http://echa.europa.eu

# Guidance on information requirements and chemical safety assessment

## Chapter R.16: Environmental Exposure Estimation

Version: 2.1

October 2012

LEGAL NOTICE:

This document contains guidance on REACH explaining the REACH obligations and how to fulfil them. However, users are reminded that the text of the REACH regulation is the only authentic legal reference and that the information in this document does not constitute legal advice. The European Chemicals Agency does not accept any liability with regard to the contents of this document.

***Guidance on information requirements and chemical safety assessment***
***Chapter R.16: Environmental Exposure Estimation***

**Reference:** ECHA-10-G-06-EN
**Publ.date:** October 2012
**Language:** EN

© European Chemicals Agency, 2012.
Cover page © European Chemicals Agency

Reproduction is authorised provided the source is fully acknowledged in the form "Source: European Chemicals Agency, http://echa.europa.eu/", and provided written notification is given to the ECHA Communication Unit (publications@echa.europa.eu).

If you have questions or comments in relation to this document please send them (quote the reference and issue date) using the information request form. The information request form can be accessed via the Contact ECHA page at: http://echa.europa.eu/about/contact_en.asp

**European Chemicals Agency**

Mailing address: P.O. Box 400, FI-00121 Helsinki, Finland
Visiting address: Annankatu 18, Helsinki, Finland

# 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. After acceptance by the Member States Competent Authorities the guidance documents had been handed over to ECHA for publication and further maintenance. Any updates of the guidance are drafted by ECHA and are then subject to a consultation procedure, involving stakeholders from Member States, industry and non-governmental organisations. For details of the consultation procedure, please see:

http://echa.europa.eu/documents/10162/13559/mb_14_2011_consultation_procedure_guidance_en.pdf[1]

These guidance documents can be obtained via the website of the European Chemicals Agency at: http://echa.europa.eu/web/guest/support/guidance-on-reach-and-clp-implementation

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 2006[2] and its amendments as of 31 August 2011.

[1] Please note, that this guidance document was updated following the previous guidance consultation procedure.

2 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).

**Document History**

| Version | Comment | Date |
|---|---|---|
| Version 1 | First edition | May/July 2008 |
| Version 2 | • Redrafting the section about the general workflow of exposure estimation:<br>o The workflow for environmental exposure assessment has been completely redrafted (R.16.1.2). A diagram has been introduced to better illustrate it. First tier assumptions and the iteration/refinement alternatives are also shown. The diagram is consistent with the text and makes clear references to other chapters of the IR-CSA Guidance. Many of the changes in this section and in the whole guidance have been triggered by the need to make the guidance R.16 more relevant for release estimation under REACH, and, in particular, consistent with its general approach which aims to make registrants describing the conditions of safe use.<br>• Reworking chapter structure and headings. In particular:<br>o The exposure assessment workflow (R.16.1.2) and general principles (R.16.2: local assessment, regional assessment and time frame) have been described first, before the release estimation, fate, distribution and exposure estimation sections. In the previous guidance, these introductory principles were spread in several paragraphs.<br>o Both, in the release estimation and in the exposure estimation parts, a clear distinction has been made between first tier assumptions and refinement options for the eventual iteration. The different options for refinement have been listed in two separate paragraphs, one for release estimation (R.16.3.5) and the other for exposure estimation (R.16.8). In the previous version of the guidance, they were spread across different paragraphs.<br>• Revision of scenarios for the local assessment<br>o Two different scenarios for the local assessment have been introduced. The “Industrial setting” scenario (R.16.2.1.1) describes the releases from industrial point sources. The “Wide dispersive use” scenario (R.16.2.2) describes releases derived from consumers, professional and service life uses. Since releases to water from wide dispersive uses are associated with a municipal sewage treatment plant, they can be assessed as a point source at the local scale. A scenario for outdoor wide dispersive uses, based on releases onto an urban paved surface, collection into a public sewer and treatment in an STP has been added. A method has been provided to attribute a default tonnage for wide dispersive uses at a local scale. Since all releases to water from each identified wide disperse use will by default enter into the same sewage | May 2010 |

| | | |
|---|---|---|
| | system, combined risk should be considered. In previous versions of the guidance, the local scenario for wide disperse uses was less visible, and there was no suggestion to add up all disperse uses at local scale for assessing combined risks.<br><br>• Tonnage attribution<br><br>o Default conservative assumptions are now clearly described for the definition of a tonnage for each identified use and at local (R.16.3.2), regional and continental scale (R.16.3.3). If market data or information from downstream users is available, the registrant can overwrite these default values.<br><br>• Operational conditions described in the exposure scenario<br><br>o The parameters determining the release rate in the local scenario are expressed in a way now suitable for describing operational conditions in exposure scenarios under REACH (e.g. daily and annual use at an industrial site and daily wide dispersive use, see section R.16.3.2). Compared to the previous version of the guidance, the parameters themselves have not changed.<br><br>• Continental release estimation<br><br>o A sub-paragraph has been inserted to illustrate the method for calculating the releases at the continental scale starting from the tonnage at EU level, the regional tonnage and the same release factors used at the local and regional scale (within R.16.3.3). No content changes with respect to TGD (2003).<br><br>• Review of the chapter on Measured data (R.16.4):<br><br>o The previous paragraph, focused on environmental concentrations, has been expanded to consider also release measurements. The consistency need with RMM/OC, as described in the exposure scenario, has been stressed.<br><br>• Review of fate, distribution and exposure estimation sections (R.16.5).<br><br>o These section has undergone minor revisions mainly aimed at avoiding duplication with concepts already mentioned in the previous paragraphs and ensuring consistency with the new release estimation part.<br><br>• The Appendix R.16.1 has been updated<br><br>o The link between ERCs and release estimation is limited now to default release factors. All other defaults that may be applied in a tier 1 default assessment have been removed for reasons of consistency.<br><br>o Two new Environmental Release Categories, ERC 12A and ERC 12B, related to industrial processing of articles with abrasive techniques have been introduced. | |

| | | |
|---|---|---|
| | o Release factors for direct regional releases onto industrial soil (ERC 1-7) have been introduced, to be taken into account for regional exposure estimates.<br><br>o Also, the description of some other ERCs has been slightly refined, including the explanation on the associated default release factor The following default release factors have been changed:<br><br>▪ ERC 4 to air: 100% instead of 95%;<br><br>▪ ERC 8D to soil: 20% instead of 1%;<br><br>▪ ERC 9A to water: 5% instead of n.a.;<br><br>▪ ERC 10A to water: 3.2% instead of 0.16 × Tservice. | |
| Version 2.1 | Corrigendum:<br>(i) replacing references to DSD/DPD with references to CLP<br>(ii) implementing minor recommendations for nanomaterials from the RIP-oN3 report<br>(iii) implementing further minor editorial changes / corrections (notably to correct over-zealous replacements of "preparation" by "mixture" in some contexts in version 2). | October 2012 |

## GUIDANCE FOR IMPLEMENTING THE UPDATES

Most updates in this Guidance are of explanatory nature, or bring previously existing parameters into a shape supporting exposure scenario building under REACH.

A registrant having already finalised the environmental exposure assessment based on the R.16 Guidance as published in May 2008 may wish to take the following advice into account:

- Read the document history to get informed what has been updated;
- Check whether the changes in the guidance put into question
  - the scope of the exposure scenarios already worked out and
  - the outcome of the risk characterization related to these exposure scenarios.

  If both questions can be answered with "no", it is unlikely that the adaptation of the already existing CSR to the Guidance update is of highest priority.

- To answer the questions mentioned above the registrant is advised to take in particular the following changes/clarifications in the current guidance into account:

  - The exposure should contain information (about operational conditions and risk management measures) based on which the assumed release factors and daily use rates can be justified. Exposure scenarios making reference to the A and B tables of the TGD (2003) without providing more specific information on the conditions of use are considered insufficient to meet the REACH requirements.

Releases to water from wide disperse uses are to be assessed in a local scenario. Since all releases to water from each identified wide disperse use will by default enter into the same sewage system, combined risk should be considered. For assessing the combined risk, the local releases to water of all wide dispersive uses should be summed up.

**Convention for citing the REACH regulation**

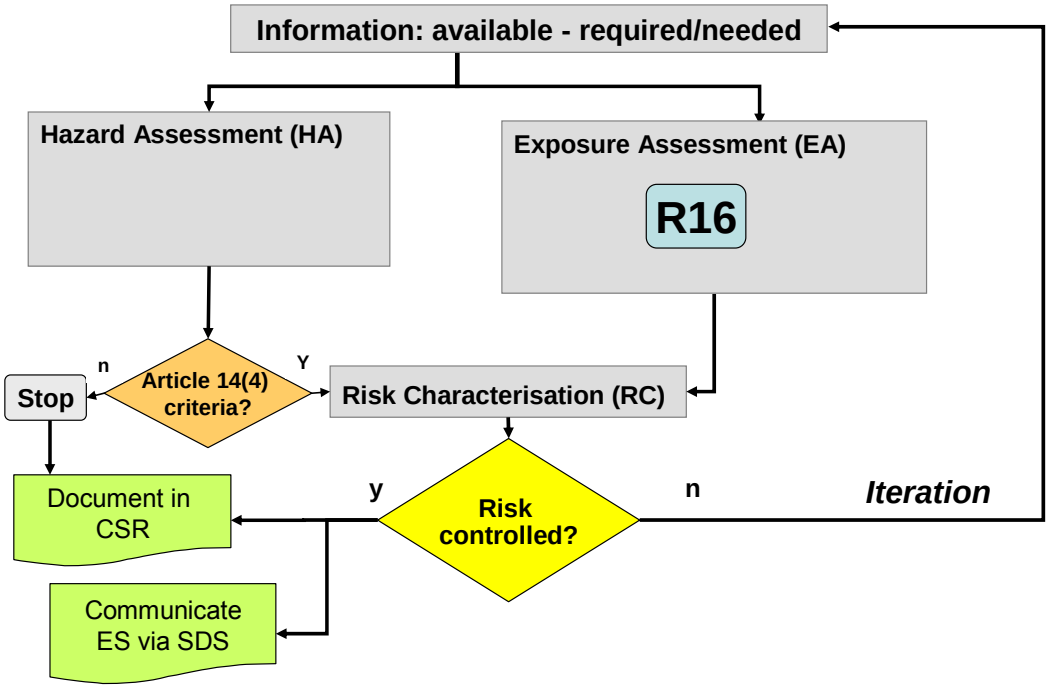
Where the REACH regulation is cited literally, this is indicated by text in italics between quotes.

**Table of Terms and Abbreviations**

See Chapter R.20

**Pathfinder**

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



# TABLE OF CONTENTS


R.16. ESTIMATION OF ENVIRONMENTAL EXPOSURE ..... 1
R.16.1. Introduction ..... 1
R.16.1.1. Aim ..... 1
R.16.1.2. Workflow for environmental exposure estimation ..... 1
R.16.2. Exposure assessment principles ..... 4
R.16.2.1. Local assessment ..... 4
R.16.2.1.1. Releases from industrial settings ..... 5
R.16.2.1.2.Releases from wide dispersive uses ..... 6
R.16.2.2. Regional assessment ..... 6
R.16.2.3. Time frame ..... 8
R.16.3. Release estimation ..... 9
R.16.3.1. Information needed for release estimation ..... 9
R.16.3.1.1. Life cycle stages of a substance ..... 9
R.16.3.1.2.Tonnage ..... 11
R.16.3.1.3. Operational conditions and RMM ..... 12
R.16.3.1.4. Release factors ..... 12
R.16.3.2. Local release estimation ..... 13
R.16.3.2.1.Industrial setting scenario ..... 13
R.16.3.2.2.Wide dispersive use scenario ..... 15
R.16.3.3. Regional release estimation ..... 16
R.16.3.4. Summary of the release patterns ..... 17
R.16.3.5. Refinement options for iteration ..... 18
R.16.3.5.1. Daily/annual use ..... 18
R.16.3.5.2. Release factor/rate ..... 19
R.16.4. Measured data ..... 21
R.16.4.1. Introduction and general principles ..... 21
R.16.4.2. Selection of adequate measured data ..... 22
R.16.4.3. Allocation of the measured data to a local or a regional scale ..... 28
R.16.5. Partitioning and degradation ..... 28
R.16.5.1. Information needed for assessing the partitioning and degradation behaviour ..... 28
R.16.5.2. Output from the calculations ..... 29
R.16.5.3. Partition coefficients ..... 29
R.16.5.3.1. Adsorption to aerosol particles (gas-aerosol partitioning) ..... 29
R.16.5.3.2. Volatilisation (air-water partitioning) ..... 30
R.16.5.3.3. Adsorption/desorption (solids-water partitioning) ..... 31
R.16.5.3.4. Partition coefficients in the marine environment ..... 32
R.16.5.3.5. Bioconcentration and biomagnification (biota-water/solids partitioning) ..... 33
R.16.5.3.6. Ionising substances ..... 35
R.16.5.4. Degradation rates in the environment ..... 36
R.16.5.4.1. Hydrolysis ..... 36
R.16.5.4.2. Photolysis in water ..... 37
R.16.5.4.3. Photochemical reactions in the atmosphere ..... 38

R.16.5.4.4.Biodegradation in a sewage treatment plant ..... 38
R.16.5.4.5.Biodegradation in surface water, sediment and soil ..... 39
R.16.5.4.6. Overall rate constant for degradation in surface water ..... 42
R.16.5.4.7. Biodegradation in the marine environment ..... 42
**R.16.6. Exposure and intake estimation ..... 43**
**R.16.6.1. Output from the exposure and intake calculations ..... 43**
**R.16.6.2. Input to exposure estimation calculations ..... 45**
**R.16.6.3. Principles ..... 46**
R.16.6.3.1. Local environmental distribution ..... 46
R.16.6.3.2. Regional distribution ..... 47
R.16.6.3.3. Continental distribution ..... 47
R.16.6.3.4. Distribution in a sewage treatment plant ..... 47
**R.16.6.4. Characterization of environmental compartments ..... 48**
**R.16.6.5. Wastewater treatment – estimation of PECstp ..... 50**
R.16.6.5.1. Wastewater treatment ..... 50
R.16.6.5.2. Measured data in full scale STP ..... 51
R.16.6.5.3. Simulation test data ..... 51
R.16.6.5.4. Modelling STP ..... 52
R.16.6.5.5. Calculation of the STP-effluent concentration ..... 54
R.16.6.5.6. Calculation of the STP concentration for evaluation of inhibition to microorganisms ..... 56
**R.16.6.6. Derivation of PEC ..... 58**
R.16.6.6.1.Calculation of PEClocal for the atmosphere ..... 59
R.16.6.6.2. Calculation of PEClocal for the aquatic compartment ..... 62
R.16.6.6.3.Calculation of PEClocal for the sediment compartment ..... 65
R.16.6.6.4. Calculation of PEClocal for the marine aquatic compartment ..... 66
R.16.6.6.5. Calculation of PEClocal for the marine sediment compartment ..... 68
R.16.6.6.6.Calculation of PEClocal for the soil compartment ..... 69
R.16.6.6.7. Calculation of concentration in groundwater ..... 76
R.16.6.6.8. Calculation of PECregional ..... 79
R.16.6.6.9. Decision on the environmental concentrations used for exposure estimation ..... 85
**R.16.6.7. Predators (secondary poisoning) ..... 86**
R.16.6.7.1. Output ..... 86
R.16.6.7.2. Input ..... 86
**R.16.6.8. Humans exposed indirectly via the environment ..... 92**
R.16.6.8.1. Introduction ..... 92
R.16.6.8.2. Output ..... 93
R.16.6.8.3. Input ..... 94
R.16.6.8.4. Exposure via the environmental compartments ..... 95
R.16.6.8.5. Exposure via food consumption ..... 95
R.16. 6.8.6. Total daily intake for humans ..... 96
**R.16.7. Tools based on models presented in section R.16.6. ..... 96**
R.16.7.1. EUSES ..... 96
R.16.7.2. TGD excel sheet ..... 100
**R.16.8. Refinement of exposure estimation ..... 100**
**R.16.9. Summary of default and refined assessment ..... 103**

## Tables

Table R.16-1: Direct releases to environmental compartments considered in the different scenarios ..... 18
Table R.16-2: Quality criteria for use of existing measured data (based on OECD, 2000) ..... 23
Table R.16-3: Default BMF values for organic substances with different log $K_{ow}$ or BCF in fish..... 35
Table R.16-4: Elimination in sewage treatment plants: ..... 39
Table R.16-5: First order rate constants and half-lives for biodegradation in surface water ..... 40
Table R.16-6: Half-lives (days) for (bulk) soil based on results from standardised biodegradation test results..... 41
Table R.16-7: Recommended mineralisation half-lives (days) for use in marine risk assessment ..... 43
Table R.16-8: Derivation of PEC-values ..... 45
Table R.16-9: Characterisation of environmental compartments ..... 49
Table R.16-10: Standard characteristics of a municipal sewage treatment plant ..... 54
Table R.16-11: Characteristics of soil and soil-use for the three different endpoints..... 75
Table R.16-12: Proposed model parameters for regional model ..... 81
Table R.16-13: Intermedia mass transfer coefficients ..... 82
Table R.16-14: Parameters for the continental model ..... 85
Table R.16-15: Environmental concentrations used as input for indirect exposure calculations ..... 94
Table R.16-16: Human daily intake of food and water (from EUSES) ..... 94
Table R.16-17: Information requirements for Tier 1 assessment of environmental distribution ..... 98
Table R.16-18 EUSES – output: Predicted environmental concentrations, PECs..... 99
Table R.16-19: Determinants and input information for refined assessment..... 101
Table R.16-20: Assumptions for the determinants of the default and refined assessment..... 103
Table R.16-21: Name and description of Environmental Release Categories..... 109
Table R.16-22: Specification of the use conditions reflected in the environmental use categories. ..... 113
Table R.16-23: Default parameters to derive the environmental release rate ..... 115
Table R.16-24: Proportion of the Population served by a Wastewater Treatment Plant (Eurostat/EC/EEA, 1998)..... 136

## Figures

Figure R.16-1: Workflow for environmental exposure assessment ..... 3
Figure R.16-2: Local distribution calculation (for an industrial setting scenario)..... 5
Figure R.16-3: Schematic representation of the model for calculating the regional PECs ..... 7
Figure R.16-4: The relationship between the continental, regional, and local scale..... 8
Figure R.16-5: Schematic design of the sewage treatment plant model SimpleTreat ..... 53
Figure R.16-6: Fate processes in the air compartment ..... 59
Figure R.16-7: Fate processes in the surface water..... 62
Figure R.16-8: Calculation of PECsoil ..... 69
Figure R.16-9: Accumulation in soil due to several years of sludge application ..... 71
Figure R.16-10: The concentration in soil after 10 years..... 72
Figure R.16-11: Regional calculations ..... 79
Figure R.16-12: Assessment of secondary poisoning ..... 87
Figure R.16-13: Secondary poisoning food chain ..... 89
Figure R.16-14: Schematic representation of the exposure routes considered in human exposure ..... 92
Figure R.16-15: The CHARM model ..... 103
Figure R.16-16: Development in Collection and Treatment Capacity EU14 (Source: EC, 1999) ..... 135

## Examples

Example R.16-1: Removal in the STP continued from Example R.16-2 ..... 57
Example R.16-2: Concentration in surface water ..... 65
Example R.16-3: Concentration in agricultural soil..... 77

## Appendices

Appendix R.16-1: Environmental Release Categories ..... 109
Appendix R.16-2: Overview of Emission Scenario Documents (ESDs) ..... 122
Appendix R.16-3: Fate of chemicals in a wastewater treatment plant based on the SimpleTreat model ..... 129
Appendix R.16-4: Connection to Sewage Treatment Plants in Europe ..... 135

# R.16. ESTIMATION OF ENVIRONMENTAL EXPOSURE

## R.16.1. Introduction

### R.16.1.1. Aim

This chapter will provide guidance on how to estimate environmental exposure. More specifically, it will deal with:

- Estimation of the releases to air, water (either wastewater and/or surface water), and soil at local and regional scale.
- Fate and distribution of the releases in environmental compartments (air, soil, surface water, sediment, biota) and sewage treatment plants;
- Calculation of exposure concentrations in / doses for, respectively:
    - Environmental compartments (Section R.16.6.1), in terms of Predicted Environmental Concentrations (PECs), at both local and regional scales, covering both direct exposure of organisms and exposure via the food chain for predators
    - Man via the environment (Section R.16.6.8) in terms of human daily intake of the substance through drinking water, fish, leaf crops, root crops, meat and dairy products, at local and regional scale.

Most of the current guidance on environmental exposure estimation has been developed mainly for organic substances. Metals and metal compounds present particularities (natural background and historical releases, speciation, adsorption/desorption behaviour, differences in bioavailability) which require specific adaptations when performing the exposure assessment. These issues are considered in the Appendix R.7.13-2.

### R.16.1.2. Workflow for environmental exposure estimation

The estimation of environmental exposure is built upon the following previously performed processes: collection of information on relevant **substance properties** and **mapping of uses**.

Information on substance properties consists of a minimum set of data (e.g. from IUCLID) including vapour pressure, water solubility, molecular weight, octanol-water partition coefficient, melting point and information on ready biodegradability which are needed for the environmental exposure estimation. Mapping of uses consists of definition of relevant life cycle stages (see part D and Chapter R.12), identification of uses, assignment of the appropriate descriptor, including the Environmental Release category - ERC, describing the conditions of use from the environmental perspective (see Chapter R.12), and the definition of an appropriate tonnage.

The whole exposure estimation is therefore built upon the definition of the life cycle stages of the substance giving rise to release/exposure (see part D and Chapter R.12) and the identification of the covered uses for each life cycle step. Once this framework has been completed, the proper exposure estimation can start.

The exposure estimation consists of the following steps:

1. Determination of **operational conditions (OC)** and **risk management measures (RMM)**, including, for example, amount of substance, process temperature, duration and frequency of use or activity etc, and industrial wastewater treatment plants, filters, scrubbers, municipal sewage treatment plants etc. (Chapter R.13);

2. **Release estimation** consisting of the determination of the local and regional release rates for each use (Sections R.16.3.2 and R.16.3.3), starting from the appropriate release factors and the tonnage assigned to any identified use;

3. **Environmental distribution and fate** and **exposure estimation**. The distribution and fate of a substance in the environment (Sections R.16.5 and R.16.6) is assessed at local and regional scale. Consecutively, PEC (Predicted Environmental Concentrations) values for each environmental compartment and the daily intake of humans via the environment (Section R.16.6.8) are derived at local and regional scale. A single overall PEC is derived for (top-)predators (Section R.16.6.7) based on local and regional contributions. PEC values for the sewage treatment plant are calculated at local scale (Sections R.16.6.5 and R.16.6.6).

Exposure estimation can be an iterative process. If the **risk characterisation** (Guidance Part E) indicates that the applied risk management measures and operational conditions are not adequate to control risks occurring from the manufacture and all identified use(s) (Risk Characterization Ratio, RCR > 1), the exposure estimation may need to be refined. This refinement is possible at every step in the workflow.

Inter alia, it might be possible to:

- refine or add more specific **RMM/OC;**
- refine the parameters in the applied release estimation method based on representative on-site data, such as **release measurement**, which should be linked with the RMM/OC;
- refine the **mapping of uses** and the tonnage assigned to each identified use (e.g. using market data);
- use environmental **measured data** (representative environmental concentrations or properties of the receiving environment such as measured river flow rates) ;
- use **higher tier exposure** estimation tools;
- refine the **substance properties** (e.g. degradation rates, partitioning coefficient).

The following flowchart (Figure R.16-1) illustrates the steps described above; the darker blue boxes are related to the exposure assessment, while the light ones are related to other steps in the safety assessment that have an impact on the exposure. The rectangular boxes represent the processes, while parallelepiped boxes show the outcome of the process.

