB_17	
Antifouling products		14/16/15/0	21	EUB_18	
Embalming and taxidermist fluids		15/0	22	EUB_19	

REFERENCES

- OECD 2004/D1: OECD Series on Emission Scenario Documents, No. 2, Emission Scenario Document for Wood Preservatives. OECD, Environment Directorate, 2003
- OECD 2004/D2: OECD Series on Emission Scenario Documents, No. 3, Emission Scenario Document on Plastics Additives. OECD, Environment Directorate, June 2004.
- OECD 2004/D3: OECD Series on Emission Scenario Documents, No. 4, Emission Scenario Document on Water Treatment Chemicals. OECD, Environment Directorate, June 2004.
- OECD 2004/D4: OECD Series on Emission Scenario Documents, No. 5, Emission Scenario Document on Photographic Industry. OECD, Environment Directorate, June 2004.
- OECD 2004/D5: OECD Series on Emission Scenario Documents, No. 6, Emission scenario document on Additives in Rubber Industry. OECD, Environment Directorate, June 2004.
- OECD 2004/D6: OECD Series on Emission Scenario Documents, No. 7, Emission Scenario Document on Textile Finishing Industry. OECD, Environment Directorate, June 2004.
- OECD 2004/D7: OECD Series on Emission Scenario Documents, No. 8, Emission Scenario Document on Leather Processing. OECD, Environment Directorate, June 2004.
- OECD 2004/D8: OECD Series on Emission Scenario Documents, No. 9, Emission Scenario Document on Photoresist Use in Semiconductor Manufacturing. OECD, Environment Directorate, June 2004.
- OECD 2004/D9: OECD Series on Emission Scenario Documents, No. 10, Emission Scenario Document on Lubricants and Lubricant Additives. OECD, Environment Directorate, November 2004.
- OECD 2004/D10: Series on Emission Scenario Documents, No. 11, Emission Scenario Document on Coating Application via Spray-painting in the Automotive Refinishing Industry. OECD, Environment Directorate, November 2004.
- OECD 2004/D11: OECD Series on Emission Scenario Documents, No. 12, Emission Scenario Document on Metal Finishing. OECD, Environment Directorate, November 2004.
- OECD 2006/D12: OECD Series on Emission Scenario Documents, No. 13, Emission Scenario Document on Antifouling Products. OECD, Environment Directorate, April 2005.
- OECD 2006/D13: OECD Series on Emission Scenario Documents, No. 14, Emission Scenario Document for Insecticides for Stables and Manure Storage Systems. OECD, Environment Directorate, January 2006.
- OECD 2006/D14: OECD Series on Emission Scenario Documents, No. 15, Emission Scenario Document on Kraft Pulp Mills. OECD, Environment Directorate, February 2006.
- OECD 2006/D15: OECD Series on Emission Scenario Documents, No. 16, Emission Scenario Document on Non-Integrated Paper Mills. OECD, Environment Directorate, February 2006.
- OECD 2006/D16: OECD Series on Emission Scenario Documents, No. 17, Emission Scenario Document on Recovered Paper Mills. OECD, Environment Directorate, February 2006.
- EU 2003: Technical guidance document in support of commission directive 93/67/EEC on risk assessment for new notified substances and commission regulation (EC) No 1488/94 on risk assessment for existing substances. Part I-III <http://ecb.jrc.it/cgi-bin/reframer.pf?A=ECB&B=/TGD/>

Appendix R.16-3: Fate of chemicals in a wastewater treatment plant based on the SimpleTreat model

The tables in this appendix provide values for the fate of substances that enter the sewage treatment plant, estimated according to the SimpleTreat 3.0 model (Struijs et al., 1996). The tables provide information on how much of a substance that enters the sewage treatment plant goes to air, surface water and to sewage sludge and how much is degraded. Separate tables are given depending on the categorization of a substance according to the results of screening biodegradation tests (see [Table R.16-6](#)).

