Evaluation Manual for the Authorisation of plant protection products and biocides

EU part

Biocides

Chapter 5 Behaviour and fate in the environment; behaviour in surface water, sediment and sewage treatment plant (STP)

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Chapter 5 Behaviour and fate in the environment; behaviour in surface water, sediment and sewage treatment plant (STP)

Category: biocides

GENERAL INTRODUCTION

This chapter describes the data requirements for estimation of the behaviour of a biocide and the active substance in surface water and sediment, and the behaviour in sewage treatment plants (STPs), and which evaluation methodologies are applied for the EU framework (§1 - §1.5).

This chapter consists of two parts, one part about behaviour in surface water and sediment (I), and a second part about behaviour in sewage treatment plants (STPs) (II).

I BEHAVIOUR IN SURFACE WATER AND SEDIMENT

1. EU FRAMEWORK

The procedure for inclusion of active substances in Annex I to Biocides Directive 98/8/EC [1] is described under EU framework (§1 - §1.5) where only the procedure laid down in the EU is described. The NL procedure for evaluation of a substance, described in In the NL part §2 - §2.5, is reverted to where no EU procedure has been laid down.

1.1. Introduction

This chapter serves to determine estimated or measured concentrations in surface water, which are used for risk assessment for organisms that depend on surface water (aquatic organisms, birds and mammals).

In view of the above, there is a relationship with the following chapters Ecotoxicology aquatic organisms (see Chapter 6 Ecotoxicology; aquatic) and Ecotoxicology terrestrial organisms (see Chapter 6 Ecotoxicology; terrestrial).

The concentration in surface water depends, inter alia, on direct emissions to surface water or indirect emissions via sewage treatment plants (STPs), or on the extent to which a substance leaches from treated materials and reaches the water via drainage pipes. Via this last route and specifically the potential application of surplus activated sludge on land, there is a relationship with Chapter 5 Behaviour and fate in the environment; behaviour in soil; Leaching to groundwater.

Calculation methods for the behaviour in water and sediment are described in the Technical Guidance Document on Risk Assessment (TGD) [4].

Determination of the relevance of the emission routes and quantification of emissions are based on emission scenarios drawn up for various product types (see the ex-ECB web site for emission scenario documents [2]). Objective of these emission scenarios is the harmonisation of the annex I inclusion and authorisation process for biocidal products. The emission scenario documents relevant for various product types are briefly summarized in Appendix A to the environmental section.

A decision tree with corresponding explanatory notes is included in Appendix 1. This decision tree summarises the evaluation system for behaviour in water and sediment.

1.2. Data requirements

The data requirements laid down in the TNsG on data requirements [3] corresponding with the Biocides Directive (98/8/EC) are listed below; the data requirements for the active substance and the product for evaluation of the risk of the behaviour in water and sediment. This is the verbatim text of the Directive (grey frames). Numbering of the studies corresponds with the numbering of the TNsG on data requirements. Numbering in square brackets follows the numbering of the Biocides Directive. Where relevant, the result of the study has been added.
The data requirements are divided into standard data requirements (core data) that apply for each product type, product-type-specific data for different product types (summarised in the table with product type specific data in Part C of Chapter 2 of de TNsG on data requirements), and additional data requirements in case higher tier data are required (summarised in Chapter 3 of the TNsG on data requirements).

One aspect that has not yet been elaborated in EU framework is presented in the NL part §2.2.
If in EU framework clarity will be provided about these currently not elaborated aspects, these will be followed.

Information on fate and behaviour of the active substance and its metabolites is required to be able to determine exposure of the environment (compartments water, sediment, soil and air).

1.2.1. Data requirements for the active substance

Standard data requirements

The following data are required for an initial evaluation:

7.1.1.1.1 Hydrolysis as function of pH and identification of breakdown products;
7.1.1.1.2 Phototransformation in water including identity of the products of transformation;
7.1.1.2.1 Ready biodegradability;
7.1.1.2.2 Inherent biodegradability;
7.1.3 Adsorption/desorption screening test

For the initial risk assessment the biodegradability aspect only requires a ready test. If a substance is not readily biodegradable, the result of an inherent test can be used supplementary. If no inherent test is available, an STP simulation study is preferred as supplementary test.

7.1 Fate and Behaviour in Water

7.1.1 Degradation, initial studies

7.1.1.1 Abiotic [Ann. IIA, VII.7.6.2.]

7.1.1.1.1 Hydrolysis as a function of pH and identification of breakdown products [Ann.IIA, VII.7.6.2.1.]

- Must be examined at least at three different pH-values. For substances with a low hydrolysis rate, just the preliminary test carried out at 50 °C for five days may be sufficient. A substance of which less than 10% hydrolyses in 5 days at 50°C (i.e. is considered hydrolytically stable) need not to be further tested for hydrolysis.