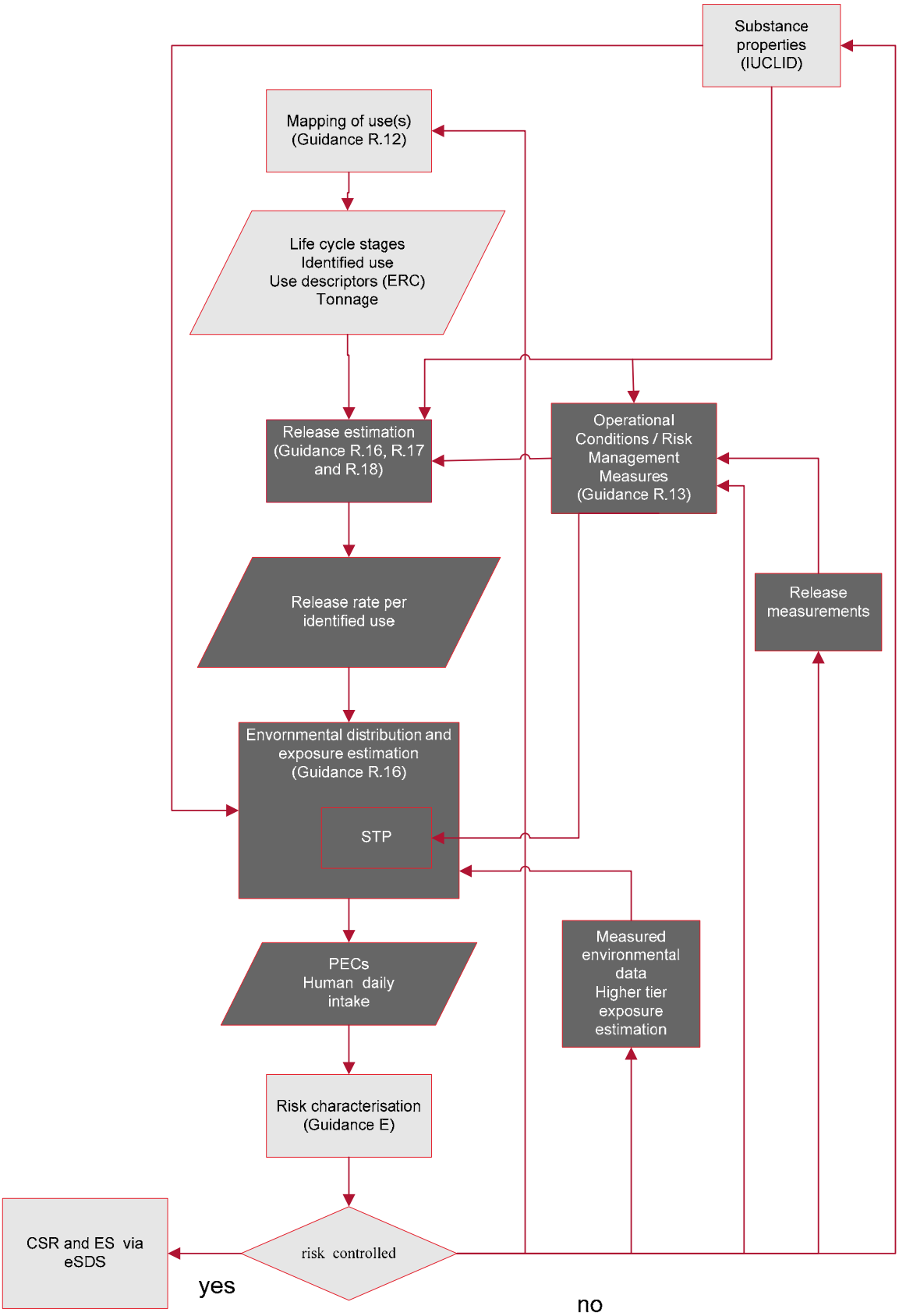



**Figure R.16-1**: Workflow for environmental exposure assessment

## R.16.2. Exposure assessment principles

The exposure to the environment is in principle assessed on two spatial scales: locally in the vicinity of point sources of release to the environment, and regionally for a larger area which includes all point sources and wide dispersive sources in that area. Releases at the continental scale are considered to provide inflow concentrations for the regional environment. The end results of the exposure estimation are concentrations (PECs) in the environmental compartments air, surface water (fresh and marine), soil, sediment, and biota (e.g. earthworms and fishes for secondary poisoning) and human daily intake of the substance via the environment for both local and regional scale. Continental concentrations are not used as endpoints for exposure.

### R.16.2.1. Local assessment

The concentrations of substances released from a single point source are assessed for a generic local environment. This is not an actual site, but a hypothetical site with predefined characteristics, defined by a 'standard environment' (for its description see Section R.16.6.4) and a standard town of 10000 inhabitants. The exposure targets are assumed to be exposed in, or at the border of, the site. In general, concentrations during a release episode are calculated. This means that local concentrations are calculated on the basis of a daily release rate, regardless of whether the discharge is intermittent or continuous (see Section R.16.2.3). They represent the concentrations expected at a certain distance from the source on a day when the release occurs.

For the exposure assessment of terrestrial organisms, of predators and of man indirectly exposed via the environment a longer term average is used instead of daily release rates. This is because exposure is assumed not to be influenced by temporal fluctuation in release rates.

In principle, degradation and distribution processes should be taken into consideration at the local scale. However, because of the relatively short time between release and exposure, concentrations at local scales are entirely controlled by initial mixing (dilution into environmental compartment) and adsorption on suspended matter. No other process is considered in the calculation of local PEC.

A fixed dilution factor is applied to the effluent concentration of an STP (by default assumed to be present). 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 the PEClocal can be carried out using actual environmental conditions around the point source.

Figure R.16-2 shows the relationship between the local release routes and the subsequent distribution process modelled for the environmental compartments.

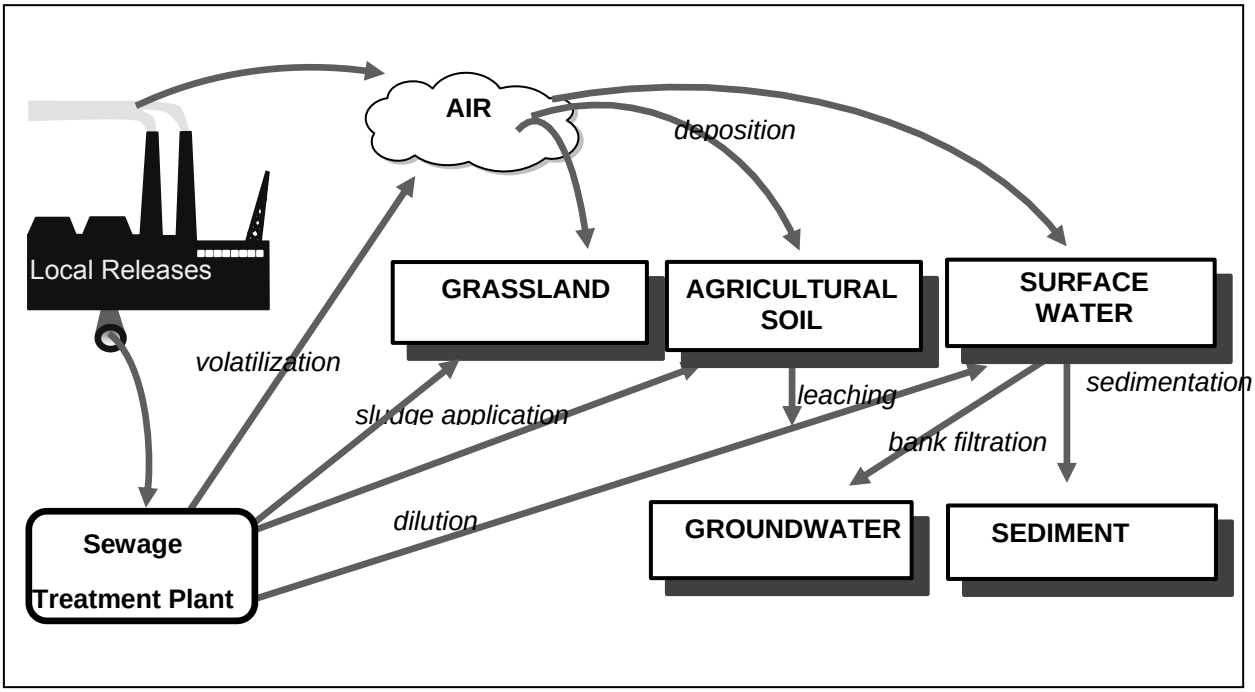



**Figure R.16-2**: Local distribution calculation (for an industrial setting scenario)

Further guidance on local exposure assessment for metals and metal compounds can be found in Guidance Chapter R.7, Appendix R.7.13-2.

Two scenarios are distinguished to assess the release to the environment at the local scale: (1) release from industrial settings and (2) release from wide dispersive uses.

#### R.16.2.1.1. Releases from industrial settings

Releases from uses in industrial settings are assessed as independent point source releases; it means that each identified use of the substance is assumed to occur at a different site. However, in some cases, it is needed to combine those assessments in the "combined risk" section of the CSR, e.g. when manufacture and formulation take place at the same site.

The industrial setting scenario considers releases to water, air and soil.

Releases to water can be treated in an on-site industrial waste water treatment plant (WWTP) or in a municipal sewage treatment plant (STP). For industrial or municipal biological treatment plants, a standard model is available to calculate the releases after treatment (Section R.16.6.5). By default, a municipal STP is available as a standard RMM for local release from industrial settings. Indirect releases to air via the STP, as a result of water treatment in the STP, are also considered in the industrial setting scenario

Release to soil at the local scale will occur via application of sludge from an STP to agricultural soil and via atmospheric deposition of substances released to air. Direct releases to soil from industrial settings are not assessed at the local scale, but only at the regional scale.

#### R.16.2.1.2.Releases from wide dispersive uses

A wide disperse use of a substance is characterised by the assumption that the substance is used by consumers or by many users in the public domain, including small, non industrial companies[3]. A wide dispersive use of a substance is by default associated with a point source release of a local municipal STP of a standard 10000 inhabitants town, that collects the releases to water from that use. This is not the case for direct releases to air and soil from wide dispersive uses. Therefore, these are not considered at the local scale, but only at the regional one.

The local tonnage used by consumers or by many users in the public domain (including small companies) is calculated from the manufactured tonnage (for more details see Section R.16.3.2.2). This calculation is carried out for each wide disperse use of the substance. Since all these releases will by default enter into the same sewage system, combined risk should be considered in section 10 of the CSR (see part F)

### R.16.2.2. Regional assessment

The concentrations of substances released from point and wide dispersive sources in a larger area are assessed for a generic regional environment. The fate of substances at the regional scale differs from the fate at the local scale in the sense that more time is available for transport and transformation processes. At longer distances from point sources or when releases are wide dispersive and not collected into a single point source, the further distribution and fate of the substance are taken into account. It can be assumed that inter-media transport and degradation become relatively more important. For calculating the regional PEC, a multi-media fate-modelling approach is used (e.g. the SimpleBox model).

All releases to each environmental compartment for each use, assumed to constitute a constant and continuous flux, are summed and averaged over the year, and steady-state concentrations in the environmental compartments are calculated. The regional concentrations are used as background concentrations in the calculation of the local concentrations. Figure R.16-3 gives a general overview of the distribution processes in the regional model. For details see Section R.16.6.6.8.

A standard region is represented by a typical densely populated EU-area located in Western Europe (~ 20 million inhabitants, 200 × 200 $km^2$).

[3] Whether a company is industrial or not from an environmental point of view can, for example be determined on the base of the obligation to apply for a permit to discharge waste water into the environment. Please note: The allowance to use the public sewage system is not regarded an “environmental permit” in this respect. .

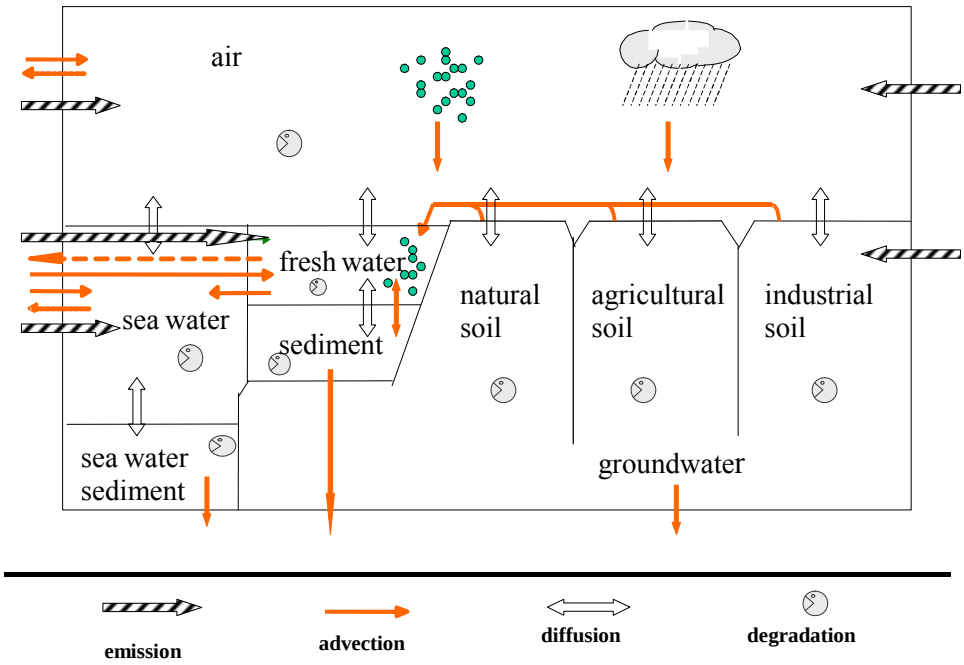



**Figure R.16-3**: Schematic representation of the model for calculating the regional PECs

Regardless of the assumptions made at local scale, regional releases to water are based on a scenario where 80% (representing the EU average) of the wastewater is treated in a biological STP and the remaining 20% is released directly into surface waters.

Further guidance for the regional exposure assessment for metals and metal compounds can be found in Appendix R.7.13-2.

Continental distribution

Concentrations in air and water are also estimated at a continental scale (Europe) to account for the chemical flux - due to passive transport of the substance with air and water - into the regional area. Both continental and regional concentrations are calculated using a multimedia fate model. The continental concentrations are not used as endpoints for exposure in the risk characterisation. Figure R.16-4 illustrates the relationships between continental, regional and local scale.

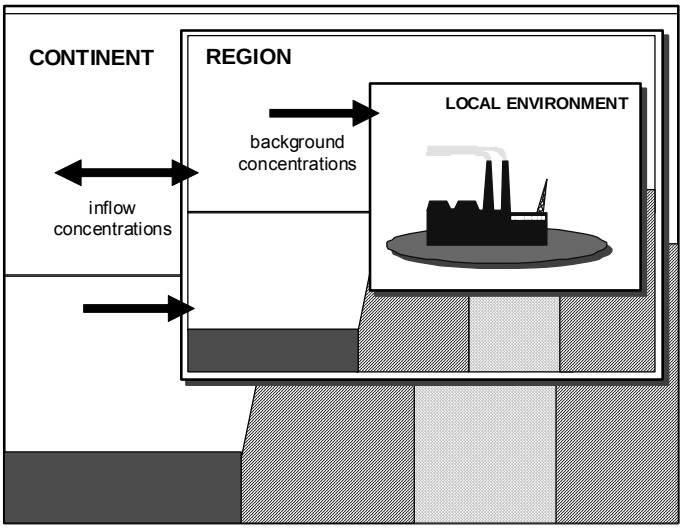



**Figure R.16-4**: The relationship between the continental, regional, and local scale

### R.16.2.3. Time frame

Local releases of substances can be either continuous or intermittent. Intermittent releases are for example caused by batch processes leading to discharges for not more that 12 times a year for not more than 24 hours. Continuous releases are characterized by an almost constant release rate over a prolonged period (e.g. 220 working days). Intermittent releases are defined as occurring infrequently, i.e. less than once per month and for no more than 24 hours.

The release rate is given averaged per day (24 hours). This implies that, even when a release takes place only a few hours per day, it will be averaged over 24 hours.

In case of continuous releases, organisms with a relatively short life-span, like aquatic organisms, are exposed locally to toxic concentrations of the substance for a considerable proportion of their lifetime. Therefore, for these organisms, the average exposure levels during release episodes are assumed to be continuous. It follows from this assumption that the estimated environmental concentrations can be considered as estimates of long-term exposure levels for these organisms, which can be compared to no effect concentrations derived from long-term toxicity data.

If intermittent release is identified, only short-term effects are considered for the aquatic ecosystem and no-effect levels are derived from short-term toxicity data only.

Since most substances are not released directly to soil and because of its less dynamic nature than air or surface water, the exposure of terrestrial organisms is assumed not to be influenced by temporal fluctuations in release rates. Also in the case of predators and human beings, these fluctuations are of a rather short-term nature compared to their life span and the time scale on which chronic effects are considered. Predators, humans and terrestrial organisms are therefore assumed to be exposed to levels averaged over a longer period, and derived from average release rates (i.e. annual average).

Regional releases of substances are assumed to occur continuously over the year. Therefore average exposure levels are calculated by the steady state model for the regional scale using annual release rates and they are compared with long term toxicity data.

For substances as such and in mixtures it is assumed that the releases take place in the year of manufacture. However, for the article service life and the subsequent waste life stage this assumption is often not applicable since the release occurs over a longer period after manufacture.

In particular, it is assumed that the release to the environment takes place continuously 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. Steady state in this case 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 share from competitors. In such case the current annual production volume can be taken to estimate the annual releases by multiplying it by the release factor of the article over its service life.

## R.16.3. Release estimation

Releases can occur to air, surface fresh and marine water, wastewater and soil and are estimated separately for every environmental compartment and each relevant stage of the life cycle.
Release estimation is the process whereby releases to the environment are quantified during the life cycle stages and uses of a substance, taking into account the different release pathways, receiving environmental compartments and the spatial scale of the releases.

Therefore, the aim of the release estimation is to calculate the following parameters:

- Release rates (expressed in kg/day) to wastewater, surface water, air and soil for each relevant life cycle stage and use at the local scale (Section R.16.3.2).
- Release rates (expressed in kg/day) to wastewater, surface water, air and soil at the regional scale (Section R.16.3.3).

### R.16.3.1. Information needed for release estimation

Proper release estimation can only start after the definition of the life cycle stages for the substance and the identification of the uses for each of them..

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

- Life cycle stages of a substance
- Supplied tonnage for the use, or group of uses, for each life cycle stage of a substance
- Information on Operational Conditions (OC) and Risk Management Measures (RMM)
- Release factors (expressed in kg/kg or %) depending on the type of use, the stage in the life cycle and the OC and RMM

#### R.16.3.1.1. Life cycle stages of a substance

The generalised life cycle stages of a substance are given in Figure R.16-5. The release pattern and the estimated release factor are closely related to the life cycle stages of a substance. The release estimate in a registration should in principle be seen from the perspective of the entire life cycle of a substance, as described here.

**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. Different types of intermediates (substances used to make other substances) can be manufactured and distinguished.

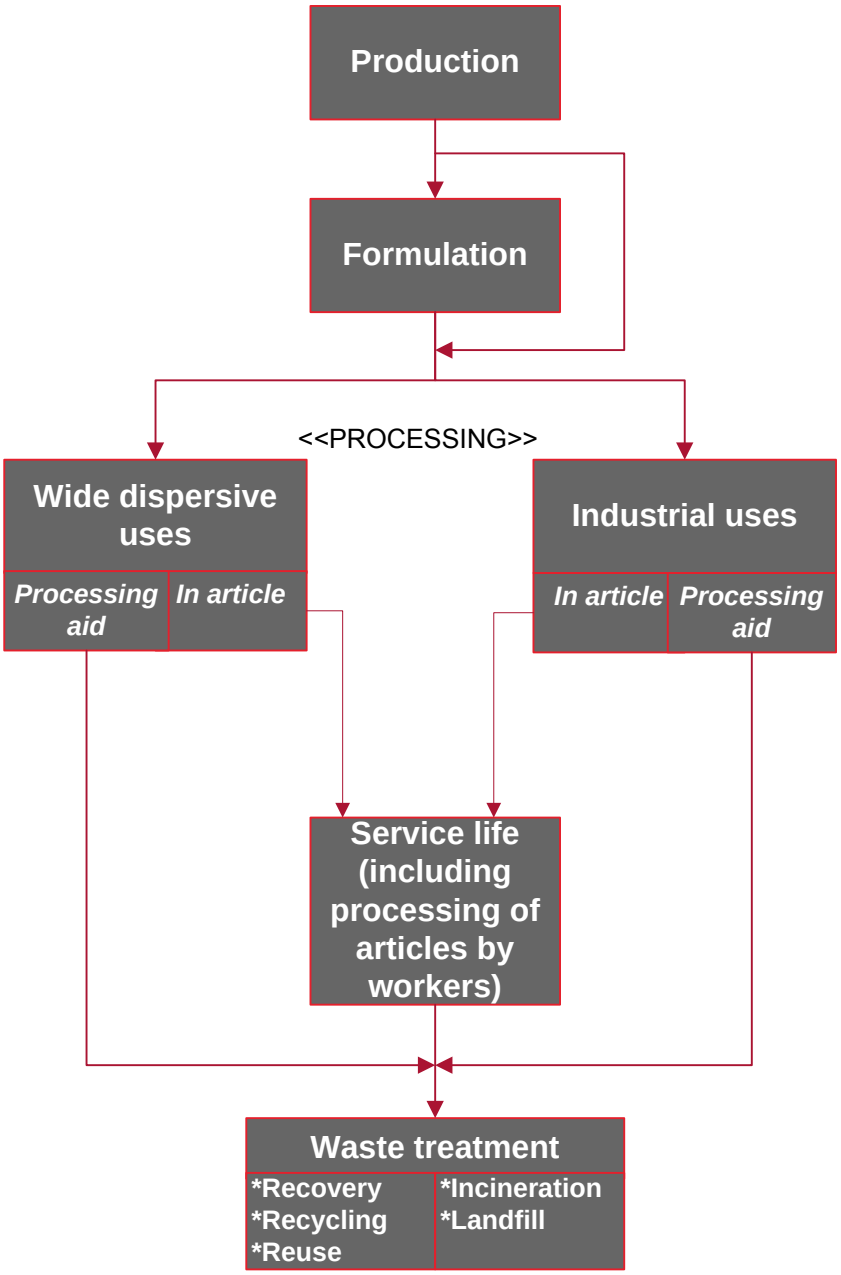



**Figure R.16-5**: Life cycle stages of substances[4]

**Formulation**: Mixing and blending into a mixture. Formulation is the stage where substances are combined in a process of blending and mixing to obtain a mixture. This may be a formulation such as a paint, or a mixture on a carrier material, 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**: Use of the substance as such or in a mixture, in an industrial process with the purpose of incorporating the substance into an article, or technically supporting the production 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.

[4] The waste treatment box will be brought in line with guidance R.18 (Estimation of exposure from waste life stage) once this is updated.

**Wide dispersive uses**: Application of the substance or mixture by professionals or the public at large outside industrial installations. They consist in professional and consumer uses:

a) Professional use may include the use of substances as such or in mixtures, in order to deliver services to business or private customers. This may include sophisticated equipment and specialised, trained personnel.

b) Consumer use includes the use of substances as such or in mixtures. 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"[5] of articles or the polymer matrix of a mixture (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, mixtures or articles are disposed of after their service life, such as for example used lubricants or solvents, old tyres or home appliances. Unintended losses of mixtures may also 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, landfilling, or recovery of the basis material or substance. For more information about exposure assessment for the waste life cycle stage see Chapter R.18.

At each of the life-cycle stages a larger or smaller fraction of the substance is lost via releases and will therefore not enter the next life cycle stage. In case a refinement of the release is needed, this aspect could be taken into account. Between the various life cycle stages transport, storage, and handling may occur. This has not been indicated in Figure R.16-1. Releases 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 further under REACH.

#### R.16.3.1.2.Tonnage

The starting point for release estimation is the tonnage of substance manufactured/imported by the registrant and the tonnage associated with each use (or group of uses) during the life cycle of the substance for which exposure scenarios need to be developed.

The manufacturer's annual production or the importer's annual import of a substance will be distributed in the EU market, and flows down the supply chains. The registrant usually knows his own production/import tonnage and the markets to which he sells the substance. However, often he has little information on the annual or daily tonnage used by the downstream users (including formulators and industrial users).

If the registrant is able to get information of the tonnage used by his downstream users and if he has enough market data, he can assign a tonnage to every life cycle step (formulation, industrial use, consumer and professional use, service life articles) and uses identified in the use mapping section (Chapter R.12). For each downstream use, it is possible to consider as a worst case assumption, the tonnage used by the largest customer. It is assumed that for each use, the evaluation performed using this tonnage ensures control of risk for all smaller customers[6].

If specific and reliable data are not available, conservative assumptions (like the use of the total manufactured volume for every identified use) need to be made by the registrant to assign the tonnage to identified uses for releases estimation. In doing so, the calculated exposure estimates

[5]Handling or processing of articles is not a "use" in the meaning of REACH. It is considered as life cycle stage subsequent to the use.

[6]Guidance for downstream users on how to define the relevant tonnage for his own use in the case of multiple suppliers of the same substance or in case of use of recycled amounts (particularly relevant for the metals industry) is out of the scope of the present R.16 Guidance.

and corresponding RCR will help the registrant to set priorities for collection of more specific information.

#### R.16.3.1.3. Operational conditions and RMM

Both operational conditions and risk management measures have an impact on the type and amount of release and the resulting exposure.