The data in the tables have been obtained from calculations with the SimpleTreat 3.0 model with the following settings: the volume of wastewater is set at 200 l per capita per day in line with [Table R.16-12](#). Assuming that the total amount of solids in raw sewage produced per inhabitant per day is $0.150 \text{ (m}^{-3} \cdot \text{d}^{-1}) \cdot 0.6 \text{ (kg} \cdot \text{m}^{-3}) = 90 \text{ g}$ per inhabitant per day, the concentration of suspended matter in influent has been set to $0.45 \text{ (kg} \cdot \text{m}^{-3})$ (see [Table R.16-12](#)). In order to maintain the main characteristics of the sludge flow, the steady-state concentration of suspended solids in the primary settler has been set at 150 mg dry weight per l, implying that still 2/3 of the solids in raw sewage is separated by the primary settler. Consequently, settled sewage flowing from the primary settler into the aeration tank contains an oxygen requirement (R_o) of 176 mg BOD per l.

The mode of operation is defined by the input parameter sludge loading rate which specifies the BOD loading of the plant. The operation of the activated sludge reactor is largely specified by this parameter. This input parameter is in units of kg BOD per kg dry weight per day and is related to the sludge retention time (SRT) or sludge age and the hydraulic retention time (HRT). A medium sludge loading rate of $0.15 \text{ kg BOD kg}_{\text{dw}}^{-1} \cdot \text{d}^{-1}$ is used with a SRT of 9.2 d and an HRT of 7.1 hr.

SimpleTreat 3.0 contains a correction for stripping chemicals, as the process description is only valid for volatile chemicals ($H > 250 \text{ Pa} \cdot \text{m}^3 \cdot \text{mol}^{-1}$). The overall mass transfer coefficient during surface aeration (k_{surf}) was assumed proportional to the dissolved oxygen overall transfer rate coefficient (K_{LaO}), estimated from the oxygen requirement (R_o), hydraulic retention time (HRT) and the difference between the oxygen saturation and the actual O_2 concentration in the aerator (ΔO_2). In order to account also for the gas phase resistance ($H < 250 \text{ Pa} \cdot \text{m}^3 \cdot \text{mol}^{-1}$) the proportionality constant Ψ , still having the default value of 0.6, should be multiplied by a factor containing the dimensionless Henry constant (K_H) and the ratio of the mass transfer rate coefficients of a chemical in air and water. Munz and Roberts (1987) recommend to apply 40 as a default value for this ratio. As a result the first order rate constant for surface aeration is written as:

$$k_{\text{surf}} = \Psi \left(\frac{40 \cdot K_H}{40 \cdot K_H + 1} \right) \frac{R_o}{HRT \cdot \Delta O_2}$$

In the following tables H (Henry's law constant) should be used in $\text{Pa} \cdot \text{m}^3 \cdot \text{mol}^{-1}$.

a) No biodegradability

Fate of chemicals that are not degradable: $k_{bio_{stp}} = 0 \text{ hr}^{-1}$ in the aqueous phase of activated sludge.

		log H									
		% to air									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	2	15	64	91	95	95
	1	0	0	0	0	2	15	64	91	95	95
	2	0	0	0	0	2	15	64	91	94	95
	3	0	0	0	0	2	14	62	89	92	92
	4	0	0	0	0	1	12	52	77	80	80
	5	0	0	0	0	1	5	28	48	51	51
	6	0	0	0	0	0	1	9	23	27	27

		log H									
		% to water									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	100	100	100	100	98	85	36	9	5	5
	1	100	100	100	100	98	85	36	9	5	5
	2	99	99	99	99	97	84	36	9	5	5
	3	96	96	96	96	94	82	35	8	5	5
	4	79	79	79	79	77	68	30	8	5	4
	5	39	39	39	39	39	35	19	6	4	4
	6	15	15	15	15	15	14	11	6	4	4

		log H									
		% to sludge									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
	3	4	4	4	4	4	4	3	3	3	3
	4	21	21	21	21	21	20	18	16	15	15
	5	61	61	61	61	60	59	53	46	45	45
	6	85	85	85	85	85	85	80	71	69	69

		log H									
		% degraded									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	0	0	0	0	0	0	0	0	0	0
	3	0	0	0	0	0	0	0	0	0	0
	4	0	0	0	0	0	0	0	0	0	0
	5	0	0	0	0	0	0	0	0	0	0
	6	0	0	0	0	0	0	0	0	0	0

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% removal										
	0	0	0	0	0	2	15	64	91	95	95
	1	0	0	0	0	2	15	64	91	95	95
	2	1	1	1	1	3	16	64	91	95	95
	3	4	4	4	4	6	18	65	92	95	95
	4	21	21	21	21	23	32	70	92	95	96
	5	61	61	61	61	61	65	81	94	96	96
6	85	85	85	85	85	86	89	94	96	96	

b) Inherent biodegradability

Fate of chemicals that are “inherently biodegradable” in an OECD/EU test: $k_{bio_{stp}} = 0.1 \text{ hr}^{-1}$ in the aqueous phase of activated sludge.