- Identification is required for breakdown products that at any sampling time account for more than 10% of the active substance added. Annex to Chapter 1 on metabolites currently drafted for plant protection products could be re-written to cover metabolites for biocides as well).
- Test according to EC method C.7 or the corresponding OECD guideline 111 (Hydrolysis as a function of pH).

Result
→ DT_{50} hydrolysis active substance and identification metabolite(s)

7.1.1.1.2 Phototransformation in water including identity of the products of transformation [Ann.IIA, VII.7.6.2.2.]

- Test according to the SETAC procedures (SETAC 1995) or e.g. US-EPA guideline OPPTS 835.2210 (US-EPA, 1998). [Note: There is an OECD draft guideline available.
- The data must be submitted for a purified active substance of stated specification.
- Identification is required for transformation products that at any sampling time account for more than 10% of the active substance added.
- The results submitted should correspond to the light intensities and spectral distribution from northern to southern European regions, for example, in 40 and 65 degrees (proposed average 50 degrees) northern latitude during spring and autumn. This may be presented e.g. by extrapolation.
- Further guidance for conducting the study may be found in an OECD Guidance Document (OECD 1997).

Result
→ DT_{50} photolysis active substance and identification metabolite(s)

7.1.1.2 Biotic [Ann.IIA, VII.7.6.1.]

7.1.1.2.1 Ready biodegradability [Ann.IIA, VII.7.6.1.1.]

- At least a screening test on ready biodegradation is always required of organic compounds, unless a simulation test is required. (More details are given in Chapter 3, 7.0.2 testing strategy on biodegradation of biocidal active substances and testing methods).
- Test according to any of the EC methods C.4-A-F or the corresponding ECD guideline 301 A-F taking especially notice of the Annex to these methods concerning the evaluation of the biodegradability of chemicals suspected to be toxic to the inoculum.
- See Chapter 3 for guidance on further studies.

Result
→ substance “ready biodegradable” or “not ready biodegradable”, percentage DOC removal.

7.1.1.2.2 Inherent biodegradability, where appropriate [Ann.IIA, VII.7.6.1.2.]

- May be performed if the compound is not readily degradable unless a simulation test is performed. Simulation tests are preferred instead of new tests on inherent biodegradability. The testing strategy to follow is described in Chapter 3, 7.0.2.2.2.
- EC method C.12 and EC.C.9 or the corresponding guidelines OECD 302 A-B and OECD 302 C. (7.1.2 An additional data requirement on rate and route of degradation in aquatic systems; guidance is given in Chapter 3).

Where these inherent tests are available, the test results should fulfil specific criteria to assign a degradation rate constant for STP modelling. Some criteria are listed in the table below. It should be demonstrated that biodegradation actually takes place, that no persistent metabolites are formed, and that the adaptation time is limited.
See also Chapter 3 of the TGD [4] 2.3.6.4 and Appendix II, pp. 278 -283.

OECD 302B (Zahn-Wellens test:)	Pass level is ≥ 70% loss of DOC. This pass level must be reached within 7 days[a], lag-phase should be no longer than 3 days, percentage removal in the test before biodegradation occurs should be below 15%.
OECD 302C (MITI-II test)	Pass level is ≥ 70% loss of DOC. This pass level must be reached within 14 days, lag-phase should be no longer than 3 days.
OECD 302A ((modified) SCAS test)	Pass levels are 20% loss of DOC: evidence of inherent biodegradation; ≥ 70% loss of DOC: evidence of ultimate biodegradation. If a substance is not biodegradable according to the SCAS test, the degradation rate is zero and further (simulation) tests are generally not required (unless metabolite formation is considered relevant).

[a]: The OECD guideline proposes 14 days degradation period.

Result
→ substance “inherently biodegradable” or “not inherently biodegradable”, percentage DOC removal.