Operational conditions consist of a set of actions, tools, parameters such as amount of substance, process temperature and pH, duration and frequency of release, type of use (e.g. indoor or outdoor), containment of process (open or closed), continuous or batch process (leading to an intermittent release), capacity of surroundings, etc. having, as a side effect, an impact on the release and the exposure.

Risk management measures consist of technologies and procedures aimed at either reducing the releases and/or preventing a release pathway.

Examples of risk management measures intended to reduce release are filters, scrubbers, biological or physico-chemical wastewater treatment plants etc.

An example of exclusion of a release pathway is when sludge from a waste water treatment is incinerated and not spread on agricultural soil.

If a specific RMM is applied as standard practice, can be controlled on-site and its effectiveness is known, release factors can be decreased and taken into account in the development of the ES (see Section D and Chapter R.13). Since a municipal biological sewage treatment plant (STP) is a standard practice in Europe, it is assumed as a standard RMM for industrial waster water treatment. The use of specific waste water treatment plants (WWTP) or the absence of the municipal STP associated with industrial settings should be taken into account in the exposure estimation and may need to be taken into account for development of the ES.

For a general overview of abatement techniques, the RMM library

http://www.cefic.org/files/downloads/Guidance%20on%20REACH%20-%20Dec%202007.pdf

can be consulted. EU BREF Documents under the EU Directive on Integrated Pollution Prevention and Control (IPPC) are also a valuable source of information.

#### R.16.3.1.4. Release factors

Release factors express the fraction (either kg/kg or %) of the used amount being released to the environmental compartment under consideration.

The release of a substance from a certain use (e.g. technical processes in installations or vehicles, application of mixtures in private households) depends on the operational conditions (like e.g. temperature, pressure, level of containment of machinery, level of internal regeneration of processing fluids, dry or wet process, dipping or spraying) and risk management practices (OC/RMM).

Special considerations have to be taken into account on the derivation of the release factors from service life of long-life articles and waste disposal, see Guidance Chapters R.17 and R.18, respectively.

To streamline the release estimation and to support data collection in and communication across the supply chain, environmental release categories (ERCs) have been developed. The ERCs are listed and described in Section R.12.3.4, Appendices R.12.4.1 and R.12.4.2.

ERCs are linked to conservative default release factors to be used as a starting point for a first tier environmental exposure assessment. The source of these release factors and their value

(expressed in %) is documented in Appendix R.16-1. Examples on how to work with ERCs are given in Part D.

The use of an ERC does not require any explicit information on substance properties for a first tier release estimate. In addition, the default assumption is that onsite RMM are not in place. If a specific RMM is applied in current practice (for example according to the best available technologies) and the effectiveness of such a technique is known, release factors can be reduced accordingly and taken into account in the development of the ES (see Guidance Part D and Chapter R.13).

In first instance, ERCs are use descriptors. In addition they are linked to a set of default release factors for a first tier environmental exposure assessment. When refining the release factor, the same ERC description may correspond to different ESs (depending on RMM and OC) resulting in different release factors.

ERCs are based on the following aspects (see Appendix R.16-1 and R.12.3.4):

1. life cycle stage;
2. level of containment;
3. type of use and technical fate of a substance;
4. dispersion of release sources;
5. indoor or outdoor use;
6. release potential during service life and waste stage.

Alternative release factors, such as those based on Emission Scenario Documents (ESD, Appendix R.16-2) or those developed by industrial sectors (SPERC fact sheets) can be used as a refinement option (Section R.16.3.5). If a refined release factor is applied, the operational conditions and RMM leading to this factor need to be documented in the environment related section of the exposure scenario.

### R.16.3.2. Local release estimation

Two scenarios are distinguished to assess the release to the environment at the local scale, as discussed in Section R.16.2:

- Industrial setting.
- Wide dispersive use.

The default parameters used in the release rates calculation, proposed in the present section are conservative and are suitable for a first iteration of the exposure assessment. The release estimation could be refined when more specific on-site data, including RMM and OC, are available (Section R.16.3.5).

#### R.16.3.2.1.Industrial setting scenario

The release rate (kg/day) to the environmental compartments is estimated on the basis of the tonnage used at the site.

The releases to water are by default treated in a municipal STP, before being discharged into surface water; however the availability and type of STP should always be checked and, adapted to site specific situation.

In order to estimate the release to the environment for an industrial setting, the following parameters are needed:

i. daily use at a site (tonnes/day); this is the amount used at one site and in one day for each life cycle stage (manufacture, formulation and industrial end use). It is used for the calculation of the exposure concentrations for the environment;

ii. annual use at a site (tonnes/year); this is the amount used in one site and in one year for each life cycle stage (manufacture, formulation and industrial end use). It is the starting point for the calculation of the exposure of man via the environment and (top) predators.

The two above mentioned parameters, together with other operational conditions and risk management measures, guarantee control of risk for all downstream users covered by the same exposure scenario .

By default, the daily use at a site is calculated from the total registrant's tonnage at the EU level for identified use, divided by the default number of release days depending on the tonnage of the substance manufactured or tonnage of mixture[7] formulated per year. It is assumed that the total tonnage is processed by at a single site (worst case).

The calculation of the default daily use, for each identified use, is reported in the following tables for manufacture, formulation and industrial end uses. "Tonnage" in the following tables is the total registrant's tonnage at EU level of manufactured substance or mixture containing the substance, supplied to an identified use, expressed in tonnes/year. The underlying assumption is that large tonnages are more likely to be manufactured or used continuously.

For manufacture

| Tonnage of the substance manufactured per year | N. of release days (days/year) | Daily use (tonnes/day) |
|---|---|---|
| Tonnage < 1000 | 20 | Tonnage/20 |
| 1000 < Tonnage < 10000 | 100 | Tonnage /100 |
| Tonnage> 10000 | 300 | Tonnage /300 |

For formulation

| Tonnage of mixture for the use (or group of uses) per year | N. of release days (days/year) | Daily use (tonnes/day) |
|---|---|---|
| Tonnage < 100 | 10[8] | Tonnage/10 |
| 100 < Tonnage < 2000 | 100 | Tonnage /100 |
| Tonnage > 2000 | 300 | Tonnage /300 |

For industrial end uses

| Tonnage of mixture for the use (or group of uses) per year | N. of release days (days/year) | Daily use (tonnes/day) |
|---|---|---|
| Tonnage < 1000 | 20 | Tonnage/20 |
| 1000 < Tonnage < 5000 | 100 | Tonnage /100 |
| Tonnage > 5000 | 300 | Tonnage /300 |

[7] The tonnage of mixture formulated or used in industrial uses, shown in the tables below, are used to set the number of emission days. Please remember that it is then necessary to refer the following assessment to the substance tonnage only. By default it is possible to assume that the percentage of substance in the mixture is 100 and therefore the tonnage of substance is equal to the tonnage of the mixture. It is possible to modify the percentage of substance in the mixture in further iterations and calculate the tonnage of substance according to the following formula: tonnage of substance (tonnes/year) = tonnage of mixture (tonnes/year) × fraction of substance in mixture.

[8] The 10 days for formulation compared to 20 days for manufacture and industrial end-uses is based on the consideration that very short production campaigns are more likely in processes of low complexity (like e.g. mixing).

The annual use at a site is set equal, by default, to 100% of the total registrant's tonnage at EU level for an identified use.

The release rate to an environmental compartment for an identified use is then calculated using the following general equation.

$$E_{local,IU,j} = Q_{daily,IU} \cdot RF_{IU,j} \cdot 1000 \qquad \textbf{(Equation R.16-1)}$$

Where:

$E_{local, IU, j}$: Release rate (kg/day) to the compartment "j" at the local scale for an identified use (IU).

$Q_{daily,IU}$ : Daily use (tonnes/day) at a site for an identified use (daily use and/or annual use divided by 365 days[9]).

$RF_{IU, j}$: Release factor (% or kg/kg) to compartment "j" for identified use. The default value is set by ERCs (see Section R.16.3.1.4)

For further iteration, the registrant can overwrite the daily and annual use, by using suitable and specific on-site, downstream user, market data, etc. if available or use specific release factors by describing the operational conditions and/or risk management measures (OC and RMM) controlling the release (e.g. with specific release factors which consider abatement strategies put in place at the site).

The refinement process is described in Section R.16.3.5.

#### R.16.3.2.2.Wide dispersive use scenario

The tonnage used for the release calculation for the wide dispersive use scenario is a fraction of the total registrant's tonnage at EU level which is used in a standard town of 10000 inhabitants.

In relation to releases to water, the scenario for both indoor and outdoor wide dispersive uses is based on the assumption that they occur in the urban infrastructure, are collected in a central public sewage system and are then treated by an STP.

For outdoor uses, this scenario can be considered as a reasonable worst case. Assuming that all releases occur on a paved surface of an urban infrastructure and are collected in a sewage system may be conservative, but this is balanced by the assumption that all releases to water are treated in an STP.

Direct releases to air and soil are not considered in the wide dispersive use scenario.

For wide dispersive uses, a daily wide dispersive use (average over a year) is assumed (tonnes/day). Consequently the same releases are used for the assessment of the risk for the environment and for man via the environment (and (top) predators).

The default daily wide dispersive use is estimated starting from the total registrant's tonnage at EU level for an identified use, and dividing it by:

- 10: fraction of the total registrant's tonnage at EU level used in the region (regional tonnage);
- 2000: fraction of the regional tonnage used in the standard town (20,000,000 inhabitants in the region / 10000 inhabitants in the standard town[10]);

[9] The annual use divided by 365 days is used for the calculation of the exposure of man via the environment and (top) predators.

[10] The reason why this factor is used for wide dispersive uses and not for industrial settings is that wide dispersive uses are assumed to be evenly distributed in the region.

- 365 (days/year): number of days in a year.

The resulting tonnage is multiplied by a safety factor of 4 to take into account geographical or temporal peaks in the use and the release of a substance, for example the use of anti-freeze compounds in window washing fluids for cars.

Therefore the fraction F of the total registrant's tonnage at EU level for identified use to be used by default at local scale (standard town) for a wide dispersive scenario is set equal to

$$F\ (\text{year/day}) = 4 / (10 \times 2000 \times 365\ \text{day/year}) = 5{,}5 \times 10^{-7}\ \text{year/day}.$$

The daily wide dispersive use is then calculated according to the following equation:

$$Q_{daily,IU}\ (\text{tonnes/day}) = \text{total registrant's tonnage at EU level (tonnes/year)} \times F\ (\text{year/day})$$

The same general equation (Equation R.16-1) is used when assessing the release rate to an environmental compartment for the identified wide dispersive use.

### R.16.3.3. Regional release estimation

All regional releases associated with the different identified uses, both industrial and wide disperse sources, are cumulated to estimate the total regional release (kg/day) to surface water, wastewater, air and soil. The regional releases associated with the different identified uses are based on the tonnage at regional level for each use and the same release factors used at local scale.

By default, the tonnage at the regional level for the industrial settings (i.e. manufacture, formulation and industrial uses) is set equal to 100% of the tonnage at EU level, while for wide dispersive uses it is set equal to the 10% of the registrant's supply volume at EU level. Releases at the regional scale are assessed for water, air and soil (including industrial soil). At this scale, also direct releases to soil are considered.

The default regional releases are therefore calculated, for each use, according to the following formula:

$$E_{regional,IU,j} = Q_{regional\ daily,IU} \cdot RF_{IU,j} \cdot 1000$$

Where:

J = environmental compartment (air, soil, wastewater)

$E_{regional,IU,j}$ (kg/day): release rate to the compartment "j" at the regional scale for an identified use (IU);

$Q_{regional\ daily,IU}$ (tonnes/day): average daily use at the regional scale for an identified use (IU) = regional tonnage for each use/365 days;

Regional tonnage for each use (tonnes/year) = 100% × total registrant's tonnage at EU level (for industrial setting);

Regional tonnage for each use (tonnes/year) = 10% × total registrant's tonnage at EU level (for wide dispersive uses);

$RF_{IU,j}$: Release factor (% or kg/kg) to compartment "j" for identified use. The default value is set by ERCs (see Section R.16.3.1.4)

If the registrant has more information (market data), the volume to be used for the regional calculation could be refined. The refinement process is describe in Section R.16.3.5.

As stated before, when calculating the total regional releases, by default, 80% (representing the EU average) of the wastewater is assumed to be treated in a STP and 20% to go directly to surface water without any treatment, regardless of the assumptions made about STP connection at local scale.

The formulas to be applied for the calculation of the total regional release to air, surface water, wastewater and soil are the following:

$E_{total,regional,air} = \sum E_{regional,IU,air}$

$E_{total,regional,soil} = \sum E_{regional,IU,soil}$

$E_{total,regional,wastewater} = \sum E_{regional,IU,wastewater} \times 80/100$

$E_{total,regional,surface\ water} = \sum E_{regional,IU,wastewater} \times 20/100$

where:

$E_{total,regional,wastewater}$ passes through an STP and, subsequently, is discharged in surface water.

**Continental release estimation**

As long as the activities related to a specific stage of the life cycle of a substance can be assumed to take place within a region, as it is often the case for manufacture, formulation and industrial uses, 100% of the whole registrant's tonnage at EU level is attributed to the regional scale.

When activities are more widely distributed over the EU, as is assumed for wide dispersive uses, only a fraction of the whole registrant's tonnage at EU level is attributed to the region (10% by default) while most of it (90% by default) is attributed to the continental scale. Therefore, for these life cycle stages, releases at continental scale will contribute as background to the regional concentration.

The continental release for each environmental compartment and for each stage can be calculated multiplying the continental tonnage by the release factor :

Continental release (kg/day) = continental tonnage (tonnes/year) × release factor × 1000 / 365

where continental tonnage = total registrant's tonnage at EU level– regional tonnage.

The total continental release for each environmental compartment is obtained by summing over all life cycle stages. If the fraction going to the region is changed in iteration, the continental release will also change.

A continental release estimation is also carried out for PBT substances. In this case, the whole EU-level tonnage is used for each life cycle stage to estimate the overall releases to the continental scale, due to registered tonnage as whole.

### R.16.3.4. Summary of the release patterns

As mentioned before, three scenarios (see Section R.16.2) are applied to reflect the pattern of release in space and time:

- Industrial setting scenario at a local scale (Section R.16.3.2.1)
- wide dispersive scenario at local scale (Section R.16.3.2.2)
- releases in a standard region for all identified uses (Section R.16.3.3)

The following table summarizes the environmental compartment where direct releases are considered, for each of these scenarios. The rationale behind these assumptions is explained throughout the previous paragraphs.

**Table R.16-1**: Direct releases to environmental compartments considered in the different scenarios

| Release compartment / Scenario | air | Water – Via STP[11] | Water – Direct | soil |
|---|---|---|---|---|
| Industrial setting - local scale | Y | Y | N | N |
| Wide dispersive uses - local scale | N | Y | N | N |
| Industrial settings –Total Regional / Wide dispersive uses – Total Regional | Y | Y (80%) | Y (20%) | Y |

*Y: release pattern taken into account in the exposure estimation scenario*
*N: release pattern not supported by the scenario*

## R.16.3.5. Refinement options for iteration

The release estimation as described in the previous Sections R.16.3.2 (local scale) and R.16.3.3 (regional scale) should be seen as a conservative first tier evaluation, for example when assessing a tentative ES. If specific information on market data, downstream uses and release of the substance is available, a higher tier assessment may be performed.

The release estimation can most directly be improved by refining the daily or annual use and the release factor, as will be detailed later.

Furthermore, the DU can demonstrate that he operates within the conditions of the ES by scaling up or scaling down the factors used for the release calculation, for example using the actual use amount, type of risk management measures and their actual effectiveness, and operational condition (e.g using the actual dilution factor in a river) having an effect on the release rate or the exposure calculation. This means that different combinations of local daily amounts, release factors (driven by OC/RMM) and receiving water volume may result in exactly the same local concentration. Please note: Where the downstream user scales down the local amount and/or scales up the dilution factor in the river, in order to compensate for a less effective risk management measures or higher initial release factors, this has an impact on the regional assessment carried out by the registrant. The registrant may need to correct the assumed release factor in order to keep his assessment valid. Thus, a downstream user should communicate back to the supplier/registrant, that he has implemented risk management measures with a lower effectiveness as required in the ES and provide some details on the nature and the effectiveness of these measures.

### R.16.3.5.1. Daily/annual use

**Local scale**

In the context of the *industrial setting scenario*, the daily or annual use at a site of a substance for an identified use can be overwritten by the registrant, on the basis of:

[11] The releases to water are by default treated in a municipal STP, before being discharged into surface water; however the availability and type of STP should always be checked and, adapted to site specific situation.

- Site specific information, such as the actual daily use in the manufacturing stage (readily accessible to the registrant)
- Information on the actual amount used by the largest downstream user (formulators and industrial end uses).

When overwriting either the daily or the annual use the number of release days should be set equal to the Annual Use (tonnes/year) divided by the Daily Use (tonnes/day), but should never be higher than 365 days.

The daily or annual use at the site should ensure control of risk for all registrant's downstream users.

The sales database of the registrant or supplier may be able to identify the highest sales tonnage per year for a single user, assuming that the large users buy directly without a distributor in between. By contrast, the real daily use at the users' sites is generally unknown to the registrant. If the registrant wants to overwrite the daily use from the default assessment for a specific identified use, he needs to collect information from representative downstream users, asking them for the amount used in a single day.

For wide dispersive uses, it is generally more difficult to have data useful for refining the daily wide dispersive use. However, should they be available, they can be used by the registrant. Moreover, if the registrant has sufficient information to demonstrate that the use of the substance is evenly distributed in space and time throughout the region (e.g. for detergents), it is possible to divide the default tonnage by a factor of 4 (Section R.16.3.2.2) and to use this tonnage when performing the calculations. This has to be justified and documented in the CSR.

**Regional scale**

The estimation of the regional tonnage depends on the geographical distribution of the substance's use. By default, 100% of the whole registrant's tonnage at EU level is assigned to the region for manufacture, formulation and industrial uses and 10% of it for wide dispersive uses . However, market data could be used to overwrite the default for the region with a percentage that corresponds to the actual situation.

The refined regional tonnage can also be used for the local scale calculation of releases from wide dispersive uses (Section R.16.3.2.2) instead of the default 10% of the registrant's tonnage at EU level..

When refining the regional tonnage for both industrial settings and wide dispersive uses, the corresponding release to the continental scale needs to be adjusted.

### R.16.3.5.2. Release factor/rate

The release factor associated with Environmental Release Categories can be used for a first tier assessment. However, better information may be available that could then be used instead. In particular for identified point sources, specific information on release factors or release rates[12] may be available. If this is the case, they should be refined and these data used for higher tier assessment.

The release factor or rate can also be refined by taking into account Risk Management Measures and Operational Conditions (RMM/OC). In this case, it is important to explicitly link such RMM/OC to the release factor/rate and communicate them properly to the downstream user. Examples of this kind of refinement is the use of actual settings for the local STP (based on refined substance

[12] They are linked to the release factor by the formula: release factor = release rate/used amount, both expressed in the same units and relative to the same period of time (see equation R.16-1)

properties and/or modified versions of the SimpleTreat model, see Section R.16.6.5.4) rather than default parameters.

It is also possible to refine the default release factors by taking into consideration substance parameters such as vapour pressure, water solubility and boiling point.

There are several sources for the refinement of release factors or release rates. One of them is the above mentioned Emission Scenario Documents (ESDs) (see Appendix R.16-2). An ESD is a document that describes the sources, production processes, pathways and use patterns with the aim of quantifying the releases of a substance into water, air, soil and/or solid waste.

Care needs to be taken to provide an appropriate description of the link between the release factors derived from ESDs and the corresponding OC/RMM to be described in the exposure scenario.

Other sources of information can be considered when refining release factors:

- Sector specific ERCs, the so called SPERCs, developed by industrial sector organisations can be used in place of the conservative ERCs. As far as possible, SPERCs have to be linked to the RMM and OC driving the release estimation;
- Standard practice of RMM/OC normally adopted by an industrial sector
- Site specific RMM/OC put in place by single industries, mainly at the manufacturing stage, where a high level of information is expected to be accessible to the registrant.
- Permits set by authorities, determining maximum release rates into environmental compartments (surface water and air).
- Release rate measurements, mainly when licence and permits set by authorities require frequent and regular monitoring of releases to environmental compartments. These data are normally available for the first three life cycle stages: (i) Production, (ii) Formulation, and (iii) Industrial Use.
- A and B tables of the TGD (2003) are acceptable as long as they clearly provide more specific information on RMM/OC. Otherwise, they are considered insufficient to meet the REACH requirements.

With respect to the outdoor use of long-life articles with a low release, the release factor also takes into account the service lifetime of the article. By default this is set to 20 years which is multiplied with a default average release from a single article of 0.16% over a year (see appendix R16.1). Both the release factor from a single article and the service lifetime can be refined. The default service lifetime can be refined based on market data. The release factor from the single article can be refined based on measured data or other models. Please note: The factors provided here are derived for additives in plastic (see Emission Scenario Document on plastic additives, OECD 2004b). If relevant, the registrant should also make himself aware whether the default assumptions also apply to other materials.

If the release rate at local scale is overwritten, the release factor should be updated accordingly (on the basis of the overwritten release rate and the local daily tonnage) and used to compute the regional and continental release.

# R.16.4. Measured data

## R.16.4.1. Introduction and general principles

A general introduction to the use of measured exposure data in the process of estimating exposure can be found in Section D.5.2. The use of measurements encompasses

a) actual measured concentrations of the substance in a particular environmental compartment which can be used to facilitate the interpretation of model output and, eventually can be used as Predicted Environmental Concentrations (PEC)[13]

b) other measured parameters that can be used to support the release and exposure calculation (e.g. measured release rates and measured removals in sewage treatment facilities). Concentrations can be measured either in the receiving environment or in the release.

Measurements can be used as:

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

Measured data at the local scale, representative for situation a) have to be clearly linked with the operational conditions and risk management measures described in the Exposure Scenario.

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 quality and representativeness according to the criteria below. They are used together with calculated environmental concentrations when deciding on the environmental concentration to be used for exposure estimation (see also 0). 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 values.

The evaluation should follow a stepwise procedure:

- adequate measured 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.16.4.2);
- the data should be assigned to local or regional scenarios by taking into account the sources of release and the environmental fate of the substance (Section R.16.4.3);
- 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 comparison of measured data and a calculated PEC (Section R.16.6.6.9).

Further guidance on metal-specific aspects in selecting measured data can be found in Appendix R.7.13-2.

[13] In the default assessment, initial full mixing is assumed between the wastewater and the river water. Therefore calculated PECs describe an equal distribution. In contrast, measured concentrations can be influenced by plumes. Depending on the point of sampling this could lead to an under-/overestimation of the PEC.

### R.16.4.2. Selection of adequate measured data

The available measurements have to be assessed first, before using them in release and exposure estimation. The following aspects should be considered:

- Quality of the sampling and analytical techniques
- Selection of representative data for the environmental compartment of concern
- Outliers
- Treatment of values below the limit of quantification (LOQ)
- Data comparability

Registrant should also consider local regulatory requirements where applicable. Local agencies may have specific requirements on how data should be statistically analysed. It is advisable to obtain as much useful information on release and 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, based on the available contextual information, are given in Table R.16-2 (based on 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 and the availability of information necessary to assess the representativeness of the sample.

**Table R.16-2**: Quality criteria for use of existing measured data (based on OECD, 2000)

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

Notes to Table R.16-2

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 substance. 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 substance under study is released as a discontinuous emission showing variations in both volume and concentration with time.

*Quality of the sampling and analytical techniques*

A quality check should be performed for both sampling and analytical techniques. The applied sampling techniques (e.g. use clean and appropriate containers to avoid contamination of the sample), sample shipping and storage, sample preparation for analysis and analysis must take into account the physico-chemical properties of the substance (e.g. the substance may degrade in presence of light, oxygen, may be volatile, etc. ). For further information, see EC, 2009a. Measured data that are of insufficient quality should not be used in the release and exposure estimation.

*Selection of representative data for the environmental compartment of concern*

The representativeness of the monitoring data is related to the objective of the monitoring programme from which they originate. Monitoring programmes may be designed to cover a large spatial area (high number of stations over a large territory), to achieve a high spatial resolution (high number of stations per area unit), or to monitor only one point source release. Monitoring programmes may be designed to assess temporal trends (high sampling frequency), or to monitor the status of a site at a given time.

For the purpose of risk assessment, there are two distinct aspects to consider:

- 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.

- Whether the sampling site(s) represent a local or regional scenario. Samples taken at sites directly influenced by the release should be used to describe the local scenario, while samples taken at larger distances may represent the regional concentrations.

For example, when evaluating the representativeness of discharges from a wastewater treatment plant, the number of samples and the sampling frequency should be adapted *inter alia* to the type of treatment process (including retention time), environmental significance and nature of the substance and effluent variability. Effluent quality and quantity vary over time in terms of volumes discharged and constituent concentrations. Variations occur due to a number of factors, including changes in human activity, changes in production cycles, variation performance of wastewater treatment systems in particular in responses to influent changes and changes in climate. Even in industries that operate continuous processes, maintenance operations, such as back-washing of filters, cause peaks in effluent constituent concentrations and volumes (US-EPA, 1991).