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to air										
	0	0	0	0	0	1	10	50	85	91	91
	1	0	0	0	0	1	10	50	85	91	91
	2	0	0	0	0	1	10	50	85	90	91
	3	0	0	0	0	1	9	49	83	88	89
	4	0	0	0	0	1	8	41	72	77	77
	5	0	0	0	0	0	4	23	45	49	49
6	0	0	0	0	0	1	8	22	26	26	

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to water										
	0	59	59	59	59	58	52	28	8	5	5
	1	59	59	59	59	58	52	28	8	5	5
	2	59	59	59	59	58	52	27	8	5	5
	3	57	57	57	57	56	50	27	8	5	5
	4	48	48	48	48	48	43	24	7	5	4
	5	28	28	28	28	27	25	16	5	4	3
6	13	13	13	13	13	13	10	6	4	4	

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to sludge										
	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
	3	4	4	4	4	4	4	3	3	3	3
	4	19	19	19	19	19	19	17	16	15	15
	5	56	56	56	56	56	55	51	46	45	45
6	83	83	83	83	82	82	78	71	69	68	

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% degraded										
	0	41	41	41	41	41	38	22	7	4	4
	1	41	41	41	41	40	38	22	7	4	4
2	41	41	41	41	40	38	22	7	4	4	

3	39	39	39	39	39	37	21	6	4	4
4	33	33	33	33	32	31	18	6	4	3
5	17	17	17	17	16	16	10	4	2	2
6	4	4	4	4	4	4	4	2	1	1

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% removal	41	41	41	41	42	48	72	92	95	95
	0	41	41	41	41	42	48	72	92	95	95
	1	41	41	41	41	42	48	73	92	95	95
	2	43	43	43	43	44	50	73	92	95	95
	3	52	52	52	52	52	57	76	93	95	96
	4	72	72	72	72	73	75	84	95	96	97
	5	87	87	87	87	87	87	90	94	96	96

c) pass levels within 28 days in a test on “ready biodegradability”, 10-day window criterion is not fulfilled

Fate of chemicals that reach the biodegradation pass levels within 28 days in an OECD/EU test on “ready biodegradability but not within the 10 day time window: $k_{bio_{stp}} = 0.3 \text{ hr}^{-1}$ in the aqueous phase of activated sludge.

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to air	0	0	0	0	1	6	36	76	84	85
	0	0	0	0	0	1	6	36	76	84	85
	1	0	0	0	0	1	6	36	75	83	84
	2	0	0	0	0	1	6	35	73	81	82
	3	0	0	0	0	1	5	30	64	71	71
	4	0	0	0	0	0	3	17	40	45	46
	5	0	0	0	0	0	1	7	20	24	25

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to water	33	33	33	33	32	29	19	7	5	4
	0	33	33	33	33	32	29	19	7	5	4
	1	32	32	32	32	32	29	19	7	5	4
	2	32	32	32	32	31	29	18	7	5	4
	3	27	27	27	27	27	25	16	6	4	4
	4	18	18	18	18	17	16	12	5	3	3
	5	11	11	11	11	11	10	9	5	4	4

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
% to sludge											
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
	3	3	3	3	3	3	3	3	3	3	3
	4	17	17	17	17	17	17	16	16	15	15
	5	51	51	51	51	51	51	49	46	45	45
	6	79	79	79	79	79	78	76	70	68	68

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
% degraded											
log Kow	0	67	67	67	67	67	64	45	17	12	11
	1	67	67	67	67	67	64	45	17	12	11
	2	67	67	67	67	67	64	45	17	12	11
	3	65	65	65	65	65	62	44	17	11	11
	4	55	55	55	55	55	53	38	15	10	9
	5	31	31	31	31	31	30	22	9	6	6
	6	11	11	11	11	11	10	9	5	3	3

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% removal	67	67	67	67	68	71	81	93	95	96
	0	67	67	67	67	68	71	81	93	95	96
	1	67	67	67	67	68	71	81	93	95	96
	2	68	68	68	68	68	71	81	93	95	96
	3	68	68	68	68	69	71	82	93	95	96
	4	73	73	73	73	73	75	84	94	96	96
	5	82	82	82	82	83	84	88	95	97	97
6	89	89	89	89	89	90	91	95	96	96	

d) pass levels within 28 days in a test on “ready biodegradability”, 10-day window criterion is fulfilled

Fate of chemicals that are “readily biodegradable” in an OECD/EU test: $k_{bio_{stp}} = 1 \text{ hr}^{-1}$ in the aqueous phase of activated sludge.