Data from a prolonged monitoring programme, where seasonal fluctuations are already included, are of special interest. However too old data may not be representative of the risk management measures and operating conditions described in the exposure scenario. Indeed, pollution may have been reduced or increased by the implementation of risk management measures or of operation conditions, by new releases or change in release pattern.

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 90$^{th}$ percentile if the distribution function has only one mode), and the required 90$^{th}$ percentile values, mean or median values of this distribution could be used in the PEC prediction. The mean of the 90$^{th}$ 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. A 90$^{th}$ percentile concentration may also be calculated. In most instances a log-normal distribution of concentrations can be assumed. 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 release episodes of short duration but of high concentration discharge. In these cases, mainly for PEClocal calculations, a more realistic picture of the release pattern can be obtained from the highest value of average concentrations during release episodes.

When considering data about dilution, it should be taken into account that flow rates of receiving waters are typically highly fluctuating. In this case, the 10$^{th}$ percentile, corresponding to the low flow rate, should always be used. If only time averaged flow rates are available, the flow rate for dilution purposes should be estimated as one third of the average (Section R.16.6.6.2).

When releases 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 also be used to extend flux measures to long-term estimates. Release data of higher quality may become available when the European Pollutant Release and Transfer Register (E-PRTR) is fully implemented[14].

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 time lags. 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

[14] http://ec.europa.eu/environment/air/pollutants/stationary/eper/index.htm

future situation. This should be considered when comparing such a PEC with measured data representing a non-steady-state.

Representative and reliable measured data from monitoring programmes or from literature should be compiled as tables and annexed to the risk assessment report. The measured data should be presented with the relevant contextual information in the following manner:

| Location | Substance | Concentration | Period | Remark | Reference |
|---|---|---|---|---|---|
| Country<br>Location | substance or metabolite | Units: [µg/L], [ng/L] [mg/kg], etc<br>Data<br>- mean<br>- average<br>- range<br>- percentile<br>- daily<br>- weekly<br>- monthly<br>- annual<br>- etc. | month, year | limit of quantitation (LOQ)<br>relevant information on analytical method<br>analytical quality control<br>Number of measured values and number of values above the LOQ. | Literature reference |

Concentrations can be measured in the receiving environment or in the release. If the reported concentration has been measured directly in the release, this should be clearly indicated in the reporting table.

*Outliers*

Outliers can be defined as unexpectedly high or low values. Outliers may reflect:

- sampling or analytical flaws
- other errors (e.g. in data capture or treatment)
- random variability
- an accidental, increased or new release, a recent change in release pattern or a newly discovered occurrence in a specific environmental compartment

Sampling or analytical errors could potentially be demonstrated after quality check of the sampling and analytical methodologies (see previous section).

Data with evident mistakes (e.g. wrong units, errors in data capture, etc.) should be discarded or corrected.

Measured concentrations caused by an accidental release should not be considered in the exposure estimation.

Outliers are, by definition, infrequent and implausible measurements, i.e. unlikely to be explained by the random variability of the data alone. The probability of deviation of a measurement from the rest of the measurements due to random variability of the data can be quantified assuming a

statistical distribution of the data (e.g. using the Grubbs' test (Grubbs, 1969)). But simpler empirical criteria may also be applied to detect outliers[15] (EC, 1999; USEPA (2006)).

Where outliers have been identified their inclusion/exclusion should be discussed and justified. The data should be critically examined with regard to the possible explanations listed above. Extreme values may reflect an actual sudden increase of releases, discharges or losses of the substance, and this should of course be considered in the assessment.

*Treatment of measurements below the limit of quantification*

A commonly encountered problem when working with monitoring data is the use of concentrations below the limit of quantification (LOQ) of the analytical method. At very low concentration levels, random fluctuations become preponderant and the uncertainty of the measurement is significantly high. Clearly at concentrations approaching the LOQ of an analytical method, percentage errors will be greater than at higher concentrations.

All measurements below the LOQ constitute a special problem and should be considered on a case-by-case basis. It should be checked first that the matrix analysed is the most appropriate (e.g. hydrophobic substances should be analysed in sediment or biota rather than in water) and that the analytical technique being used is suitable and sensitive enough (EC, 2009a). In the absence of adequate method of analysis for the substance or in case of substances that are toxic in extremely low concentrations, one approach that could be considered would be to use a value corresponding to LOQ/2 (EC, 2009b). As this method could heavily influence the assessment (e.g. when calculating a mean or a standard deviation), other methods may also be considered (e.g. assuming same distribution of data below and above the LOQ) (EC, 1999).

*Data comparability*

Another important point to check is the comparability of the data. 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).

Samples of living organisms (= biota) 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 a release 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. But concentrations in biota can vary depending on species (mainly because of different feeding habits and different metabolic pathways) and on other factors such as age, size, lipid content, sex, season etc. These pieces of information should be considered carefully before comparing or aggregating measured concentrations in biota. For instance, normalisation for the lipid content is a common practice when working with monitoring data in biota. A specific guidance on chemical monitoring of sediment and biota is currently under preparation for the implementation of the Water Framework Directive.

[15] For example the following approach may be used: $\log(X_i) > \log(p_{75}) + K(\log(p_{75}) - \log(p_{25}))$

Where Xi is the concentration, above which a measured value may be considered an outlier, pi is the value of the ith 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.

### R.16.4.3. Allocation of the measured data to a local or a regional scale

Concentrations measured in the receiving environment should be allocated to a local or regional scale in order to define the nature of the environmental concentration that is derived.

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

## R.16.5. Partitioning and degradation

In this section the derivation of the substance's fate and distribution characteristics is described. After entering the environment, substances 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 substance in an organism than in its immediate environment, including food. Substances may also be transformed into other substances ('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.16.5.3.1)
- Partitioning between air and water (volatilisation) (detailed in Section R.16.5.3.2)
- Partitioning between solids and water in soil, sediment and suspended matter (adsorption and desorption) (detailed in Section R.16.5.3.3 and R.16.5.3.4)
- Partitioning between water/solids and biota (bioconcentration and biomagnification) (detailed in Section R.16.5.3.5)
- Transformation processes in the environment. Both biological (biotic, detailed in Sections R.16.5.4.4, R.16.5.4.5) and abiotic (detailed in Sections R.16.5.4.1, R.16.5.4.2, R.16.5.4.3) 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. Most of the guidance has been developed mainly from the experience gained on organic substances. This means that the used methodology cannot always be applied directly to metals without modifications. Specific guidance on how to model fate and distribution characteristics for metals can be found in Appendix R.7.13-2.

There are significant limitations in the applicability of any of the environmental fate models (e.g. fugacity models for various compartments and overarching models like EUSES) which depend on LogKow and Henry's law for use with soluble nanomaterials (and other insoluble particles or substances). As no broadly accepted and scientifically valid models are available for estimating environmental fate of nanomaterials, M/Is are advised to collect measurement information on environmental release, fate (including (dis)aggregation and (dis)agglomeration) and level in the environment where possible.

### R.16.5.1. 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.16.5.2. 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.16.5.3. Partition coefficients

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

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.16.5.3.6. 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.16.5.3.1. 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.

$$Fass_{aer} = \frac{CONjunge \bullet SURF_{aer}}{VPL + CONjunge \bullet SURF_{aer}} \qquad \textbf{(Equation R.16-2)}$$

Explanation of symbols

| | | | |
|---|---|---|---|
| CONjunge | constant of Junge equation | [Pa·m] | * |
| $SURF_{aer}$ | surface area of aerosol particles | [$m^2 \cdot m^{-3}$] | * |
| VPL | Sub-cooled liquid vapour pressure | [Pa] | |
| $Fass_{aer}$ | fraction of the substance associated with aerosol particles | [-] | |

* as a default the product of CONjunge and SURFaer 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):

$$VPL = \frac{VP}{e^{6.79 \bullet (1-\frac{TEMP_{melt}}{TEMP})}}$$ **(Equation R.16-3)**

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.16.5.3.2. 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 $K_{air\text{-}water}$ (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.16-5). For water miscible compounds, direct measurement of the Henry's Law constant is recommended. For detailed information, see Section R.7.1.22.

$$HENRY = \frac{VP \bullet MOLW}{SOL}$$ **(Equation R.16-4)**

$$K_{air\text{-}water} = \frac{HENRY}{R \bullet TEMP}$$ **(Equation R.16-5)**

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$^{-1}$] | |
| $K_{air\text{-}water}$ | 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.16.5.3.3. 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.16.6.5) 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 Koc 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.16-9.

$$Kp_{comp} = Foc_{comp} \bullet Koc \quad with\ comp \in \{soil\ ,\ sed\ ,\ susp\}$$ **(Equation R.16-6)**

Explanation of symbols

| | | | |
|---|---|---|---|
| Koc | partition coefficient organic carbon-water | [l·kg$^{-1}$] | data set/Ch. 4 |
| $Foc_{comp}$ | weight fraction of organic carbon in compartment *comp* | [kg·kg$^{-1}$] | Table R.16-9 |
| $Kp_{susp}$ | partition coefficient solid-water in suspended matter | [l·kg$^{-1}$] | |
| $Kp_{sed}$ | partition coefficient solid-water in sediment | [l·kg$^{-1}$] | |
| $Kp_{soil}$ | partition coefficient solid-water in soil | [l·kg$^{-1}$] | |

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

$$K_{comp-water} = \frac{Ctotal_{comp}}{Cporew_{comp}}$$

$$K_{comp-water} = Fair_{comp} \cdot K_{air-water} + Fwater_{comp} + Fsolid_{comp} \cdot \frac{Kp_{comp}}{1000} \cdot RHOsolid$$

**(Equation R.16-7)**

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

Explanation of symbols

| | | | |
|---|---|---|---|
| $Fwater_{comp}$ | fraction water in compartment *comp* | $[m^3 \cdot m^{-3}]$ | Table R.16-9 |
| $Fsolid_{comp}$ | fraction solids in compartment *comp* | $[m^3 \cdot m^{-3}]$ | Table R.16-9 |
| $Fair_{comp}$ | fraction air in compartment comp (only relevant for soil) | $[m^3 \cdot m^{-3}]$ | Table R.16-9 |
| RHOsolid | density of the solid phase | $[kg \cdot m^{-3}]$ | 2,500 |
| $Kp_{comp}$ | solids-water part. coeff. in compartment *comp* | $[l \cdot kg^{-1}]$ | Equation R.16.-6 |
| $K_{air-water}$ | air-water partitioning coefficient | [-] | Equation R.16.5 |
| $K_{soil-water}$ | soil-water partitioning coefficient | $[m^3 \cdot m^{-3}]$ | |
| $K_{susp-water}$ | suspended matter-water partitioning coefficient | $[m^3 \cdot m^{-3}]$ | |
| $K_{sed-water}$ | sediment-water partitioning coefficient | $[m^3 \cdot m^{-3}]$ | |

### R.16.5.3.4. 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.16.5.3. However, the techniques that allow such an extrapolation are also largely based on freshwater data sets. Therefore, to assess the distribution of substance 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 substance with other compartments. To a large extent, these effects are associated with differences in water solubility and/or speciation of the substance, compared with freshwater. The relatively high levels of dissolved inorganic salts in seawater generally decrease the solubility of a substance (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 substances 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.16.5.3.5. Bioconcentration and biomagnification (biota-water/solids partitioning)

Bioconcentration and bioaccumulation may be of concern for lipophilic organic substances 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:

$$BCF_{org} = \frac{C_{org}}{C_{water}} \; or \; \frac{k_1}{k_2}$$ **(Equation R.16-8)**

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 substances, 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 these substances 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 BCFfish*

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.16.6.7.

*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.16-3 can be used (see also Section R.7.10.4.4). For further explanation, see Section R.16.6.7 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.16-3 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.16-3**: Default BMF values for organic substances with different log $K_{ow}$ or BCF in fish

| log Kow | 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 substances 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 Kow, 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.16.5.3.6. 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.16.5.4. 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 Appendix R.7.13-2.

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.16.5.4.1. 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.16-9. 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:

$$DT50(X\,°C) = DT50(t) \cdot e^{(0.08 \cdot (T - X))}$$ **(Equation R.16-9)**

where X = 12°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:

$$khydr_{water} = \frac{\ln 2}{DT50\, hydr_{water}}$$ **(Equation R.16-10)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $DT50hydr_{water}$ | half-lifetime for hydrolysis in surface water | [d] | data set |
| $khydr_{water}$ | first order rate constant for hydrolysis in surface water | [$d^{-1}$] | |

### R.16.5.4.2. 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:

$$kphoto_{water} = \frac{\ln 2}{DT50\, photo_{water}}$$ **(Equation R.16-11)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $DT50photo_{water}$ | half-lifetime for photolysis in surface water | [d] | data set |
| $kphoto_{water}$ | first order rate constant for photolysis in surface water | [$d^{-1}$] | |

### R.16.5.4.3. 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 (kOH in cm3.molecule-1.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:

$$kdeg_{air} = k_{OH} \bullet OHCONC_{AIR} \bullet 24 \bullet 3600$$ **(Equation R.16-12)**

Explanation of symbols

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

*The global annual average OH-radical concentration can be assumed to be 5.105 molecules.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 substance 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.16.5.4.4.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.16-4 were derived from the biodegradation screening tests. All constants in Table R.16-4 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. SimpleTreat[16], are based. The same applies to STP-measured data, i.e., in-situ influent/effluent measurements.

**Table R.16-4**: Elimination in sewage treatment plants:

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

| Test result | Rate constant k·($h^{-1}$) |
|---|---|
| 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.16.5.4.5.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 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.16-9. 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.16-5 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.16-5) and 300 – 30,000 days in soil and sediment (Table R.16-6) will only affect the predicted regional concentration provided that the residence time of the substance is

[16] 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

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.16-5 and Table R.16-6.

**Table R.16-5**: 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.16-5:

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.16-5 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.16-5) should therefore be regarded as a “the realistic worst-case concept”. An OECD guidance document for classification of substances 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 Kp 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 Kp-values there is evidence that some sort of Kp dependence exists. Therefore degradation half-life classes for (bulk) soil, partly based on Kp are presented in Table R.16-6. 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.16-6**: Half-lives (days) for (bulk) soil based on results from standardised biodegradation test results

| $Kp_{soil}$ [$l \cdot kg^{-1}$] | 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:

$$kbio_{soil} = \frac{\ln 2}{DT50\,bio_{soil}}$$ **(Equation R.16-13)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $DT50bio_{soil}$ | half-life for biodegradation in bulk soil | [d] | Table R.16-6 |
| $kbio_{soil}$ | 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:

$$kbio_{sed} = \frac{\ln 2}{DT50\,bio_{soil}} \cdot Faer_{sed}$$ **(Equation R.16-14)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $DT50bio_{soil}$ | half-life for biodegradation in bulk soil | [d] | Table R.16-6 |
| $Faer_{sed}$ | fraction of the sediment compartment that is aerobic | $[m^3 \cdot m^{-3}]$ | 0.10 |
| $kbio_{sed}$ | 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.16.5.4.6. 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 PECregional, 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.

$$k\deg_{water} = khydr_{water} + kphoto_{water} + kbio_{water}$$ **(Equation R.16-15)**

Explanation of symbols

| | | | |
|---|---|---|---|
| khydrwater | first order rate constant for hydrolysis in surface water | $[d^{-1}]$ | Equation R.16-11 |
| kphotowater | first order rate constant for photolysis in surface water | $[d^{-1}]$ | Equation R.16-10 |
| kbiowater | first order rate constant for biodegradation in surface water | $[d^{-1}]$ | Table R.16-5 |
| Kdegwater | Total first order rate constant for degradation in surface water | $[d^{-1}]$ | |

### R.16.5.4.7. 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 substance 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 substances, no test data from marine simulation tests are yet available. For many substances 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.16-7.

**Table R.16-7**: 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.16-7:

1) Half-lives from Table R.16-7.
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.16.6.6.8.

The half-lives for the marine environments that are described in Table R.16-7 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.16-7).

## R.16.6. Exposure and intake estimation

Exposure of the environment is the result of the release of substances (Section R.16.3), which may partly be degraded/removed due to treatment facilities (Section R.16.6.3.3), subsequent distribution and degradation within the environment (Section R.16.5). Secondary poisoning (section R.16.6.7) of predators and intake of man via the environment (Section R.16.6.8) is calculated based on the environmental exposure concentrations in water, air, soil.

### R.16.6.1. 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.16.6.8).

**Table R.16-8**: Derivation of PEC-values

| Target | Medium of exposure | Exposure scenario | | | | |
|---|---|---|---|---|---|---|
| | | regional | Section | local | Section | |
| Aquatic com-partment (incl. Marine environ-ment) | surface water | steady-state concentration in surface water | R.16.6.6.8 | concentration during release period taking into account dilution, sorption, and, if relevant, sedimentation, volatilisation and degradation | | R.16.6.6.2 |
| | sediment | steady-state concentration in sediment | | equilibrium concentration in freshly deposited sediment, related to the local surface water concentration | | R.16.6.6.3 |
| 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 | | R.16.6.6.6 |
| | ground water | steady-state concentration in groundwater under agricul-tural soil | | concentration in groundwater under agricultural soil. | | R.16.6.6.7 |
| Air compartment | air | steady-state concentration in air | | concentration in air, at 100 m from point source or STP | | R.16.6.6.1 |
| Microorganisms | STP aeration tank | - | - | concentration during release period | | R.16.6.6.2 |

## R.16.6.2. Input to exposure estimation calculations

Input into the exposure estimation calculations are:

- Substance properties as described in Section R.16.5.1
- Release rates as described in Section R.16.3
- Removals and distribution in waste treatment systems derived in Section R.16.6.5.4,

- Partition coefficients and degradation rates derived in Section R.16.5

For full details, read Section R.16.6 and Section R.16.6.7

## R.16.6.3. Principles

Two types of PEC-values are derived to be used in the further risk assessment: the regional concentration (PECregional) and the local concentration (PEClocal). 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 substance 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 releases 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 substances 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.16.6.6.8.

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 PEClocal 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.16.6.4 the main generic characteristics of the ‘standard’ environments are presented.

The environmental distribution estimation of a substance 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.16.6.6.8.

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.16-4: 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 release is counted twice at the local scale: not only due to the local release, but the same release is also responsible for the background concentration of the region.

### R.16.6.3.1. Local environmental distribution

Distribution on the local scale is assessed in the vicinity of point sources. (Figure R.16-2) shows the relationship between the local release 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.16.6.4.

#### R.16.6.3.2. Regional distribution

For calculating the regional PEC, the multi-media fate-model SimpleBox[17] is used. The basic characteristics of this model are shown in Figure R.16-3. A description of the assumptions made is given in Section R.16.6.6.8.

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;

#### R.16.6.3.3. Continental distribution

Concentrations in air and water are also estimated at a continental scale (Europe) to provide inflow concentrations for the regional environment (Figure R.16-4). These concentrations are also derived using the SimpleBox model. The continental concentrations are not used as endpoints for exposure in the risk characterisation.

#### R.16.6.3.4. 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.16.7.1 and R.16.7.2).

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 substance 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.16.6.5.

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

### R.16.6.4. Characterization of environmental compartments

In this section, the following parameters are derived:

- definition of the standard environmental characteristics;
- 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.16-9, 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.16-9. When more specific information is available on the location of the release sources, this information can be applied in refinement of the PEC by deviating from the parameters of Table R.16-9.

Several other generic environmental characteristics, mainly relevant for the derivation of PECregional (e.g. the sizes of the environmental compartments, mass transfer coefficients) are given in Section R.16.6.6.8, Table R.16-12 and Table R.16-14.

**Table R.16-9**: Characterisation of environmental compartments

| Parameter | Symbol | Unit | Value |
|---|---|---|---|
| General | | | |
| Density of the solid phase | RHOsolid | $[kg_{solid} \cdot m_{solid}^{-3}]$ | 2,500 |
| Density of the water phase | RHOwater | $[kg_{water} \cdot m_{water}^{-3}]$ | 1000 |
| Density of air | RHOair | $[kg_{air} \cdot m_{air}^{-3}]$ | 1.3 |
| Temperature (12°C) | TEMP | [K] | 285 |
| Surface water | | | |
| Concentration of suspended matter (dry weight) | $SUSP_{water}$ | $[mg_{solid} \cdot l_{water}^{-1}]$ | 15 |
| Suspended matter | | | |
| Volume fraction solids in susp. Matter | $Fsolid_{susp}$ | $[m_{solid}^{3} \cdot m_{susp}^{-3}]$ | 0.1 |
| Volume fraction water in susp. Matter | $Fwater_{susp}$ | $[m_{water}^{3} \cdot m_{susp}^{-3}]$ | 0.9 |
| Weight fraction organic carbon in susp. solids | $Foc_{susp}$ | $[kg_{oc} \cdot kg_{solid}^{-1}]$ | 0.1 |
| Sediment | | | |
| Volume fraction solids in sediment | $Fsolid_{sed}$ | $[m_{solid}^{3} \cdot m_{sed}^{-3}]$ | 0.2 |
| Volume fraction water in sediment | $Fwater_{sed}$ | $[m_{water}^{3} \cdot m_{sed}^{-3}]$ | 0.8 |
| Weight fraction organic carbon sediment solids | $Foc_{sed}$ | $[kg_{oc} \cdot kg_{solid}^{-1}]$ | 0.05 |
| Soil | | | |
| Volume fraction solids in soil | $Fsolid_{soil}$ | $[m_{solid}^{3} \cdot m_{soil}^{-3}]$ | 0.6 |
| Volume fraction water in soil | $Fwater_{soil}$ | $[m_{water}^{3} \cdot m_{soil}^{-3}]$ | 0.2 |
| Volume fraction air in soil | $Fair_{soil}$ | $[m_{air}^{3} \cdot m_{soil}^{-3}]$ | 0.2 |
| Weight fraction organic carbon in soil solids | $Foc_{soil}$ | $[kg_{oc} \cdot kg_{solid}^{-1}]$ | 0.02 |
| Weight fraction organic matter in soil solids | $Fom_{soil}$ | $[kg_{om} \cdot kg_{solid}^{-1}]$ | 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:

$$RHO_{comp} = Fsolid_{comp} \bullet RHOsolid + Fwater_{comp} \bullet RHOwater + Fair_{comp} \bullet RHOair$$
$$with\ comp \in \{soil, sed, susp\}$$

**(Equation R.16-16)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Fx_{comp}$ | fraction of phase x in compartment comp | $[m^3 \cdot m^{-3}]$ | Table R.16-9 |
| RHO*x* | density of phase *x* | $[kg \cdot m^{-3}]$ | Table R.16-9 |
| $RHO_{comp}$ | 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.16.6.5. Wastewater treatment – estimation of PECstp

In this section, the following parameters are derived:

- release from a sewage treatment plant to air (to be further used in PECair estimation);
- concentration in sewage sludge (to be further used in PECsoil estimation);
- concentration in effluent of a sewage treatment plant (to be further used in PECwater 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.16.6.5.1. 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 releases 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.16.6.6.8) 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.16.6.5.2. 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.16.6.5.3. 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.16.6.5.4. 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.16.5.3.2), 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.

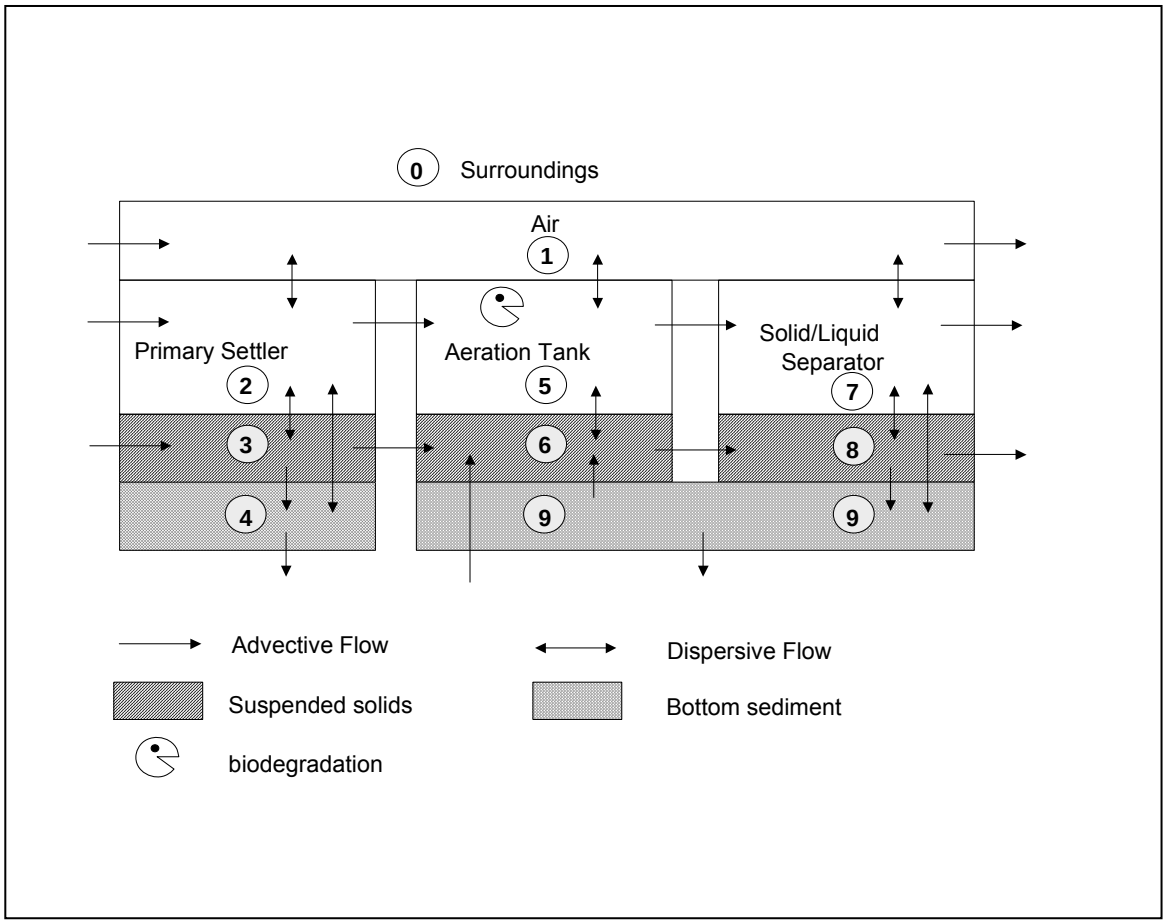



**Figure R.16-5**: Schematic design of the sewage treatment plant model SimpleTreat

For the purpose of modelling a STP, the rate constants presented in Table R.16-4 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 release data pertaining to air, water, and sludge as a function of Henry's Law constant and log Kow for the different biodegradation categories. If no specific measured biodegradation rate data are available for a particular substance, the tabulated values from Table R.16-4 and Appendix R.16-3 should be used.

Typical characteristics of the standard sewage treatment plant are given in Table R.16-10. 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.16-10**: 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 | [$l \cdot d^{-1} \cdot eq^{-1}$] | 200 |
| Surplus sludge per inhabitant | SURPLUSsludge | [$kg \cdot d^{-1} \cdot eq^{-1}$] | 0.011 |
| Concentration susp. matter in influent | $SUSPCONC_{inf}$ | [$kg \cdot m^{-3}$] | 0.45 |

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

Input

| | | | |
|---|---|---|---|
| HENRY | Henry's law constant | [$Pa \cdot m^3 \cdot mol^{-1}$] | Equation R.16.4 |
| Kow | octanol-water partitioning coefficient | [-] | data set |
| $kbio_{stp}$ | first-order rate constant for biodegradation in STP | [$d^{-1}$] | Table R.16-4 |

Output

| | | |
|---|---|---|
| $Fstp_{air}$ | fraction of release directed to air by STP | [-] |
| $Fstp_{water}$ | fraction of release directed to effluent by STP | [-] |
| $Fstp_{sludge}$ | fraction of release 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 release to wastewater and the influent flow to the STP. The influent flow equals the effluent discharge.

$$Clocal_{inf} = \frac{Elocal_{water} \cdot 10^6}{EFFLUENT_{stp}}$$ **(Equation R.16-17)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Elocal_{water}$ | local release rate to (waste) water during episode | [$kg \cdot d^{-1}$] | Equation R.16-1 |
| $EFFLUENT_{stp}$ | effluent discharge rate of STP | [$l \cdot d^{-1}$] | Equation R.16-19 |
| $Clocal_{inf}$ | concentration in untreated wastewater | [$mg \cdot l^{-1}$] | |

### R.16.6.5.5. 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:

$$Clocal_{eff} = Clocal_{inf} \cdot Fstp_{water}$$ **(Equation R.16-18)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{inf}$ | concentration in untreated wastewater | [mg·l$^{-1}$] | Equation R.16-17 |
| $Fstp_{water}$ | fraction of release directed to water by STP | [-] | Appendix R.16-3 |
| $Clocal_{eff}$ | concentration of substance in the STP effluent | [mg·l$^{-1}$] | |

If no specific data are known, EFFLUENTstp 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.16-10):

$$EFFLUENT_{stp} = CAPACITY_{stp} \cdot WASTEWinhab$$ **(Equation R.16-19)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $CAPACITY_{stp}$ | capacity of the STP | [eq] | Table R.16-10 |
| WASTEWinhab | sewage flow per inhabitant | [l·d$^{-1}$·eq$^{-1}$] | Table R.16-10 |
| $EFFLUENT_{stp}$ | effluent discharge rate of STP | [l·d$^{-1}$] | |

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

Calculation of the release to air from the STP

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

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water}$$ **(Equation R.16-20)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Fstp_{air}$ | fraction of the release to air from STP | [-] | Appendix R.16-3 |
| $Elocal_{water}$ | local release rate to water during release episode | [kg·d$^{-1}$] | Equation R.16-1 |
| $Estp_{air}$ | local release to air from STP during release episode | [kg·d$^{-1}$] | |

Calculation of the STP sludge concentration

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

$$C_{sludge} = \frac{Fstp_{sludge} \cdot Elocal_{water} \cdot 10^6}{SLUDGERATE}$$ **(Equation R.16-21)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Elocal_{water}$ | local release rate to water during episode | [kg·d$^{-1}$] | Equation R.16-1 |
| $Fstp_{sludge}$ | fraction of release directed to sludge by STP | [-] | Appendix R.16-3 |
| SLUDGERATE | rate of sewage sludge production | [kg·d$^{-1}$] | Equation R.16-22 |
| $C_{sludge}$ | 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:

$$SLUDGERATE = \frac{2}{3} \cdot SUSPCONC_{inf} \cdot EFFLUENT_{stp} + SURPLUSsludge \cdot CAPACITY_{stp}$$

**(Equation R.16-22)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $SUSPCONC_{inf}$ | concentration of suspended matter in STP influent | [kg·m$^{-3}$] | Table R.16-10 |
| $EFFLUENT_{stp}$ | effluent discharge rate of STP | [m$^3$·d$^{-1}$] | Equation R.16-19 |
| SURPLUSsludge | surplus sludge per inhabitant equivalent | [kg·d$^{-1}$·eq$^{-1}$] | Table R.16-10 |
| $CAPACITY_{stp}$ | capacity of the STP | [eq] | Table R.16-10 |
| 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.16.6.5.6. Calculation of the STP concentration for evaluation of inhibition to microorganisms

As explained above in the section on STP modeling, the removal of a substance 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 substance 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:

$$PEC_{STP} = CLOCAL_{EFF}$$ **(Equation R.16-23)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{eff}$ | total concentration of substance in STP effluent | [mg·l$^{-1}$] | Equation R.16-18 |
| $PEC_{stp}$ | PEC for microorganisms in the STP | [mg·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 PECSTP can still be considered equal to Clocaleff. After longer intervals the specific bacteria that are capable to biodegrade the compound, may be completely lost.

If the activated sludge is de-adaptated, 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:

$$PEC_{STP} = CLOCAL_{INF}$$ **(Equation R.16-24)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{inf}$ | total concentration of substance in STP influent | [mg·l$^{-1}$] | Equation R.16-18 |
| $PEC_{stp}$ | PEC for microorganisms in the STP | [mg·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 release periods care must be taken that the release rates are in fact calculated over the actual release period (as kg.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 $Fstp_{water}$ 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: $kbio_{stp}$ = 1 $hr^{-1}$ 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 release of substance A from the STP can be estimated to:

$$Elocal_{water} = Fstp_{water} \cdot Elocal_wastewater = 0.12 \cdot 0.0625 \frac{kg}{d} = 0.0075 \frac{kg}{d}$$

## R.16.6.6. Derivation of PEC

In the following sections guidance is given for the calculation of the PEClocal for each compartment and Section R.16.6.6.8 presents the calculation of regional steady-state concentrations (PECregional).

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 (PEClocalwater) 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 PNECwater. The concentration in sediment is calculated at the same location. For exposure of aquatic organisms, having a relatively short lifespan, the concentration during an release 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 (PEClocalsoil) 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.16.6.6.6) (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 (PEClocalair) 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.16.6.6.1). Deposition is used as input for the soil module, annual average deposition fluxes are used.

#### R.16.6.6.1.Calculation of PEClocal for the atmosphere

In this section, the following parameters are derived:

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

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

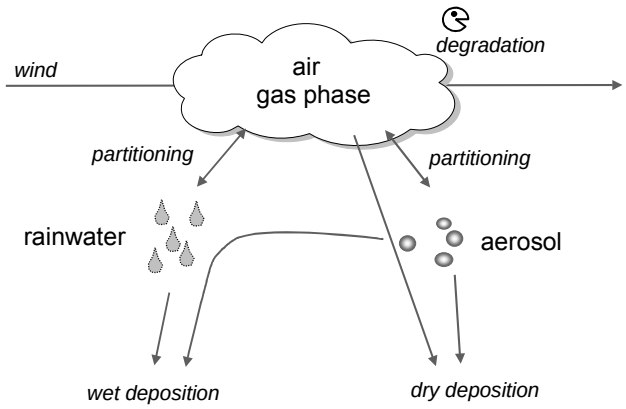



**Figure R.16-6**: Fate processes in the air compartment

PEClocal for air cannot be compared with the PNEC for air because the latter is usually not available. The PEClocal for air is used as input for the calcu-lation of the intake of substances through inhalation in the indirect exposure of humans. Deposition fluxes are used as input for the calculation of PEClocal 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, release 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.16-2);
- 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;
  - 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 release 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 release 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 PEClocal for air both release from a point source as well as the release from a STP is taken into account. The concentration on the regional scale (PECregional) 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 substance is calculated at a 100 m distance from it. The maximum from the two concentrations (direct and via STP) is used as the PEClocal:

$$Clocal_{air} = \max\left( Elocal_{air} \, , \, Estp_{air} \right) \cdot Cstd_{air}$$ **(Equation R.16-25)**

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365}$$ **(Equation R.16-26)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Elocal_{air}$ | local direct release rate to air during episode | [kg·d$^{-1}$] | eq. (5) |
| $Estp_{air}$ | local indirect release to air from STP during episode | [kg·d$^{-1}$] | Equation R.16-20 |
| $Cstd_{air}$ | concentration in air at source strength of 1 kg·d$^{-1}$ | [mg·m$^{-3}$] | 2.78.10$^{-4}$ |
| Temission | Number of emission days equal to:<br>Annual Use (kg·y$^{-1}$) / Daily Use (kg·d$^{-1}$) | [d·y$^{-1}$] | Section R.16.3.2.1 |
| $Clocal_{air}$ | local concentration in air during release episode | [mg·m$^{-3}$] | |
| $Clocal_{air,ann}$ | annual average concentration in air, 100 m from point source | [mg·m$^{-3}$] | |

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air}$$ **(Equation R.16-27)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{air,ann}$ | annual average local concentration in air | [mg·m$^{-3}$] | Equation R.16-26 |
| $PECregional_{air}$ | regional concentration in air | [mg·m$^{-3}$] | Section R.16.6.6.8 |
| $PEClocal_{air,ann}$ | annual average predicted environmental conc. in air | [mg·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 releases from the two sources (direct and STP) are summed:

$$DEPtotal = \left( Elocal_{air} + Estp_{air} \right) \cdot \left( Fass_{aer} \cdot DEPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right)$$

**(Equation R.16-28)**

$$DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365}$$ **(Equation R.16-29)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Elocal_{air}$ | local direct release rate to air during release episode | [kg·d$^{-1}$] | Equation R.16-1 |
| $Estp_{air}$ | local indirect release to air from STP during episode | [kg·d$^{-1}$] | Equation R.16-20 |
| $Fass_{aer}$ | fraction of the substance bound to aerosol | [-] | Equation R.16-2 |
| $DEPstd_{aer}$ | standard deposition flux of aerosol-bound compounds at a source strength of 1 kg·d$^{-1}$ | [mg·m$^{-2}$·d$^{-1}$] | $1 \cdot 10^{-2}$ |
| $DEPstd_{gas}$ | deposition flux of gaseous compounds as a function of Henry's Law constant, at a source strength of 1 kg·d$^{-1}$ | [mg·m$^{-2}$·d$^{-1}$] | |
| | $^{10}$logHENRY ≤ -2: | | $5 \cdot 10^{-4}$ |
| | -2 < $^{10}$logHENRY ≤ 2: | | $4 \cdot 10^{-4}$ |
| | $^{10}$logHENRY > 2: | | $3 \cdot 10^{-4}$ |
| Temission | Number of emission days equal to: Annual Use (kg·y$^{-1}$) / Daily Use (kg·d$^{-1}$) | [d·y$^{-1}$] | Section R.16.3.2.1 |
| DEPtotal | total deposition flux during release episode | [mg·m$^{-2}$.d$^{-1}$] | |
| $DEPtotal_{ann}$ | annual average total deposition flux | [mg.m$^{-2}$.d$^{-1}$] | |

### R.16.6.6.2. Calculation of PEClocal for the aquatic compartment

In this section, the following parameters are derived:

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

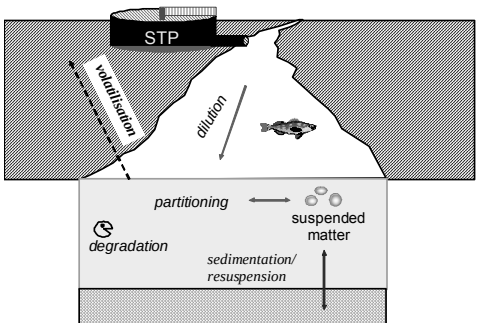



**Figure R.16-7**: Fate processes in the surface water

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.

The calculation of the PEClocal 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 PECsurface water and underestimation of PECsediment. 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 release 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 releases 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 release 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, Kpsusp, it can be estimated from the $K_{oc}$ of the substance, determined for other sorbents like soil or sediments (Section R.16.5.3.3) 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 release pattern as well as river parameters.

The local concentration in surface water is calculated as follows:

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION}$$ **(Equation R.16-30)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{eff}$ | concentration of the substance in the STP effluent | [mg·l$^{-1}$] | Equation R.16-18 |
| $Kp_{susp}$ | solids-water partitioning coefficient of suspended matter | [l·kg$^{-1}$] | Equation R.16-6 |
| $SUSP_{water}$ | concentration of suspended matter in the river | [mg·l$^{-1}$] | 15 |
| DILUTION | dilution factor | [-] | 10 |
| $Clocal_{water}$ | local concentration in surface water during release 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 10$^{th}$ 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):

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}}$$ **(Equation R.16-31)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $EFFLUENT_{stp}$ | effluent discharge rate of stp | [l·d$^{-1}$] | Equation R.16-19 |
| 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:

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365}$$ **(Equation R.16-32)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{water}$ | local concentration in surface water during release episode | [mg·l$^{-1}$] | Equation R.16-30 |
| Temission | Number of emission days equal to:<br>Annual Use (kg·y$^{-1}$) / Daily Use (kg·d$^{-1}$) | [d·y$^{-1}$] | Section R.16.3.2.1 |
| $Clocal_{water,ann}$ | annual average local concentration in surface water | [mg·l$^{-1}$] | |

The concentration at the regional scale (PECregionalwater) is used as background concentration for the local scale. Therefore, these concentrations are summed:

$$PEClocal_{water} = Clocal_{water} + PECregional_{water}$$ **(Equation R.16-33)**

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECregional_{water}$$ **(Equation R.16-34)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{water}$ | local concentration in surface water during episode | [mg·l$^{-1}$] | Equation R.16-30 |
| $Clocal_{water,ann}$ | annual average concentration in surface water | [mg·l$^{-1}$] | Equation R.16-32 |
| $PECregional_{water}$ | regional concentration in surface water | [mg·l$^{-1}$] | Section R.16.6.6.8 |
| $PEClocal_{water}$ | predicted environmental concentration during episode | [mg·l$^{-1}$] | |
| $PEClocal_{water,ann}$ | annual average predicted environmental concentration | [mg·l$^{-1}$] | |

**Example R.16-2: Concentration in surface water**

**See Section R.16.6.6.2 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:

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

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.16.6.6.3.Calculation of PEClocal for the sediment compartment

In this section, the following parameter is derived:

- local concentration in sediment during the release episode.

PEClocal 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):

$$PEClocal_{sed} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water} \cdot 1000 \qquad \textbf{(Equation R.16-35)}$$

Explanation of symbols

| | | | |
|---|---|---|---|
| $PEClocal_{water}$ | concentration in surface water during release episode | [mg.l$^{-1}$] | Equation R.16-33 |
| $K_{susp\text{-}water}$ | suspended matter-water partitioning coefficient | [m$^3$.m$^{-3}$] | Equation R.16-7 |
| $RHO_{susp}$ | bulk density of suspended matter | [kg.m$^{-3}$] | Equation R.16-16 |
| $PEClocal_{sed}$ | 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.16.6.6.4. Calculation of PEClocal 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 ($Clocal_{seawater}$). 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 release 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 ($Clocal_{seawater}$).

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:

$$Clocal_{seawater} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION}$$

**(Equation R.16-36)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{eff}$ | concentration of the substance in the STP effluent | [mg·l$^{-1}$] | Equation R.16-18 |
| $Kp_{susp}$ | solids-water partitioning coefficient of suspended matter | [l·kg$^{-1}$] | Equation R.16-6 |
| $SUSP_{water}$ | concentration of suspended matter in the seawater | [mg·l$^{-1}$] | 15 |
| DILUTION | dilution factor | [-] | 100 |
| $Clocal_{seawater}$ | local concentration in seawater during release episode | [mg·l$^{-1}$] | |

$Kp_{susp}$ is derived as for inland risk assessment. For a specific estimation of the partitioning behaviour of substances in saltwater environments see Section R.16.5.3.4

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 m$^3$/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 m$^3$/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:

$$Clocal_{seawater,ann} = Clocal_{seawater} \cdot \frac{Temission}{365}$$ **(Equation R.16-37)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{seawater}$ | local concentration in seawater during release episode | [mg·l$^{-1}$] | Equation R.16-36 |
| Temssion | Number of emission days equal to:<br>Annual Use (kg·y$^{-1}$) / Daily Use (kg·d$^{-1}$) | [d·y$^{-1}$] | Section R.16.3.2.1 |
| $Clocal_{seawater,ann}$ | annual average local concentration in seawater | [mg·l$^{-1}$] | |

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

$$PEClocal_{seawater} = Clocal_{seawater} + PECregional_{seawater}$$ **(Equation R.16-38)**

$$PEClocal_{seawater,ann} = Clocal_{seawater,ann} + PECregional_{seawater}$$ **(Equation R.16-39)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{seawater}$ | local concentration in seawater during episode | [mg·l$^{-1}$] | Equation R.16-36 |
| $Clocal_{seawater,ann}$ | annual average concentration in seawater | [mg·l$^{-1}$] | Equation R.16-37 |
| $PECregional_{seawater}$ | regional concentration in seawater | [mg·l$^{-1}$] | Section R.16.6.6.8 |
| $PEClocal_{seawater}$ | predicted environmental concentration during episode | [mg·l$^{-1}$] | |
| $PEClocal_{seawater,ann}$ | annual average predicted environmental concentration | [mg·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 substances is already agreed within OSPAR (OSPAR, 2000a; 2000b). For this specific exposure situation within the EU legislation, the methodology proposed by OSPAR can be taken into consideration[18];
- 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.16.6.6.5. Calculation of PEClocal 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):

$$PEClocal_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PEClocal_{seawater} \cdot 1000$$

**(Equation R.16-40)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PEClocal_{seawater}$ | Concentration in seawater during release episode | [mg·l$^{-1}$] | |
| $K_{susp-water}$ | suspended matter-water partitioning coefficient | [m$^3$·m$^{-3}$] | Equation R.16-7 |
| $RHO_{susp}$ | bulk density of suspended matter | [kg·m$^{-3}$] | Equation R.16-16 |
| $PEClocal_{sed}$ | 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 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.

[18] 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.

### R.16.6.6.6.Calculation of PEClocal 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 PEClocal in soil is given for the following exposure routes:

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

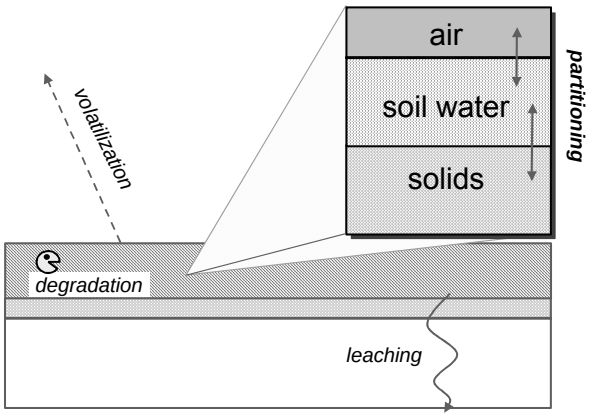



**Figure R.16-8**: Calculation of PECsoil

Direct application of substances (on the basis of the maximum recommended application rate; e.g. pesticide adjuvants or fertilisers) is 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 release calculation of a point source (Section R.16.6.6.1) 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 release episode. Averaging is done to facilitate calculation of a steady-state level. Furthermore, it is impossible to indicate when the release 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.16.6.8 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, Csoil(0), is governed by the input of the substance through sludge application.

$$\frac{dC_{soil}}{dt} = -k \cdot C_{soil} + D_{air}$$ **(Equation R.16-41)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $D_{air}$ | aerial deposition flux per kg of soil | [mg·kg$^{-1}$·d$^{-1}$] | Equation R.16-42 |
| t | Time | [d] | |
| k | first order rate constant for removal from top soil | [d$^{-1}$] | Equation R.16-46 |
| $C_{soil}$ | concentration in soil | [mg·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 ($DEPtotal_{ann}$) as follows:

$$D_{air} = \frac{DEPtotal_{ann}}{DEPTH_{soil} \cdot RHO_{soil}}$$ **(Equation R.16-42)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $DEPtotal_{ann}$ | annual average total deposition flux | [mg·m$^{-2}$·d$^{-1}$] | Equation R.16-29 |
| $DEPTH_{soil}$ | mixing depth of soil | [m] | Table R.16-11 |
| $RHO_{soil}$ | bulk density of soil | [kg·m$^{-3}$] | Equation R.16-16 |
| $D_{air}$ | aerial deposition flux per kg of soil | [mg·kg$^{-1}$·d$^{-1}$] | |

The differential Equation R.16-41 has an analytical solution, given by:

$$C_{soil}(t) = \frac{D_{air}}{k} - \left[ \frac{D_{air}}{k} - C_{soil}(0) \right] \cdot e^{-k\,t}$$ **(Equation R.16-43)**

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

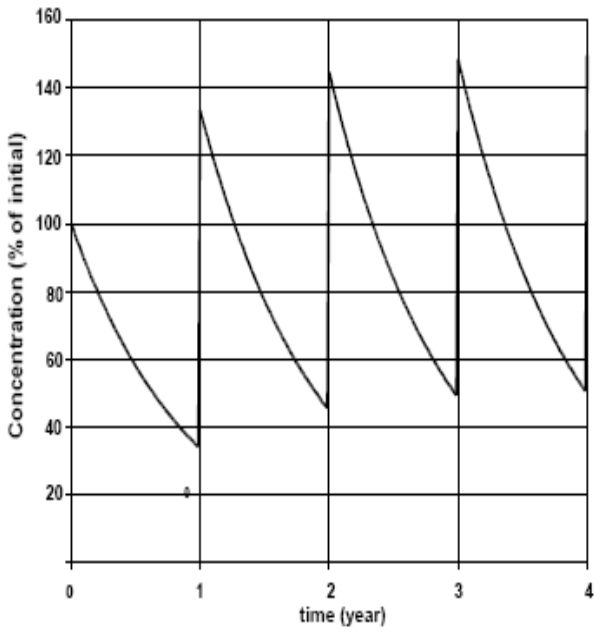



**Figure R.16-9**: Accumulation in soil due to several years of sludge application

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.

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.