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to air	0	0	0	0	0	3	19	55	66	68
	0	0	0	0	0	0	3	19	55	66	68
	1	0	0	0	0	0	3	19	54	66	67
	2	0	0	0	0	0	3	18	53	64	66
	3	0	0	0	0	0	3	16	46	56	57
	4	0	0	0	0	0	1	9	29	36	37
	5	0	0	0	0	0	1	4	15	20	20
6	0	0	0	0	0	1	4	15	20	20	

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to water	13	13	13	13	13	12	9	5	4	3
	0	13	13	13	13	13	12	9	5	4	3
	1	13	13	13	13	13	12	9	5	4	3
	2	13	13	13	13	12	12	9	5	4	3
	3	12	12	12	12	12	11	9	5	4	3
	4	11	11	11	11	11	10	8	4	3	3
	5	8	8	8	8	8	7	6	4	3	3
6	7	7	7	7	7	7	6	4	3	3	

		log H									
		-4	-3	-2	-1	0	1	2	3	4	5
log Kow	% to sludge	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	0	0	0	0	0	0	0	0	0	0
	3	3	3	3	3	3	3	3	3	3	3
	4	16	16	16	16	16	16	16	15	15	15
	5	47	47	47	47	47	47	46	45	45	45
6	72	72	72	72	72	72	71	69	67	67	

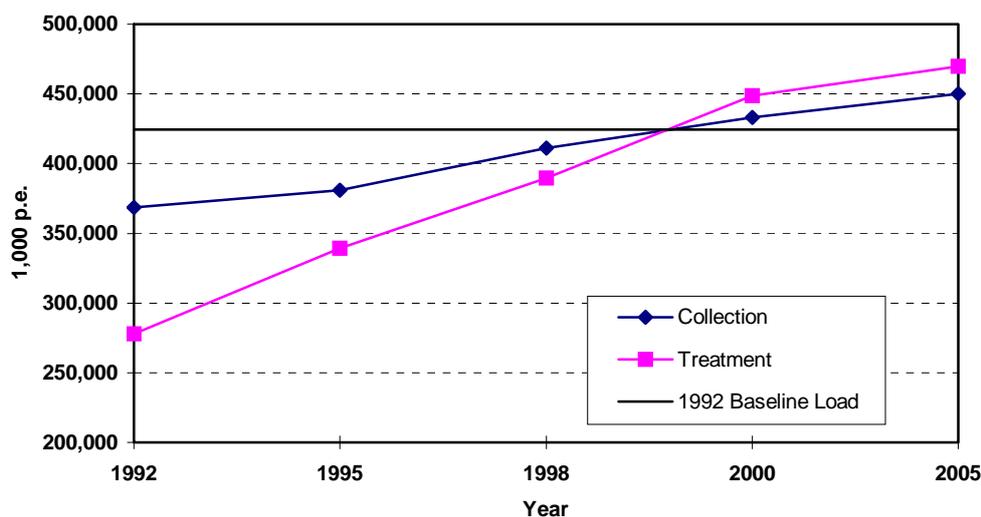
		log H										
		% degraded	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0		87	87	87	87	87	85	72	41	30	29
	1		87	87	87	87	87	85	72	40	30	29
	2		87	87	87	87	87	85	72	40	30	29
	3		85	85	85	85	84	82	70	39	29	28
	4		73	73	73	73	73	71	61	34	26	24
	5		45	45	45	45	45	44	38	22	17	16
	6		21	21	21	21	21	21	19	12	9	9

		log H										
		% removal	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0		87	87	87	87	87	88	91	95	96	97
	1		87	87	87	87	87	88	91	95	96	97
	2		87	87	87	87	88	88	91	95	96	97
	3		88	88	88	88	88	89	91	95	96	97
	4		89	89	89	89	89	90	92	96	97	97
	5		92	92	92	92	92	93	94	96	97	97
	6		93	93	93	93	93	93	94	96	97	97