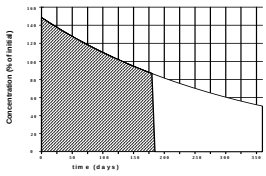


**Figure R.16-10**: The concentration in soil after 10 years.

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

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:

$$Clocal_{soil} = \frac{1}{T} \cdot \int_0^T C_{soil}(t)\,dt \qquad \textbf{(Equation R.16-44)}$$

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

$$Clocal_{soil} = \frac{D_{air}}{k} + \frac{1}{k\,T}\left[ C_{soil}(0) - \frac{D_{air}}{k} \right] \cdot \left[ 1 - e^{-kT} \right] \qquad \textbf{(Equation R.16-45)}$$

Explanation of symbols

| | | | |
|---|---|---|---|
| $D_{air}$ | aerial deposition flux per kg of soil | [mg·kg$^{-1}$·d$^{-1}$] | (Equation R.16-42) |
| T | averaging time | [d] | Table R.16-11 |
| k | first order rate constant for removal from top soil | [d$^{-1}$] | (Equation R.16-46) |
| $C_{soil}$ (0) | initial concentration (after sludge application) | [mg·kg$^{-1}$] | (Equation R.16-53) |
| $Clocal_{soil}$ | average concentration in soil over T days | [mg·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:

$$k = k_{volat} + k_{leach} + kbio_{soil}$$ **(Equation R.16-46)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $k_{volat}$ | pseudo-first order rate constant for volatilisation from soil | [$d^{-1}$] | (Equation R.16-47) |
| $k_{leach}$ | pseudo-first order rate constant for leaching from top soil | [$d^{-1}$] | (Equation R.16-48) |
| $kbio_{soil}$ | pseudo-first order rate constant for biodegradation in soil | [$d^{-1}$] | Equation R.16-13 |
| 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, $k_{volat\ i}$, becomes:

$$\frac{1}{k_{volat}} = \left( \frac{1}{kasl_{air} * K_{air-water} / K_{soil-water}} + \frac{1}{kasl_{soil}} \right) \cdot DEPTH_{soil}$$ **(Equation R.16-47)**

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.16-59 |
| $K_{air-water}$ | air-water equilibrium distribution constant | [m3.m-3] | Equation R.16-5 |
| $K_{soil-water}$ | soil-water partitioning coefficient | [m3.m-3] | Equation R.16-7 |
| $DEPTH_{soil}$ | 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:

$$k_{leach} = \frac{Finf_{soil} \cdot RAINrate}{K_{soil-water} \cdot DEPTH_{soil}}$$ **(Equation R.16-48)**

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 | [$m^3 \cdot m^{-3}$] | Equation R.16-7 |
| $DEPTH_{soil}$ | mixing depth of soil | [m] | |
| $k_{leach}$ | 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.16-45), 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 **Error! Reference source not found.** with an initial concentration of zero and 10 years of input:

$$Cdep_{soil\,10}(0) = \frac{D_{air}}{k} - \frac{D_{air}}{k} \cdot e^{-365 \cdot 10 \cdot k}$$ **(Equation R.16-49)**

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:

$$Csludge_{soil\,1}(0) = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO_{soil}}$$ **(Equation R.16-50)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $C_{sludge}$ | concentration in dry sewage sludge | [mg·kg$^{-1}$] | Equation R.16-21 |
| $APPL_{sludge}$ | dry sludge application rate | [kg·m$^{-2}$·yr$^{-1}$] | Table R.16-11 |
| $DEPTH_{soil}$ | mixing depth of soil | [m] | Table R.16-11 |
| $RHO_{soil}$ | bulk density of soil | [kg·m$^{-3}$] | Equation R.16-16 |
| $Csludge_{soil\,1}(0)$ | 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:

$$Facc = e^{-365\,k}$$ **(Equation R.16-51)**

Explanation of symbols

| | | | |
|---|---|---|---|
| k | first order rate constant for removal from top soil | [d$^{-1}$] | Equation R.16-46 |
| Facc | fraction accumulation in one year | [-] | |

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

$$Csludge_{soil\,10}(0) = Csludge_{soil\,1}(0) \cdot \left[ 1 + \sum_{n=1}^{9} Facc^{n} \right]$$ **(Equation R.16-52)**

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

$$C_{soil\,10}(0) = Cdep_{soil\,10}(0) + Csludge_{soil\,10}(0)$$ **(Equation R.16-53)**

This initial concentration can be used in Equation R.16-44 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:

$$Fst\text{-}st = \frac{C_{soil\,10}(0)}{C_{soil\,\infty}(0)}$$ **(Equation R.16-54)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $C_{soil}$ 10 (0) | initial concentration after 10 years | [mg·kg$^{-1}$] | (Equation R.16-53) |
| $C_{soil\,\infty}$ (0) | initial concentration in steady-state situation | [mg·kg$^{-1}$] | (Equation R.16-55) |
| Fst-st | fraction of steady-state in soil achieved | [-] | |

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

$$C_{soil\,\infty}(0) = \frac{D_{air}}{k} + Csludge_{soil\,1}(0) \cdot \frac{1}{1 - Facc}$$ **(Equation R.16-55)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $D_{air}$ | aerial deposition flux per kg of soil | [mg·kg$^{-1}$·d$^{-1}$] | (Equation R.16-42) |
| k | first order rate constant for removal from top soil | [d$^{-1}$] | (Equation R.16-46) |
| Facc | fraction accumulation in one year | [-] | (Equation R.16-51) |
| $Csludge_{soil\,1}$ (0) | concentration in soil due to sludge in first year at t=0 | [mg·kg$^{-1}$] | (Equation R.16-50) |
| $C_{soil\infty}$(0) | initial concentration in steady-state situation | [mg·kg$^{-1}$] | |

*Calculation of $PEClocal_{soil}$*

For soil, three different PECs are calculated, for different endpoints (Table R.16-11).

**Table R.16-11**: Characteristics of soil and soil-use for the three different endpoints

| | Depth of soil compartment | Averaging time | Rate of sludge application | Endpoint |
|---|---|---|---|---|
| | **[m]** | **[days]** | **[$kg_{dwt}$·$m^{-2}$·$year^{-1}$]** | |
| $PEClocal_{soil}$ | 0.20 | 30 | 0.5 | terrestrial ecosystem |
| $PEClocal_{agr.\ soil}$ | 0.20 | 180 | 0.5 | crops for human consumption |
| $PEClocal_{grassland}$ | 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.

$$PEClocal_{soil} = Clocal_{soil} + PECregional_{natural\ soil}$$ **(Equation R.16-56)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{soil}$ | Local concentration in soil | [mg·kg$^{-1}$] | (Equation R.16-44) |
| $PECregional_{natural\ soil}$ | regional concentration in natural soil | [mg·kg$^{-1}$] | Section R.16.6.6.8 |
| $PEClocal_{soil}$ | predicted environmental conc. in soil | [mg·kg$^{-1}$] | |

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

$$PEClocal_{soil,porew} = \frac{PEClocal_{soil} \cdot RHO_{soil}}{K_{soil\text{-}water} \cdot 1000}$$ **(Equation R.16-57)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PEClocal_{soil}$ | predicted environmental conc. in soil | [mg·kg$^{-1}$] | (Equation R.16-56) |
| $K_{soil\text{-}water}$ | soil-water partitioning coefficient | [m$^3$·m$^{-3}$] | (Equation R.16-6 |
| $RHO_{soil}$ | bulk density of wet soil | [kg·m$^{-3}$] | (Equation R.16-16) |
| $PEClocal_{soil,porew}$ | predicted environmental conc. in porewater | [mg·l$^{-1}$] | |

### R.16.6.6.7. 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.

$$PEClocal_{grw} = PEClocal_{agr.soil,porew}$$ **(Equation R.16-58)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PEClocal_{agr.soil,porew}$ | predicted environmental conc. in porewater | [mg·l$^{-1}$] | Equation R.16-57 |
| $PEClocal_{grw}$ | predicted environmental conc. in groundwater | [mg·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 $Fstp_{sludge}$ 0.03. The same release fraction can be estimated using the model SimpleTreat.

| | | 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 | 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:

$$Csludge = \frac{Fstp_{sludge} \cdot Elocal_{wastewater} \cdot 10^6}{SLUDGERATE}$$

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

The concentration is sludge is calculated to:

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

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

$$\Delta Csludge_{soil}(0) = \frac{Csludge \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO_{soil}}$$

APPLsludge is the dry sludge application rate. Default value is 0.5 kg/m$^2$/yr (when assessing the terrestrial ecosystem)

DEPTHsoil is the mixing depth of soil. Default value is 0.2 m.

RHOsoil is the bulk density of soil. Default value is 1700 kg/m$^3$

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

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

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

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

$Finf_{soil}$: 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

Ksoil-water: soil-water partitioning coefficient. For this substance, having calculated the Koc from the QSAR assuming that the substance belongs to the group “Predominantly hydrophobics”, Kpsoil is estimated atKsoil-water is calculated at 10.4 m$^3$/m$^3$

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

kbiosoil is found from the half-life in soil ($DT50bio_{soil}$), which is 30 days in Table R.16-6 (readily biodegradable substance, Kpsoil<100 l/kg):

$$kbio_{soil} = \frac{\ln(2)}{DT50bio_{soil}} = \frac{\ln(2)}{30}d^{-1} = 0.023d^{-1}$$

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

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

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

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

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

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

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

$$Clocal_{soil} = \frac{Dair}{k} + \frac{1}{k \cdot T}\left[\Delta Csludge_{soil}(0) - \frac{Dair}{k}\right] \cdot \left[1 - e^{-k \cdot T}\right]$$

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

The $PEClocal_{soil}$ is calculated by adding Clocalsoil to the regional concentration in natural soil, which is set to 0 mg/kg in this example. The $PEClocal_{soil}$ = 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 $PEClocal_{soil}$, it is concluded that the substance A does not exhibit a risk to the soil ecosystem.

### R.16.6.6.8. Calculation of PECregional

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:

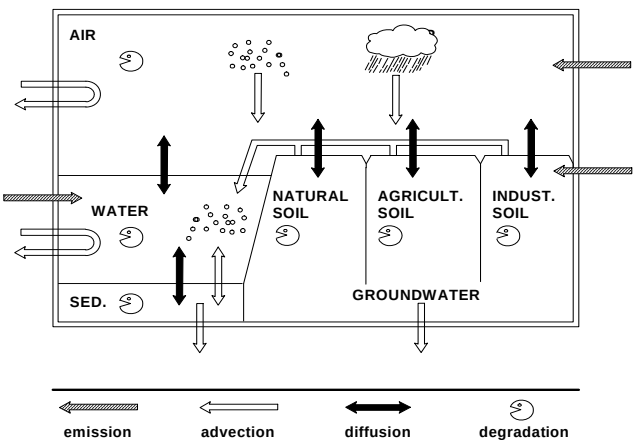



**Figure R.16-11:** Regional calculations

- release, 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 release. 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 release 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 PECregional calculation, in contrast to PEClocal, 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 PECregional*

When calculating the PECregional it is important which modelling parameters are chosen and what fraction of the total releases is used as release for the region. There are two different possibilities:

- calculation of a PECregional on the basis of a standardised regional environment with agreed model parameters;
- calculation of a PECregional on the basis of country specific model parameters.

A standardised regional environment should be used for the first approach in the calculation of PECregional. When more specific information is available on the location of production /release 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. The model parameters proposed for this standard region are given in Table R.16-12. 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.16-12 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.16-12.

**Table R.16-12**: 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 | 0.27 |
| area fraction of agricultural soil | 0.60 |
| 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://www.fao.org/corp/statistics/en/). 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 $l \cdot d^{-1}$ (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 $4.0 \cdot 10^6$ $m^3 \cdot d^{-1}$. The inflow caused by inflowing riverwater, is $6.5 \cdot 10^7$ $m^3 \cdot d^{-1}$.

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.16-13.

**Table R.16-13**: Intermedia mass transfer coefficients

| Parameter | Value |
|---|---|
| air-water interface: air side partial mass transfer coefficient | Equation R.16-68 |
| air-water interface: water side partial mass transfer coefficient | Equation R.16-69 |
| Aerosol deposition rate | 0.001 m.s-1 |
| air-soil interface: air side partial mass transfer coefficient | 1.39.10-3 m.s-1 |
| air-soil interface: soil side partial mass transfer coefficient | Equation R.16-59 |
| sediment-water interface: water side partial mass transfer coefficient | 2.78.10-6 m.s-1 |
| sediment-water interface: pore water side partial mass transfer coefficient | 2.78.10-8 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 $kasl_{soil}$ ($m.d^{-1}$) is deduced from the exponential concentration profile in an undisturbed soil:

$$kasl_{soil} = \left( Veff_{soil} + \frac{Deff_{soil}}{d_p} \right)$$ **(Equation R.16-59)**

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).

$$d_p = \frac{Veff_{soil} + \sqrt{Veff_{soil}^{\ 2} + Deff_{soil} \cdot 4 \cdot k\deg_{soil}}}{2 \cdot k\deg_{soil}}$$ **(Equation R.16-60)**

In which:

$$Veff_{soil} = FRw.soil \frac{RAINRATE \cdot F\inf_{soil}}{Fwater_{soil}} + FRs.soil.\frac{SOLIDadv.soil}{Fsolid_{soil}}$$ **(Equation R.16-61)**

$$Deff_{soil} = FRa.soil \frac{DIFFgas \cdot Fair_{soil}^{\ 1.5}}{Fair_{soil}} + FRw.soil.\frac{DIFFwater \cdot Fwater_{soil}^{\ 1.5}}{Fwater_{soil}} + FRs.soil \cdot \frac{SOLIDdiff.soil}{Fsolid_{soil}}$$ **(Equation R.16-62)**

$$FRw.soil = \frac{Fwater_{soil}}{Fair_{soil} \cdot K_{air-water} + Fwater_{soil} + Fsolid_{soil} \cdot K_{soil-water}}$$ **(Equation R.16-63)**

$$FRs.soil = \frac{Fsolid_{soil}}{Fair_{soil} \cdot K_{air-water} / K_{soil-water} + Fwater_{soil} / K_{soil-water} + Fsolid_{soil}}$$ **(Equation R.16-64)**

$$FRa.soil = 1 - FRw.soil - FRs.soil$$ **(Equation R.16-65)**

$$DIFFgas = 2.57 \cdot 10^{-5} \sqrt{\frac{18}{MOLW}}$$ **(Equation R.16-66)**

$$DIFFwater = 2.0 \cdot 10^{-9} \sqrt{\frac{32}{MOLW}}$$ **(Equation R.16-67)**

Explanation of symbols

| | | | |
|---|---|---|---|
| MOLW | molecular weight of the substance | [$kg_c \cdot mol^{-1}$] | |
| $kdeg_{soil}$ | rate constant for degradation in bulk soil | [$d^{-1}$] | |
| RAINRATE | average daily rate of wet precipitation | [$m \cdot d^{-1}$] | Table R.16-12 |
| $Finf_{soil}$ | fraction of precipitation that penetrates into the soil | [-] | Table R.16-12 |
| $d_p$ | substance-dependent penetration depth | [m] | Equation R.16-60 |
| $Veff_{soil}$ | effective advection (with penetrating porewater) | [m] | Equation R.16-61 |
| Deffsoil | effective diffusion coefficient | [$m^2 \cdot d^{-1}$] | Equation R.16-62 |
| FRa.soil | mass fraction of the substance in the air phase of soil | [-] | Equation R.16-65 |
| FRw.soil | mass fraction of the substance in the water phase of soil | [-] | Equation R.16-63 |
| FRs.soil | mass fraction of the substance in the solid phase of soil | [-] | Equation R.16-64 |
| $Fair_{soil}$ | volume fraction of air in the soil compartment | [$m_{air}^3 \cdot ms_{oil}^{-3}$] | Table R.16-9 |
| $Fwater_{soil}$ | volume fraction of water in the soil compartment | [$m_{water}^3 \cdot ms_{oil}^{-3}$] | Table R.16-9 |
| $Fsolid_{soil}$ | volume fraction of solids in the soil compartment | [$m_{solid}^3 \cdot ms_{oil}^{-3}$] | Table R.16-9 |
| $K_{air\text{-}water}$ | air-water partitioning coefficient | [$m^3 \cdot m^{-3}$] | Equation R.16-5 |
| $K_{soil\text{-}water}$ | soil-water partitioning coefficient | [$m^3 \cdot m^{-3}$] | **Error! Reference source not found.** |
| DIFFgas | molecular diffusivity of the substance in the gas phase | [$m^2 \cdot d^{-1}$] | Equation R.16-66 |
| DIFFwater | molecular diffusivity of the substance in the water phase | [$m^2 \cdot d^{-1}$] | Equation R.16-67 |
| SOLIDadv.soil | rate of advective downward transport of soil particles | [$m \cdot d^{-1}$] | $6.34 \cdot 10^{-12}$ |
| SOLIDdiff.soil | solid phase diffusion coefficient in the soil compartment | [$m^2 \cdot d^{-1}$] | $6.37 \cdot 10^{-12}$ |
| $kasl_{soil}$ | partial mass-transfer coefficient at soil side at the air-soil interface | [$m \cdot d^{-1}$] | |

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.16-12).

**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:

$$kaw_{air} = 0.01 \cdot (0.3 + 0.2 \cdot WINDSPEED) \cdot (\frac{0.018}{MOLW})^{0.335}$$ **(Equation R.16-68)**

$$kaw_{water} = 0.01 \cdot (0.0004 + 0.0004 \cdot WINDSPEED^2) \cdot (\frac{0.032}{MOLW})^{0.25}$$ **(Equation R.16-69)**

Explanation of symbols

| | | | |
|---|---|---|---|
| MOLW | molecular weight of the substance | [$kg_c \cdot mol^{-1}$] | |
| WINDSPEED | average windspeed | [$m \cdot d^{-1}$] | Table R.16-12 |
| $kaw_{air}$ | partial mass-transfer coefficient at the air side of the air-water interface | [$m \cdot d^{-1}$] | |
| $kaw_{water}$ | partial mass-transfer coefficient at the water side of the air-water interface | [$m \cdot d^{-1}$] | |

*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 substances 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 releases 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 releases 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 substances) or more (for substances 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 PECregional,marine according to this standard scenario may be sufficient for generic risk assessment If additional information is available on sources and releases 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 substances 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 in principle covers all 27 EU countries and Norway and similar percentages for water and natural, agricultural and industrial/urban soils as given in Table R.16-12. All other parameters are similar to the ones given in the preceding tables. Release 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 substance.

**Table R.16-14**: Parameters for the continental[19] 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 | 0.27 |
| area fraction of agricultural soil | 0.60 |
| area fraction of industrial/urban soil | 0.10 |

### R.16.6.6.9. 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 PECregional 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

[19] The parameters for the continental model are still based on the current 15 EU Member States and Norway

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 release 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 release 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.16.6.7. Predators (secondary poisoning)

### R.16.6.7.1. Output

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

### R.16.6.7.2. Input

For fish-eating predators, the local and regional PECs for surface water (Sections R.16.6.6.2 and R.16.6.6.4), BCF for fish and $BMF_1$/$BMF_2$ (Section R.16.5.3.5) are needed.

For worm-eating predators, the PEC for soil (Section R.16.6.6.6) and BCF for worms (Section R.16.5.3.5) 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.16.5.3.5.

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 substance 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 indications (e.g. endocrine disruption) then the substance should be considered as having the potential to cause toxic effects if accumulated in higher organisms.

In conclusion, if a substance has a bioaccumulation potential and a low degradability (e.g. not readily biodegradable or not hydrolysable) and has also a potential to cause toxic effects if accumulated in higher organisms, a detailed assessment of secondary poisoning should be conducted (see also B.7.2.7).

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.

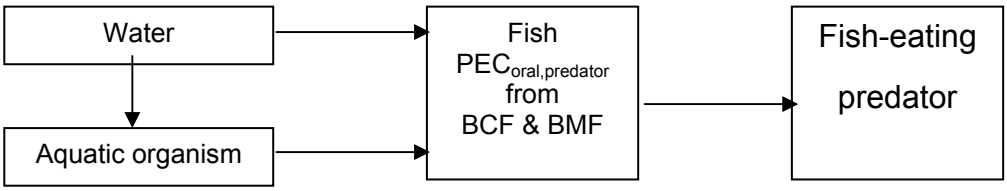



**Figure R.16-12**: Assessment of secondary poisoning

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 ($PECoral_{predator}$) 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, $PECoral_{predator}$ is calculated from the bioconcentration factor (BCF) and a biomagnification factor (BMF). Note that $PECoral_{predator}$ 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 ($PECoral_{predator}$) is calculated from the PEC for surface water, the measured or estimated BCF for fish and the biomagnification factor (BMF):

$$PEC_{oral,predator} = PEC_{water} \cdot BCF_{fish} \cdot BMF$$ **(Equation R.16-70)**

Explanation of symbols

| | | |
|---|---|---|
| $PECoral_{predator}$ | Predicted Environmental Concentration in food | $[mg \cdot kg_{wet\ fish}^{-1}]$ |
| $PEC_{water}$ | Predicted Environmental Concentration in water | $[mg \cdot l^{-1}]$ |
| $BCF_{fish}$ | bioconcentration factor for fish on wet weight basis | $[l \cdot kg_{wet\ fish}^{-1}]$ |
| 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 = Cpredator/Cprey). 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 PEClocal 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 PEClocal. However, using PECregional 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 PEClocal) and 50% of the diet comes from a regional area (represented by the annual average PECregional) 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 ($PNECoral_{predator}$). 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 ($PNECoral_{top\ predator}$). 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 PECoral and PNECoral is not based on internal concentrations but on intake rates.

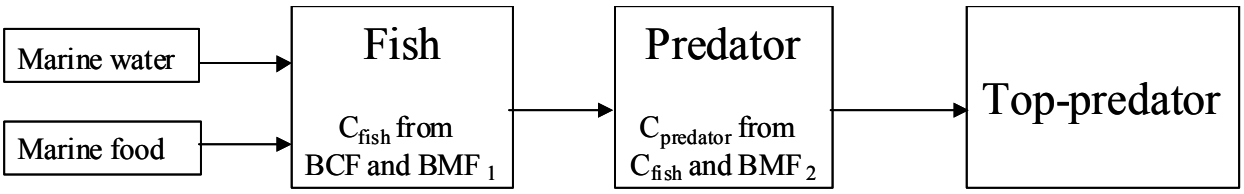



**Figure R.16-13**: Secondary poisoning food chain

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 substance.

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 substances: 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 $PECoral_{predator}$ is calculated as:

$$PEC_{oral,\,predator} = C_{earthworm}$$ **(Equation R.16-71)**

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 PEClocal is used in which with respect to sludge application the concentration is averaged over a period of 180 days (see Section R.16.6.6.6). The same scenario is used as for the aquatic food chain, i.e. 50% of the diet comes from PEClocal and 50% from PECregional.

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):

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} \cdot W_{earthworm} + C_{soil} \cdot W_{gut}}{W_{earthworm} + W_{gut}}$$ **(Equation R.16-72)**

Explanation of symbols

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

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

$$W_{gut} = W_{earthworm} \cdot F_{gut} \cdot CONV_{soil}$$ **(Equation R.16-73)**

where:

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid} \cdot RHO_{solid}}$$ **(Equation R.16-74)**

Explanation of symbols

| | | | |
|---|---|---|---|
| $CONV_{soil}$ | conversion factor for soil concentration wet-dry weight soil | $[kg_{wwt} \cdot kg_{dwt}^{-1}]$ | |
| $F_{solid}$ | volume fraction of solids in soil | $[m^3 \cdot m^{-3}]$ | Table R.16-9 |
| $F_{gut}$ | fraction of gut loading in worm | $kg_{dwt} \cdot kg_{wwt}^{-1}$ | 0.1 |
| $RHO_{soil}$ | bulk density of wet soil | $[kg_{wwt} \cdot m^{-3}]$ | (Equation R.16-16) |
| $RHO_{solid}$ | density of solid phase | $[kg_{dwt} \cdot m^{-3}]$ | Table R.16-9 |

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

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} + C_{soil} \cdot F_{gut} \cdot CONV_{soil}}{1 + F_{gut} \cdot CONV_{soil}}$$ **(Equation R.16-75)**

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 substances, 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):

$$BCF_{earthworm} = (0.84 + 0.012K_{ow}) / RHO_{earthworm}$$ **(Equation R.16-76)**

where for $RHO_{earthworm}$ by default a value of 1 ($kg_{wwt} \cdot L^{-1}$) 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.[20]

Earthworms are also able to take up substances 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 substances 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 substances.

[20] 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 logKow > 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

## R.16.6.8. Humans exposed indirectly via the environment

### R.16.6.8.1. 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.

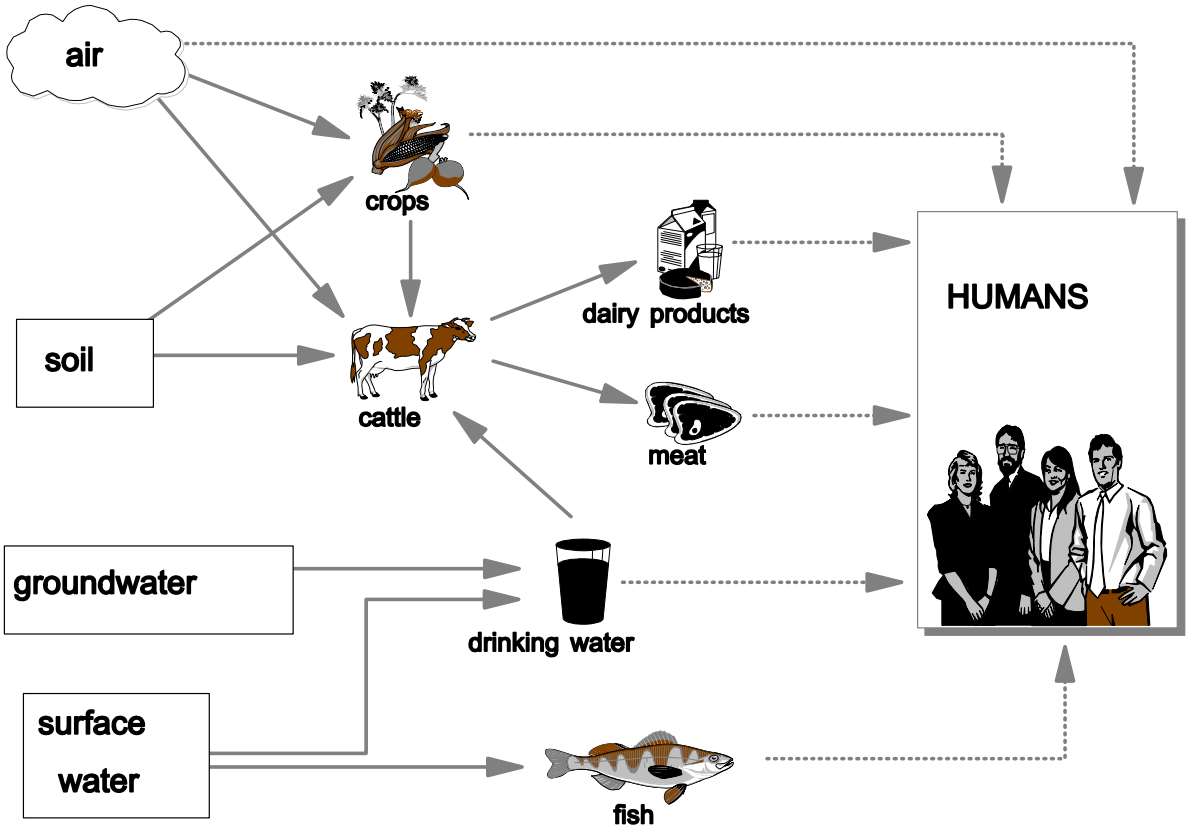



**Figure R.16-14**: Schematic representation of the exposure routes considered in human exposure

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.16.6. 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.16.6.4 and Section R.16.6.6.8. 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.16.6.8.2. 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.16.6.8.3. 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.16-15.

In addition to the data required for the environmental exposure estimation (see Section R.16.6), 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.16-16.

**Table R.16-15**: 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.16-16**: 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.16.6.8.4. Exposure via the environmental compartments

Exposure 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.16.6.6.1.

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 release. 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.16.6.8.5. 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 (Kow), indicating that lipid or fat is the main dissolving medium. The estimation of fish-water bioconcentration is more specifically discussed in Section R.16.5.3.5.

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). Kow and Kaw (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. 6.8.6. 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.16.7. Tools based on models presented in section R.16.6

### R.16.7.1. EUSES

EUSES (2.1) 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.16.3. 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 for example by including more specific information on releases (Section R.16.3) and improved data on substance properties (Section R.16.8).

Currently a new CHEmical Safety Assessment and Reporting tool (CHESAR) is being developed by ECHA. The CHESAR tool is intended to help the registrant to perform a CSA. A new dedicated release module (based on the present guidance) and the EUSES model are implemented in CHESAR in order to estimate PECs and human daily intake of a substance via the environment, both at the local and regional scale.

**Input (Tier 1 assessment)**

For Tier 1 assessments of environmental distribution, the information described in Table R.16-17 should be collected (more information on fate may be needed for metals and metal compound, see Appendix R.7.13-2).

**Table R.16-17:** 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<br>See also Section R.16.5.3.3 |
| 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<br>See also Section R.16.5.3.3 |
| 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<br>See also Section R.16.5.3.3 |
| Biode-gradability | Results of screening test on biodegradability. Not relevant for inorganic substances. | Technical dossier– chapter 9<br>See also Sections R.16.5.4.4, R.16.5.4.5, R.16.5.4.7 |
| Ej,localIU,j | Local release to compartment j (j: water, air, soil) from identified use | Release estimation based on use scenario<br>See Section R.16.3 |
| Regional Release$_i$ by use | Regional release from source and identified use to compartment j (j: water, air, soil)} | Release estimation based on exposure scenario<br>See Section R.16.3 |

### Output

The output of the Tier 1 consists of the predicted environmental concentrations (PECs) for environmental risk assessment (see Table R.16-18). 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 chemical safety assessment

**Table R.16-18 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<br>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<br>Indirect exposure of humans |
| PEClocal.grass,180 | Local PEC in grassland (total) averaged over 180 days | Secondary poisoning<br>Indirect exposure of humans |
| PECreg.water,tot | Regional PEC in surface water (total) | Risk assessment fresh water<br>Secondary poisoning<br>Indirect exposure of humans |
| PECreg.seawater,tot | Regional PEC in seawater (total) | Risk assessment marine water<br>Secondary poisoning<br>Indirect exposure of humans |
| PECreg.air | Regional PEC in air (total) | |
| PECreg.agric | Regional PEC in agricultural soil (total) | Risk assessment terrestrial environment<br>Secondary poisoning<br>Indirect exposure to man |
| PECreg.natural | Regional PEC in natural soil (total) | Risk assessment terrestrial environment<br>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.16.7.2. TGD excel sheet

The TGD excel sheet (EU TGD 2003 Risk Assessment Spreadsheet Model) can be obtained free of charge (http://cem-nl.eu/eutgd.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.16.6.

A new version of ECETOC-TRA (http://www.ecetoc.org/index.php?page=tra), combining the novel element of the REACH guidance with the algorithms of the EU TGD for the estimation of environmental exposure concentrations, has recently been developed .

## R.16.8. Refinement of exposure estimation

If risks deriving from the manufacture and all identified use(s) are not controlled, the registrant can:

- Refine the hazard or exposure assessment parts of the CSA:
- Advise against unsafe uses.

Any step of the workflow leading to exposure estimation can be modified. Refinement options related to the release estimation step (refinement or addition of more specific RMM/OC, use of release measurement, refinement of the mapping of uses) have been described in Section R.16.3.5. In this paragraph, the different options for refining the environmental distribution and exposure estimation steps are described (see Figure R.16-1).

a) use environmental **measured data**

If measured data related to environmental concentrations are available, of a suitable quality, representative of the OC/RMM that were in place when measurements were performed, supported by sufficient contextual information, and assigned to the appropriate spatial scale, they can be used for the exposure estimate. More details about these issues can be found in Section R.16.4.

b) refine the determination of the **substance properties**

The exposure assessment might lead to worst case results because of limited knowledge of the properties having an impact on fate and distribution of the substance. It might therefore be necessary to refine information related to degradation rates, partitioning coefficients, vapour pressure, water solubility etc.

The following table gives an overview of the data used as input for EUSES exposure estimation and which is possible to refine.

**Table R.16-19**: Determinants and input information for refined assessment

| Determinant | Description |
|---|---|
| Koc | Organic carbon water partition coefficient<br>In Tier 1 estimated from log Kow<br>Used for estimation of<br>1 Kpsusp (solids-water partition coefficient in suspended matter)<br>2 Kpsed (solids-water partition coefficient in sediment)<br>3 Kpsoil (solids-water partition coefficient in soil)<br>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 |
| $kbio_{stp}$ | Rate constant for biodegradation in STP. In Tier 1 estimated from Biodegradability |
| kbiowater | Rate constant for biodegradation in bulk surface water. In Tier 1 estimated from Biodegradability |
| kdegsoil<br>kdegsed | Total rate constant for biodegradation in bulk soil and sediment. In Tier 1 estimated from Biodegradability |
| DT50hydrwater | Half-life for hydrolysis in water at the temperature of the data set |
| $DT50photo_{water}$ | Half-life for photolysis in water at the temperature of the data set |
| DT50air | Half life for degradation in air at the temperature of the data set |

In particular, the Henry's Law constant (HENRY), the octanol-water partitioning coefficient (Kow) and the first order rate constant for biodegradation ($kbio_{stp}$) can be used to refine the input into the STP calculations.

c) refine the **characterization of environmental compartments**

Local and regional environments are not actual sites or regions, but standardized environments based on generic parameters (see Table R.16-12 and Table R.16-15). When more specific information is available on the location of release sources, this information can be used to deviate from these default parameters and refine the assessment. If, for example, the manufacture or use of a certain substance is confined within a specific country, parameters which are relevant for that country can be used.

d) use **higher tier exposure** estimation tools

There is a wide range of exposure estimation models which can be used to simulate fate and distribution of substances among the different environmental compartments. These models vary in their complexity and purposes. Tier 1 exposure estimation models (like EUSES and the incorporated SimpleTreat model or the spreadsheet version TGD-excel) are simple to use, require only a few data on substance properties and are specifically developed to quickly evaluate substances. However, they are inherently conservative and are therefore used for an initial screening.

More demanding models have been developed for other purposes and for specific environmental compartments and exposure routes. These models demand expert knowledge to operate them, a

characterization of the environmental compartment where they are applied and a high level of detail. However, they provide a more accurate estimate of environmental concentrations.

GREAT-ER (www.great-er.org; Boeije et al. 2000; Schowanek et al. 2001; Wind 2004) and GEMCO (CEFIF LRI, 2004) can be used to estimate adsorption, degradation and volatilization in the water compartment. They are GIS-based models providing exposure predictions of PEClocal in, respectively, a river basin or an estuary[21].

GPM and OPS are used to simulate dispersion, deposition and chemical transformations in the air compartment.

PRZM and SESOIL are used to simulate the vertical movement of substances, leaching, erosion, runoff and volatilization for the soil and groundwater compartment.

If the 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 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 EU Directive 91/414/EEC.

FOCUS has recommended a number of models to be used for soil and ground water exposure estimation (MACRO, PEARL, PELMO, PRZM_GW) and for surface water exposure estimation (STEP1-2, which is a screening tool to assess whether there is a risk to fresh water living organisms; SWASH, which is a higher tier tool combining tools for leaching, drift, run-off, and fate in surface water).

Some of the above mentioned tools, together with documentation and manuals, can be downloaded for free from:

http://viso.jrc.it/focus/index.html

In order to assess releases from offshore platforms, the CHARM model (see fig. R.16-15) can be an alternative to EUSES/TGD excel for this specific use.

CHARM has been developed for screening level risk assessment of offshore substances, 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 substances 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 substances on the basis of the PEC/PNEC ratios.

Long term exposure of persistent and bioaccumulative substances and inorganic substances cannot be assessed by CHARM.

[21] Estuaries represent another example where higher tier models can be used. By default they are covered by either the inland or the marine risk assessment.

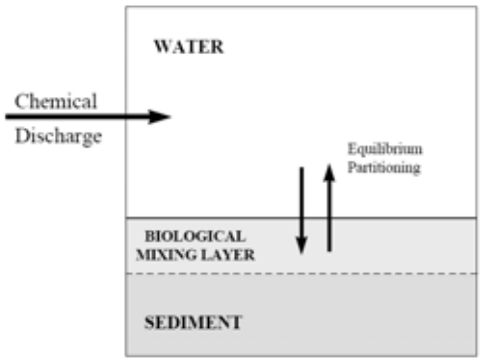



**Figure R.16-15**: The CHARM model

Most of the calculations within CHARM concern the estimation of the concentration of a substance in the waste stream, and different models are used depending on of the process for which they are used, the amount of the substance, 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 substance present in the environment will partition between the water and organic matrix in the sediment. The concentration of a substance may, therefore vary greatly from one compartment to another. Consequently, two PEC values are calculated: PECwater and PECsediment. For further details see for example

https://www.ogp.org.uk/pubs/CHARMManualFeb05.pdf

The FOCAS model (Fate of Chemicals in Amended Soils) predicts the fate of consumer product and other chemicals in soil based on amendments from sludge, compost, or irrigation water. In addition to degradation rates used in the Sludge model, FOCAS also incorporates other loss mechanisms, and is considered a Tier II model.

ASTREAT (McAvoy, et al. 1999) is a Windows executable designed to quantify chemical pathways within wastewater treatment systems. It is based on the framework developed by Lee to al. (1998). The TIER II analysis required for ASTREAT measures Henry's Law Constant, the biodegradation constants (1st Order Decay constant, Biological Reaction Coefficient or Monod parameters), and the Partition Coefficient directly.

## R.16.9. Summary of default and refined assessment

In the following table both, the default assumptions and the refinement options for the determinants of release and exposure assessment are summarized. The detailed description of these assumptions can be found in the chapters R.16.3 – R.16.8.

**Table R.16-20**: Assumptions for the determinants of the default and refined assessment

| Determinant | Default assessment | Refined assessment |
|---|---|---|
| Daily use at local scale<br>Industrial setting<br>(ERC1-7, 12) | It is calculated from:<br>▪ total registrant's tonnage (at the EU level) supplied to an identified use<br>▪ divided by the default number of release days, (depending on the annual tonnage) (see R. 16.3.2.1)<br>It is assumed that the tonnage for | The daily use at a site for an identified use can be overwritten by the registrant, on the basis of:<br>▪ Site specific information, such as the actual daily use in the manufacturing stage (readily accessible to the registrant)<br>▪ Information on the actual amount used by a large downstream users |

| Determinant | Default assessment | Refined assessment |
|---|---|---|
| | the identified use is processed by a single user. | (formulators and industrial end uses).<br>See R. 16.3.5.1 |
| Annual use at local scale<br>Industrial setting<br>(ERC1-7, 12) | It is set equal to 100% of the total registrant's tonnage (at the EU level) for identified use (see R. 16.3.2.1) | The annual use at the site can be overwritten by the registrant considering the information listed in the previous point<br>See R. 16.3.5.1 |
| Daily wide dispersive use at local scale<br>(ERC 8-11) | It is calculated from the fraction of the registrant's total EU tonnage supplied to an identified use, corresponding to the consumption in a standard town of 10.000 inhabitants (R. 16.3.2.1), multiplied by a factor of 4. | The registrant can overwrite this value, for example if he has sufficient information to demonstrate that the use of the substance is evenly distributed in space and time throughout the region (e.g. for detergents); in this case it is possible to divide the default tonnage by a factor of 4. See R. 16.3.5.1 |
| Regional tonnage | For the industrial settings (ERC1-7, 12), it is set equal to 100% of the tonnage at EU level for an identified use. For wide dispersive uses it is set equal to the 10% of the registrant's supply volume at EU level for an identified use (see R. 16.3.3) | Market data could be used to overwrite the default for the region with a percentage that corresponds to the actual situation. |
| Pattern of release to water | Continuous (see R. 16.2.3) | The pattern of release to water can be changed to *intermittent* (i.e. in case the releases take place less than once per month and for no more than 24 hours) |
| Municipal Sewage Treatment Plant (STP) | By default the releases to fresh and marine water go to the Municipal STP for both industrial setting (ERC1-7, 12) and wide dispersive use (ERC 8-11). See also R. 16.6.3.3. | The STP can be bypassed depending on the actual conditions of use of the substance. |
| Discharge rate of the Municipal Sewage Treatment Plant (STP) | 2000 m3/day (see also R. 16.6.5.4) | The flow rate can be changed according to the site specific data. |
| Incineration of the sludge of the Municipal Sewage Treatment Plant (STP) | No incineration. The sludge is by default applied to a agricultural soil (see R. 16.6.6.6) | If incineration is foreseen, then agricultural application of sludge does not take place. |
| Receiving surface water flow rate | 18.000 m3/day (corresponding to a dilution factor of 10). For marine water, the dilution factor is set equal to 100 (see R. 16.6.3.3). | The flow rate or the dilution factor can be changed according to the site specific data. |
| Release factors or rates | ERCs correspond to default release factors (see R. 16.3.1.4) which are listed in Appendix 16.1. | The release factor or rate can be refined by taking into account RMM/OC.<br>It is also possible to refine the default release factors by taking into consideration substance physico-chemical properties..<br>Measured release rate at the site can be used instead of the default values.<br>Possible sources to refine the release |

| Determinant | Default assessment | Refined assessment |
|---|---|---|
| | | factors are:<br>▪ Emission Scenario Documents (ESDs)<br>▪ Sector specific ERCs, the so called SPERCs, developed by industrial sector organizations.<br>See R. 16.3.5.2 |
| Environmental exposure model | Tier I models:<br>EUSES (2.1)<br>TGD 2003 Risk Assessment Spreadsheet Model<br>ECETOC TRA<br>See R. 16.7 | Higher tier model<br>See R.16.8, letter d) |
| PECs concentrations | PECs calculated by tier I exposure models/tools | Environmental measured concentrations of a suitable quality can be used for the exposure estimate. See R.16.4. |
| Substance properties | See table R. 16.17 for information requirements for Tier I assessment | See Table R. 16.19 related to substance properties to be used for refined environmental assessment.<br>See R. 16.8, letter b) |
| Characterization of environmental compartments | Default assumption included in the Tier I models (see Table R.16-12 and Table R.16-15) | More specific information on the location of release sources (see R. 18.8, letter c) |

**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.

Boeije, G., Wagner, J.-O., Koormann, F., Vanrolleghem, P., Schowanek, D. and Feijtel, T.C.J. (2000). New PEC definitions for river basins applicable to GIS-based environmental exposure assessment. Chemosphere, 40, 255-265.

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.

GEMCO (Generic Estuary Model for Contaminants) – Conceptual Background and User Manual. Final Report 1.0 (2004). Report available form CEFIC LRI.

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.

EC (2009a). Guidance on Surface Water Chemical Monitoring under the Water Framework Directive. Common Implementation Strategy for the Water Framework Directive (2000/60/EC) - Guidance Document No. 19. Technical Report – 2009-025. ISBN 978-92-79-11297-3. http://circa.europa.eu/Public/irc/env/wfd/library?l=/framework_directive/guidance_documents/guidance_monitoringpdf/_EN_1.0_&a=d

EC (2009b). COMMISSION DIRECTIVE 2009/90/EC of 31 July 2009 laying down, pursuant to Directive 2000/60/EC of the European Parliament and of the Council, technical specifications for chemical analysis and monitoring of water status.

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.

Grubbs, F (1969). Procedures for detecting outlying observations in samples. Technometrics 11(1):1-21

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.

Hrubec, 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.

McAvoy, D. J. Shi, W. Schecher, B. E. Rittmann, and K.-C. Lee (1999). ASTREAT: A Model for Calculating Chemical Loss Within an Activated Sludge Treatment System, Version 1. The Procter & Gamble Co, Cincinnati, OH.

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, Luttik 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.

Schowanek, D., Fox, K., Holt, M., Schroeder, F.R., Koch, V., Cassani, G., Matthies, M., Boeije, G., Vanrolleghem, P., Young, A., Morris, G., Gandolfi, C. and Feijtel, T.C.J. (2001). GREAT-ER: a new tool for management and risk assessment of chemicals in river basins. Contribution to GREAT-ER # 10 Wat. Sci. Technol., 43 (2), 179 – 185.

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.

US-EPA (1991). Technical Support Document For Water Quality-based Toxics Control. EPA/505/2-90-001.

http://www.epa.gov/npdes/pubs/owm0264.pdf

US-EPA (2006). Data Quality Assessment: Statistical Methods for Practitioners, EPA QA/G 9S. Office of Environmental Information, Washington, DC

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.

Wind, T. (2004). Prognosis of environmental concentrations by geo-references and generic models: a comparison of GREAT-ER ad EUSES exposure simulations for some consumer product ingredients in the Itter. Chemosphere 54, 1145-1153.

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.16-21**: Name and description of Environmental Release Categories

| ERC | Name | Description |
|---|---|---|
| ERC 1 | Manufacture of substances | Manufacture 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 |
| ERC 2 | Formulation of mixtures | Mixing and blending of substances into (chemical) mixtures in all types of formulating industries, such as paints and do-it-yourself products, pigment paste, fuels, household products (cleaning products), lubricants etc. |
| ERC 3 | 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 compounds. For instance a plasticizers or stabilizers in PVC master-batches or products, crystal growth regulator in photographic films etc. |
| ERC 4 | Industrial use of processing aids in processes and products, not becoming part of articles | 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 |
| ERC 5 | Industrial use resulting in inclusion into or onto a matrix | Industrial use of substances as such or in mixtures (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, dyes in textile fabrics and leather products, metals in coatings applied through plating and galvanizing processes. The category covers substances in articles with a particular function and also substances remaining in the article after having been used as processing aid in an earlier life cycle stage (e.g. heat stabilisers in plastic processing).. |
| ERC 6A | Industrial use resulting in manufacture of another substance (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. |
| ERC 6B | 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. |

| ERC | Name | Description |
|---|---|---|
| ERC 6C | Industrial use of monomers in polymerisation process | Industrial use of monomers in the production of polymers, plastics (thermoplastics), polymerization processes. For example the use of vinyl chloride monomer in the production of PVC |
| ERC 6D | Industrial use of process regulators for polymerisation processes in production of resins, rubbers, polymers | Industrial use of chemicals (cross-linking agents, curing agents) in the production of thermosets and rubbers, polymer processing. For instance the use of styrene in polyester production or vulcanization agents in the production of rubbers |
| 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. No intended contact between functional fluids and products foreseen, and thus low emissions via waste water and waste air to be expected. |
| ERC 8A | 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/sewage system, 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. |
| ERC 8B | 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 |
| ERC 8C | 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. |

| ERC | Name | Description |
|---|---|---|
| ERC 8D | 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. |
| ERC 8E | 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) |
| ERC 8F | 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. |
| ERC 9A | 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. |
| ERC 9B | 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. |
| ERC 10A | 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 in outdoor use, such as metal, wooden and plastic construction and building materials (gutters, drains, frames etc.) |
| ERC 10B | Wide dispersive outdoor use of long-life articles and materials with high or intended release (including abrasive processing) | Substances included into or onto articles and materials with high or intended release during their service life from outdoor use. Such as tyres, 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. This also includes releases from the article matrix as a result of processing by workers. These are processes typically related to PROC 21, 24, 25, for example: Sanding of buildings (bridges, facades) or vehicles (ships). |

| ERC | Name | Description |
|---|---|---|
| ERC 11A | 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) |
| ERC 11B | Wide dispersive indoor use of long-life articles and materials with high or intended release (including abrasive processing) | 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. This also includes releases from the article matrix as a result of processing by workers. These are processes typically related to PROC 21, 24, 25. For example removal of indoor paints. |
| ERC12A | Industrial processing of articles with abrasive techniques (low release) | Substances included into or onto articles and materials are released (intended or not) from the article matrix as a result of processing by workers. These are processes typically related to PROC 21, 24, 25. Processes where the removal of material is intended but the expected release remains low include for example cutting of textile, cutting, machining or grinding of metal or polymers in engineering industries. |
| ERC12B | Industrial processing of articles with abrasive techniques (high release) | Substances included into or onto articles and materials are released (intended or not) from/with the article matrix as a result of processing by workers. These are processes typically related to PROC 21, 24, 25..Processes , where the removal of material is intended and high amounts of dust may be expected include for example sanding operations or paint stripping by shotblasting. |

**Table R.16-22**: Specification of the use conditions reflected in the environmental use categories.

| ERC | Lifecycle Stage | level of containment | Intended technical fate of substance | Dispersion of release sources | indoor/outdoor | release promotion during service life |
|---|---|---|---|---|---|---|
| 1 | Manufacture | open-closed | | Industrial | Indoor | Na |
| 2 | Formulation | open-closed | No inclusion into matrix | Industrial | Indoor | Na |
| 3 | Formulation | open-closed | inclusion into/onto matrix | Industrial | Indoor | Na |
| 4 | Use | open-closed | processing aid | Industrial | Indoor | Na |
| 5 | Use | open-closed | inclusion into/onto matrix | Industrial | Indoor | Na |
| 6a | Use | open-closed | Intermediate | Industrial | Indoor | Na |
| 6b | Use | open-closed | reactive processing aid | Industrial | Indoor | Na |
| 6c | Use | open-closed | monomers for polymers | Industrial | Indoor | Na |
| 6d | Use | open-closed | Process regulators for thermosets/rubbers | Industrial | Indoor | Na |
| 7 | Use | closed system | processing aid | Industrial | Indoor | Na |
| 8a | Use | open-closed | processing aid | wide disperse | Indoor | Na |
| 8b | Use | open-closed | reaction on use | wide disperse | Indoor | Na |
| 8c | Use | open-closed | inclusion into/onto matrix | wide disperse | Indoor | Na |
| 8d | Use | open-closed | processing aid | wide disperse | Outdoor | Na |
| 8e | Use | open-closed | reaction on use | wide disperse | Outdoor | Na |
| 8f | Use | open-closed | inclusion into/onto matrix | wide disperse | Outdoor | Na |
| 9a | Use | closed systems | processing aid | wide disperse | Indoor | Na |
| 9b | Use | closed systems | processing aid | wide disperse | Outdoor | Na |
| 10a | Service life | Open | inclusion into/onto matrix | wide disperse | Outdoor | Low |
| 10b | Service life | Open | inclusion into/onto matrix<br>Removing from matrix | wide disperse | Outdoor | High |
| 11a | Service life | Open | inclusion into/onto matrix | wide disperse | Indoor | Low |
| 11b | Service life | Open | inclusion into/onto matrix<br>Removing from matrix | wide disperse | Indoor | High |

| | | | | | | |
|---|---|---|---|---|---|---|
| 12a | Service life | open-closed | Losses from matrix during article processing | Industrial | Indoor | Low |
| 12b | Service life | open-closed | Losses with matrix during article processing | Industrial | Indoor | High |