Appendix R.16-4: Connection to Sewage Treatment Plants in EuropeDefault STP Connection Rate

Marked improvements in overall EU wastewater collection (+22% relative to 1992) and treatment (+69% relative to 1992) will follow full implementation of the Urban Waste Water Treatment Directive (91/271/EEC) in 2005 (see Figure 1). Even before 2005, a provisional figure is indicated for interim use as substantial increases in wastewater collection (+12%) and treatment (+40%) capacity have already been reported from across the EU. Projected wastewater treatment capacity in the EU as a whole for 2000 is greater than baseline organic loadings (i.e., 106%), although this is not uniformly distributed throughout the EU. An interim figure of 80% connection to wastewater treatment is therefore proposed for the generic region. A figure of 90 - 95% is also proposed for use following full implementation of the UWWTD. This coincides with the likely ultimate degree of connection and treatment capacity for urban regions of the EU.

Figure R. 16-15 Development in Collection and Treatment Capacity EU14 (Source: EC, 1999)⁹.



p.e. = person equivalent

Historical Data

Data on the proportion of the total population connected to wastewater treatment in individual MS in the period 1970-95 are presented in Table 1. The population weighted average for the whole of the EU15 in 1995 was 73%. Although the apparent degree of connection to wastewater treatment is

⁹ European Commission (1999). Implementation of Council Directive 91/271/EEC of 21 May 1991 concerning urban waste water treatment as amended by Commission Directive 98/15/EC of 27 February 1998. Summary of the measures implemented by the member states and assessment of the information received pursuant to Article 17 and 13 of the directive. Available on European Union (EU) web-site at <http://www.europa.eu.int/water/water-urbanwaste/report/report.html>.

low in some countries, its absence does not necessarily always imply inadequate treatment or direct discharge. For example, the proportion of the population with individual arrangements such as septic tanks has been reported as 24% in Greece, 23% in France, 22% in Finland, 12% in Portugal, 7% in Germany, 6% in Italy, 2.5% in the UK, 1.5% in the Netherlands, 1% in Spain and 0.5% in Luxembourg (EWWG, 1997)

Table R.16-25 Proportion of the Population served by a Wastewater Treatment Plant (Eurostat/EC/EEA, 1998)

Member State	Year				
	1970	1980	1985	1990	1995
Belgium	4	23	-	-	27
Denmark	54	-	91	98	99
Germany	62 (West)	80 (West)	84 (West)	86	89
Greece	-	1	10	11	34
Spain	-	18	29	48	48
France	19	62	64	68	77
Ireland	-	11	-	44	45
Italy	14	30	-	61	61
Luxembourg	28	81	83	90	88
Netherlands	-	73	87	93	96
Austria	17	38	65	72	76
Portugal	-	2	4	21	21
Finland	16	65	72	76	77
Sweden	63	82	94	94	95
UK	-	82	83	87	86

Urban Waste Water Treatment

Details of the current situation within the EU reveal that there are 17,351 agglomerations of more than 2,000 p.e. in the 14 member states excluding Italy (EC, 1999). This represents a total organic loading of 424 million p.e. relative to an actual EU14 population of 314 million. Data from a different source indicate an organic load of 105 million p.e. (in Italy (EWWG, 1997)).

It is notable that relatively few countries (i.e., Greece, Spain, Portugal and the UK) have designated coastal/estuarine areas as less sensitive. Discharges to such areas are subject to less stringent requirements regarding treatment (i.e., primary). In p.e. terms, this corresponds to <9% of organic loads.

Details of developments in the capacity of collecting systems conforming to the provisions of the directive are presented in Figure 1. The projected increase in capacity in terms of absolute p.e. (81 million) and percent (+22%) between the baseline situation in 1992 and the final situation after implementation of the directive in 2005 is substantial. More marked increases are projected for individual MS such as Spain (+113%), Ireland (+346%) and Portugal (+76%). Separate data for Italy indicate an increase in collection capacity of 7% from a baseline of 95 million p.e. to 102 million p.e. in 2005 (EWWG, 1997).