**Table R.16-23**: Default parameters to derive the environmental release rate

| Note | No | ERC | Default worst case release factors resulting from the conditions of use described in the ERCs. Grey cells indicate release factors which are used for the regional release estimation only (and not for the local one). | | |
|---|---|---|---|---|---|
| | | | to air | to water (before STP) | to soil |
| 1,7 | 1 | Manufacture of chemicals | 5% | 6% | 0.01% |
| 2,7 | 2 | Formulation of mixtures | 2.5% | 2% | 0.01% |
| 2,7 | 2 | Formulation in materials | 30% | 0.2% | 0.1% |
| 3, 7 | 4 | Industrial use of processing aids | 100% | 100% | 5% |
| 4,7 | 5 | Industrial inclusion into or onto a matrix | 50% | 50% | 1%. |
| 5,7 | 6A | Industrial use of intermediates | 5% | 2% | 0.1% |
| 5,7 | 6B | Industrial use of reactive processing aids | 0.10% | 5% | 0.025% |
| 5,7 | 6C | Industrial use of monomers for polymerisation | 5% | 5% | 0% |
| 5,7 | 6D | Industrial use of auxiliaries for polymerisation | 35% | 0.005% | 0.025% |
| 6,7 | 7 | Industrial use of substances in closed systems | 5% | 5% | 5% |
| 3,7 | 8A | Wide dispersive indoor use of processing aids, open | 100% | 100% | n.a. |
| 5,7 | 8B | Wide dispersive indoor use of reactive substances , open | 0.10% | 2% | n.a. |
| 4,7 | 8C | Wide dispersive indoor use, inclusion into or onto a matrix | 15% | 1% | n.a. |
| 3,7,8 | 8D | Wide dispersive outdoor use of processing aids, open | 100% | 100% | 20% |
| 4,7 | 8E | Wide dispersive outdoor use of reactive substances, open | 0.10% | 2% | 1% |
| 4,7 | 8F | Wide dispersive outdoor use, inclusion in matrix | 15% | 1% | 0.5% |
| 6,7 | 9A | Wide dispersive indoor use in closed systems | 5% | 5% | n.a. |
| 6,7 | 9B | Wide dispersive outdoor use in closed systems | 5% | 5% | 5% |
| 8 | 10A | Wide dispersive outdoor use of long-life articles, low release | 0.05% | 3.2.% | 3.2% |
| 9,10 | 10B | Wide dispersive outdoor use of long-life articles, high or intended release | 100% | 100% | 100% |
| 8 | 11A | Wide dispersive indoor use of long-life articles, low release | 0.05% | 0.05% | n.a. |
| 9,10 | 11B | Wide dispersive indoor use of long-life articles, high or intended release | 100% | 100% | n.a. |
| 10 | 12A | Industrial processing of articles with abrasive techniques (low release) | 2.5% | 2.5% | 2.5% |
| 10 | 12B | Industrial processing of articles with abrasive techniques (high release) | 20% | 20% | 20% |

**Notes**

**General**

Each environmental release category is linked to default parameters to estimate the release rates to the relevant environmental compartments. For each environmental release category, the release factors are based on the highest release 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 release factors have been selected from general release information from EC (2003) for representative cases. In the conservative design of the release factors, it is assumed that no risk management measures are included. The physico-chemical properties of a substance are not taken into account. The distribution between air, water and soil is therefore not based on the properties of the substance. Also the potential waste treatment route is not considered. These characteristics lead to conservative values for release to all compartments. The background to, and the rationale for, the default parameters to derive environmental release rates (Table R.16-21) is based on the exposure assessment principles detailed in Section R.16.2. In this section, the different spatial scales of assessment are explained.

For industrial production, formulation and use (ERC 1-7), air and water releases are considered for exposure at both the local and the regional scale. Direct releases to soil are however only taken into account at the regional scale. This is due to the fact that industrial soil is not considered a protection target in the framework of chemicals assessment. The same assumptions apply to industrial processing of articles (ERC12).

For wide dispersive uses (i.e. a large number of users, including private use) and non-industrial article service life (a large number of product sources) it is assumed that a certain fraction of the estimated volume for that use is used in a standard town of 10000 inhabitants. At the local scale, the corresponding releases in such a standard town go to surface water, via a municipal sewage treatment plant (STP), resulting in a point source release. The releases to air and the direct releases to soil are considered for exposure at regional scale.

**Annotations per environmental release category**

**1) Manufacture of chemicals**

The release factors are based on the information for the manufacture of basic chemicals and chemicals used in synthesis (including monomers and catalysts). Besides basic (organic) chemicals both the production of chemicals in the petrochemical industry and the metal extraction and refining industry are included. Release factors are derived from the general release factors for the production of chemicals provided in EC (2003).

**2) Formulation**

For the life cycle stage formulation a distinction is made between mixing and blending of substances (processing aids) in mixtures like liquids, pastes or (compressed) gases for instance in aerosol cans, and on the other hand processes of mixing, which result in 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 articles. Often the processes of compounding and conversion are performed as successive process steps at the same facility. The production of master batches, which are made up to contain high concentrations of specific additives, is 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. Release factors are derived from the general release factors for formulation from EC (2003). The highest release 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 the matrix of an article. It should be stressed though that processing aids might be converted by 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. Solvents in cleaners, paints or adhesives are another example of processing aids which are released with waste air, waste water or as waste from the application process. Without release abatement or waste treatment, 100% of this type of processing aid applied will be emitted via air or water.

Release factors for industrial use of processing aids have been derived from the release factor tables for industrial use of processing aids (processing). For each compartment the highest release factors for this specific use pattern are taken from EC (2003)

In addition to industrial use, release factors have been derived for the use by the public at large (households). Release factors for wide dispersive use of processing aids have been derived from EC (2003) for the sector personal or domestic use. For air the release factor is set at 100% for instance to represent the use of propellants in aerosol cans . For water the release 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 release of these type of chemicals is assumed to be complete to either air or water.

**4) Substances processed into or onto an article matrix**

Besides the specific use of chemicals as processing aids, chemicals are also processed with the specific goal of being included into or onto a matrix. For example, pigments or fillers in paints will be included in the paint layer (matrix) after the painting process, and dyes will be included into the fibre matrix during the dyeing process. The highest release factors for air and water for this specific type of use have been taken from EC (2003), which is related for instance to dying of leather or painting or coating

Please note: If a processing aid remains in the matrix without function after processing it should be assessed under ERC 5 rather than ERC 4. An example for such a case is a heat stabiliser remaining in the polymer matrix although increased temperature was only relevant at the formulation or conversion stage.

**5) 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 have so far not been covered in the default release factors in the Technical Guidance Document (EC, 2003). Several assumptions have been made to provide release 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 a release factor of 0.1% has been assumed. A default half 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 monomers in a polymerization processes for the production of thermoplastics and thermosetting resins, and auxiliaries for polymer processing of rubbers and thermosetting resins (pre-polymers). The release factors for intermediates have been taken from available release factors for the chemical industry and the specific use of intermediates in the synthesis of other chemicals. Release factors for the use of monomers in the polymer industry have also been taken from EC (2003) for this specific type of use (polymerization processes). Releases 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.

**6) Release from closed systems**

The release factors have been based on leakage of cooling liquids from refrigerators and leakage of engine oil from cars. A leakage rate of 5% per year to air is assumed based on Matthijsen and Kroeze (1996) and Folkert and Peek (2001). The leakage rates do not include losses from recharging or filling of machinery (about 0.2% to air and 0.1% to water) but in general this is negligible compared to the annual leakage rate. Release 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 release factor can be calculated as follows: 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 a release 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 values are somewhat lower at about 0,5 up to 7 percent (OECD, 2004a). Releases to water has also been taken into account for indoor use because of the possible spills to (waste) water and the potential release of substances used in central heating systems where the heat transfers system is water.

**7) Indoor and outdoor use**

Industrial

Industrial activities are primarily considered to be indoor processes. The relevant life cycle stages are production, formulation and industrial use (ERC1-7). However this is not strictly the case for large industrial installations (e.g. at refineries) that are usually not inside a covered building.

Release to industrial soil assumed in the ERCs may result from spilling during transfer or delivery procedures or leakage from equipment like pumps, pipes (above and below ground), reactors and storage tanks (above and below ground). They may also result from the transport of waste streams like waste water due to leakage of the drain pipe (cracks, loose connections etc.) or the outside (open) storage of raw materials on the site. Releases might also result from the industrial application of certain products like hydraulic fluids and lubricants for instance in industrial transport or material handling equipment such as conveyer belts.

In many EU countries, the releases to soil will be lower due to special provisions which are compulsory to prevent them. Some typical spill prevention systems are liquid proof floors, concrete containment pits, curbs, dykes or bunds, containment buckets etc.

Wide disperse uses

For outdoor use of processing aids (ERC 8D), the release factor for soil refers to private use (consumers) of solvents. Release factors for the soil compartment for outdoor use of reactive processing aids (ERC 8E) refer to for example the use of a bleaching aid in cleaning products by the public at large. For the outdoor use of substances, which results in inclusion into or onto a matrix (ERC 8F), the release factors have been taken for the private use of paints and specifically refers to substances like fillers and pigments.

**8) Release from articles/materials during service life, low release**

Release factors are taken from the OECD emission scenario document on plastic additives (OECD, 2004b). The release factors presented in the ERC table are based on the assumption that a steady state has been reached in the market between the amounts of an article produced, the amount in use (stock) and the amount becoming waste per year. Under such an assumption, the annual release is not driven by the actual use of a substance for production of an article but by the stock of article in use. Thus the annual release is derived from the release factor multiplied by the

service life of the article. Note that for new substances recently placed on the market, there is no steady-state situation yet.

For outdoor use the release factor to water and soil is based on a worst case release of 0.16% multiplied by the service lifetime period of the article ($T_{service\ life}$) . In the Tier 1 $T_{service\ life}$ is set at 20 years, resulting in a release factor of 3.2%.

For indoor use the release factors are also taken from the OECD emission scenario document on plastic additives (OECD, 2004b).

**9) Release from articles during service life, high release**

Release factors to air and water for indoor use are taken from the emission scenario document for the textile processing industry, industrial category (IC) 13. For indoor wide dispersive use, the soil compartment is considered not to be relevant, and the same release factors are used for air and water.

For outdoor use the release factors are set to 100% per year for all compartments (steady state situation and total release of substance over service life). The reasoning behind this assumption is that complete release over service life for outdoor applications may occur either to air, water or soil.

**10) Release from processing of articles with abrasive techniques**

The processes to be addressed here are high and low energy manipulation or hot work operations with articles, resulting in releases of substances contained in these articles. The release from the articles may occur in the form of a substance as such or as particle (larger particles, dust, aerosols) where the substance is still embedded in a more or less intact solid matrix. The processes potentially relevant may include treatment of article surfaces (polishing, sanding), sawing and cutting of semi-finished articles (mechanical cutting, flame cutting) or welding and soldering. This may often correspond to PROC 21, 24 and 25.

Typical examples would be cutting of textile in the fabric industry, metal cutting, or sanding and planing of PU-foam blocks in the production of surfboards. Also chemical/mechanical paint stripping and other surface treatments of e.g. buildings or vehicles are processes to be covered under ERC 10B, 11B or ERC 12.

Particles from abrasive techniques can be quite large (fibers, wood shaving, chips, iron curls etc, and thus unlikely to become airborne or potentially give rise to intensified leaching of substances due to the increase of surface. If dusts and aerosols are formed indoor they are expected to be removed by local ventilation (efficiency not included in the release factors) or to precipitate on the ground/floor, and become waste (floor cleaning), or go to waste water if cleaned with water. This is comparable to the considerations on handling powders in paint manufacture and plastics compounding and conversion. Two different situations can be discerned, related to the type of abrasive process. When cutting or coarse grinding of textile, polymers or metals is involved, larger particles are formed as a relatively small fraction of the original material. In the low release situation (ERC12A), the release factors of 2.5% are based on the OECD ESD for plastic additives (OECD 2004), based on grinding/ machining. The release might either be to air, water or soil or a combination of these.

When surfaces are treated with high energy abrasive techniques such as sanding or shot blasting, ERC12b is applicable. The worst case release is based on dust releases due to shot blasting without any RMM, where a high release factor of 20% is estimated (Verstappen 1993). The release might either be to air, water or soil or a combination of these.

If surfaces are treated with abrasive techniques under outdoor, non industrial conditions (e.g. sanding of bridges, high pressure cleaning of walls, paint stripping of ships) substances contained

in the removed surface may be completely released into the environment if no RMMs are applied (OECD 2006). Thus such conditions can be covered under ERC 10B.

If surfaces are treated with abrasive techniques under indoor, non industrial conditions (ERC11B, e.g. paint stripping of walls, doors, floors) substances contained in the removed surface or surface coatings could be released totally when no RMMs are in place (OECD, 2006). These activities are taken into account under ERC11B when they are in a non-industrial setting with many release sources constituting wide dispersive release.

**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. Environment Directorate Organisation for Economic Co-operation and Development (OECD).

OECD (2004b). Emission Scenario Document on plastics additives. OECD series on Emission Scenario Documents number 3. Environment Directorate Organisation for Economic Co-operation and Development (OECD).

OECD (2006). Draft Emission Scenario Document on Coatings Industry. Environment Directorate Organisation for Economic Co-operation and Development (OECD).

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, 2010en 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 2

Verstappen (1993) Joint project process descriptions Dutch industry, Ship yards. RIVM report nr 773006148.

**Appendix R.16-2**: Overview of Emission Scenario Documents (ESDs)

The following table lists the existing Emission Scenario Documents

For more information, please refer to: http://www.oecd.org/document/46/0,3343,en_2649_34373_2412462_1_1_1_37465,00.html#a.

| ESD TITLE | NACE[22] | IC[23] | PT[24] | REFERENCE | REMARKS |
|---|---|---|---|---|---|
| ***Industrial manufacturing process/mixture type*** | | | | | |
| **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** | |

[22] Nomenclature générale des Activités économiques dans les Communautés Européennes. See European Commission, Competition: List of NACE Codes (2007.11.19); http://ec.europa.eu/comm/competition/mergers/cases/index/nace_all.html

[23] Industrial Category

[24] Product Type

| ESD TITLE | NACE[22] | IC[23] | PT[24] | REFERENCE | REMARKS |
|---|---|---|---|---|---|
| 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 | |
| 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 | |
| Insecticides, acaricides and products to control other arthropods for household and professional uses | | 15/0 | 18 | OECD_17 | BIOCIDAL PRODUCTS |
| Adhesive Formulation | | | | OECD_18 | |
| Coating Industry (Paints, Lacquers and Varnishes) | | 14 | | OECD_19 | |

| ESD TITLE | NACE[22] | IC[23] | PT[24] | REFERENCE | REMARKS |
|---|---|---|---|---|---|
| Pulp, Paper and Board Industry | | 12 | | OECD_20 | |
| Formulation of Radiation Curable Coatings, Inks and Adhesives | C26.6? | 0? | | OECD_21 | |
| Transport and Storage of Chemicals | H? | 0? | | OECD_22 | |
| 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 | |
| Rubber industry | | 11 | 9 | EU_1 | |
| ***Biocidal products*** | | | | | |

| ESD TITLE | NACE[22] | IC[23] | PT[24] | REFERENCE | REMARKS |
|---|---|---|---|---|---|
| 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 | |
| Preservatives for liquid-cooling and processing systems | | 2/3/9 | 11 | EUB_12 | |
| Slimicides | | 12 | 12 | EUB_13 | |

| ESD TITLE | NACE[22] | IC[23] | PT[24] | REFERENCE | REMARKS |
|---|---|---|---|---|---|
| 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, revised 2009.

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, revised January 2010.

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.

OECD 2008/D17: OECD Series on Emission Scenario Documents, No. 18, Emission Scenario Document for insecticides, acaricides and products to control other arthropods for household and professional uses. OECD, Environment Directorate, July 2008.

OECD 2008/D18: OECD Environment, Health and Safety Publications Series on Emission Scenario Documents No. 20, Emission Scenario Document on adhesive formulation . OECD, April 2009.

OECD 2008/D19: OECD Series on Emission Scenario Documents, No. 22, Emission Scenario Document on coating industry (Paints, Laquers and Varnishes). OECD, Environment Directorate, July 2009.

OECD 2008/D20: OECD Series on Emission Scenario Documents, No. 23, Emission Scenario Document on pulp, paper and board industry. OECD, Environment Directorate, July 2009.

OECD 2009/D21: OECD Series on Emission Scenario Documents, No. 21, Emission Scenario Document on the formulation of Radiation Curable Coating, Inks and Adhesives. OECD, Environment Directorate, 2009, revised January 2010.

OECD 2009/D22: OECD Series on Emission Scenario Documents, No. 24, Emission Scenario Document on transport and storage of chemicals. OECD, Environment Directorate, 2009.

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

**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.16-4).

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.16-10. Assuming that the total amount of solids in raw sewage produced per inhabitant per day is 0.150 ($m^{-3}\cdot d^{-1}$)·0.6 ($kg\cdot m^{-3}$) = 90 g per inhabitant per day, the concentration of suspended matter in influent has been set to 0.45 ($kg\cdot m^{-3}$) (see Table R.16-10). 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 kg BOD $kg_{dw}^{-1}\cdot d^{-1}$ 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 $Pa\cdot m^3\cdot mol^{-1}$). The overall mass transfer coefficient during surface aeration ($k_{surf}$) was assumed proportional to the dissolved oxygen overall transfer rate coefficient ($K_La_O$), 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 ($\Delta O_2$). In order to account also for the gas phase resistance (H < 250 $Pa\cdot m^3\cdot mol^{-1}$) the proportionality constant $\Psi$, 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:

$$k_{surf} = \psi \left(\frac{40 \cdot K_H}{40 \cdot K_H + 1}\right) \frac{R_O}{HRT \cdot \Delta O_2}$$

In the following tables H (Henry's law constant) should be used in $Pa\cdot m^3\cdot mol^{-1}$.

**a) No biodegradability**

Fate of chemicals that are not degradable: $kbio_{stp}$ = 0 $hr^{-1}$ 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 | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | % removal | -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 | 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: $kbio_{stp}$ = 0.1 $hr^{-1}$ in the aqueous phase of activated sludge.

| | % to air | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| log Kow | 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 |

| | % to water | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| log Kow | 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 |

| | % to sludge | 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 | 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 |

| | % degraded | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| log Kow | 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 |

| | % removal | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| log Kow | 0 | 41 | 41 | 41 | 41 | 42 | 48 | 72 | 92 | 95 | 95 |
| | 1 | 41 | 41 | 41 | 41 | 42 | 48 | 72 | 92 | 95 | 95 |
| | 2 | 41 | 41 | 41 | 41 | 42 | 48 | 73 | 92 | 95 | 95 |
| | 3 | 43 | 43 | 43 | 43 | 44 | 50 | 73 | 92 | 95 | 95 |
| | 4 | 52 | 52 | 52 | 52 | 52 | 57 | 76 | 93 | 95 | 96 |
| | 5 | 72 | 72 | 72 | 72 | 73 | 75 | 84 | 95 | 96 | 97 |
| | 6 | 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: $kbio_{stp}$ = 0.3 $hr^{-1}$ in the aqueous phase of activated sludge.

| | % to air | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| log Kow | 0 | 0 | 0 | 0 | 0 | 1 | 6 | 36 | 76 | 84 | 85 |
| | 1 | 0 | 0 | 0 | 0 | 1 | 6 | 36 | 76 | 84 | 85 |
| | 2 | 0 | 0 | 0 | 0 | 1 | 6 | 36 | 75 | 83 | 84 |
| | 3 | 0 | 0 | 0 | 0 | 1 | 6 | 35 | 73 | 81 | 82 |
| | 4 | 0 | 0 | 0 | 0 | 1 | 5 | 30 | 64 | 71 | 71 |
| | 5 | 0 | 0 | 0 | 0 | 0 | 3 | 17 | 40 | 45 | 46 |
| | 6 | 0 | 0 | 0 | 0 | 0 | 1 | 7 | 20 | 24 | 25 |

| | % to water | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| log Kow | 0 | 33 | 33 | 33 | 33 | 32 | 29 | 19 | 7 | 5 | 4 |
| | 1 | 33 | 33 | 33 | 33 | 32 | 29 | 19 | 7 | 5 | 4 |
| | 2 | 32 | 32 | 32 | 32 | 32 | 29 | 19 | 7 | 5 | 4 |
| | 3 | 32 | 32 | 32 | 32 | 31 | 29 | 18 | 7 | 5 | 4 |
| | 4 | 27 | 27 | 27 | 27 | 27 | 25 | 16 | 6 | 4 | 4 |
| | 5 | 18 | 18 | 18 | 18 | 17 | 16 | 12 | 5 | 3 | 3 |
| | 6 | 11 | 11 | 11 | 11 | 11 | 10 | 9 | 5 | 4 | 4 |

| | % to sludge | 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 | 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 |

| | % degraded | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 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 |

| | % removal | log H -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| log Kow | 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: $kbio_{stp}$ = 1 $hr^{-1}$ in the aqueous phase of activated sludge.

| | % to air | log H -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 |

| | % to water | log H -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 |

| | % to sludge | 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 |

| | % degraded | log H -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 |

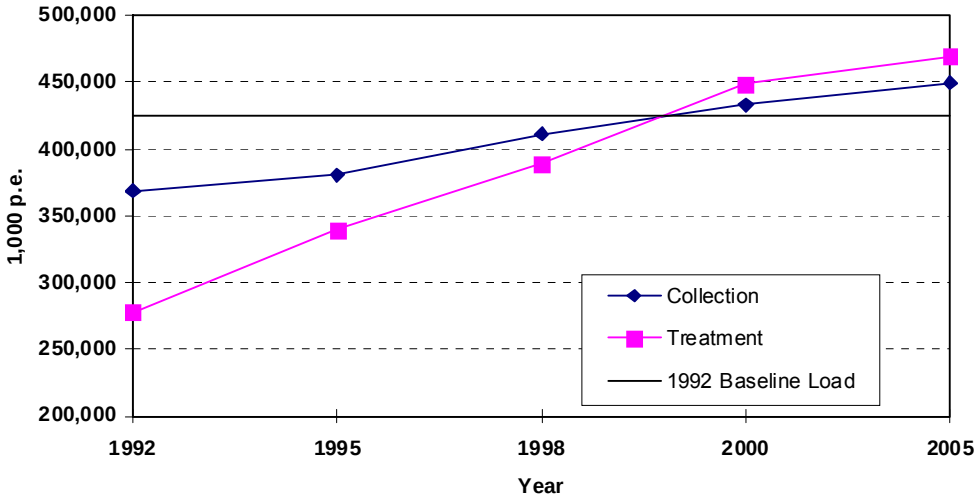
| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | 4 | 73 | 73 | 73 | 73 | 73 | 71 | 61 | 34 | 26 | 24 |
| | 5 | 45 | 45 | 45 | 45 | 45 | 44 | 38 | 22 | 17 | 16 |
| | 6 | 21 | 21 | 21 | 21 | 21 | 21 | 19 | 12 | 9 | 9 |

| | | 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 Europe

Default 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.




*p.e. = person equivalent*

**Figure R.16-16**: Development in Collection and Treatment Capacity EU14 (Source: EC, 1999)25

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 R.16-24. The population weighted average for the whole of the EU15 in 1995 was 73%. Although the apparent degree of connection to wastewater treatment is 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)

[25] 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.

**Table R.16-24**: 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 (EEWG, 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 R.16-16. 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 (EEWG, 1997).

**European Chemicals Agency**
P.O. Box 400, FI-00121 Helsinki
http://echa.europa.eu