7.1.2 Adsorption/desorption screening test [Ann.IIA, VII.7.7.]

- A screening test is always required according to, for example, to the new EC method C.18 or the corresponding OECD guideline 106 tier 2 (Adsorption/desorption)
  The adsorption is studied in five different soil types by means of adsorption kinetics at a single concentration and determination of distribution coefficients Kd and Koc. Although not explicitly mentioned in the guideline the handling procedure can also be applied to sediments.
- An alternative method is the estimation of adsorption with HPLC, OECD guidelines 121 (draft, will soon be adopted as new EC method). The method provides an estimate of a chemical’s partitioning behaviour between aqueous phases and organic surfaces of soils, sediments and sludge (Koc). This estimate is normally sufficient for a preliminary exposure assessment of substances (e.g. feed in fugacity type models). It should be noted however, that for some substances the HPLC-technique is not yet fully validated.
- Where the results of this test indicate the need to do so, the additional test described in the Chapter 3, in paragraph A7.1.4 (data set for the active substance) shall be required, and/or the additional test described in paragraph A7.2.3. A more detailed testing strategy is described in Chapter 3

Result
→ Kd and Koc values for 5 different soils (OECD 106 tier 2) or
→ Koc value by means of HPLC for a first evaluation (OECD 121)

No supplementary data are requested if direct emission to water can be ruled out and if the PEC/PNEC ratio <1 in the initial risk assessment (the PNEC is derived in Chapter 6 Ecotoxicology).

Product-type-specific and additional data

Supplementary tests are required if induced by the initial risk assessment or if direct emission to water or sediment occurs.

Simulation tests

• Simulation tests are mandatory if **direct** emission to surface water occurs.
• Simulation tests can be carried out:
  - as first step, where the screening stage biodegradation tests are skipped. This can be the case for biocides that are toxic to the inoculum.
  - if a substance is “not ready” or “not inherently” biodegradable and PEC/PNEC >1 and a further refinement of degradation rate and route is required related to metabolites.

7.1.1.2.3 Biodegradation in seawater

- If a substance is to be used or released in marine environments in considerable amounts (e.g. it is known to be repeatedly used or continuously released in marine environments), then a seawater biodegradation test according to OECD guideline 306 will be required.
- A modified version of ISO 14592 (shake flask batch test) with seawater at environmentally relevant concentrations (14C) may be performed.
- Alternatively a water/sediment degradation study (see paragraph A7.1.2.2.2) in seawater according to modified guidelines may be done.

Result

→ percentage degradation after 28 days (OECD 306)

7.1.2 Rate and route of degradation in aquatic systems including identification of metabolites and degradation products [Ann. IIIA, XII.2.1.]

- If the results from paragraphs A7.1.1.2.1 or (A7.1.1.2.2) above indicate the need to do so, or the active substance has an overall low or absent abiotic degradation, then the tests described in this paragraph shall be required. [Ann. IIIA, VII.6.]
- See section 7.0 and the testing strategy given in figure 1.
- Testing methods include: water degradation simulation test according to US-EPA guideline OPPTS 835.3100 (US-EPA 1998b); water sediment degradation test according to SETAC procedures (SETAC, 1995) or BBA guideline Part IV, 5.1 (BBA, 1990a); activated sludge biodegradation test according to Federle & Itrich (1997).

Result

→ DT_{50}

7.1.2.1.2 Anaerobic biodegradation

- An anaerobic degradation study is required if exposure to anaerobic conditions is likely. This may be the case with veterinary hygiene biocidal products and biocidal pest control products to be used in animal housing where release into manure storage facilities is possible.
- A test according to, e.g. ISO method 11734: 1995.

Result

→ DT_{50} active substance and/or metabolites (water/active sludge system)

7.1.2.2 Biodegradation in freshwater

7.1.2.2.1 Aerobic aquatic degradation study

- Test according to, for example, ISO method 14592 or US-EPA guideline OPPTS 835.3100 (US-EPA 1998b) is required with non-adapted inoculum.

7.1.2.2.2 Water/sediment degradation study

- Test according to, for example, draft OECD guideline (Aerobic and anaerobic transformation in water/sediment systems), BBA guideline Part IV, 5.1, BBA 1990a, Hoeks/Dekker or US-EPA guideline OPPTS 835.3180 (US-EPA 1998c).
- A water/sediment degradation study under anaerobic conditions should be done if the exposure of the substance to anaerobic conditions is very likely e.g. when a major proportion of the substance is absorbed in sediment).

Result

→ DT_{50} active substance and/or metabolites (water/sediment system)

7.1.3 Studies on adsorption and desorption in water/sediment systems and, where relevant, on the adsorption and desorption of metabolites and degradation products. [Ann. IIIA, XII.2.2.]

- Such studies are required where the preliminary risk assessment indicates that this is necessary.
- Screening tests on metabolites and other degradation products are required for compounds which at any sampling time during the soil degradation studies account for more than 10% of the active substance added.
- A full scale adsorption test may be appropriate to refine the PEC value in those cases where:
  - PEC/PNEC > 1 as a result from indirect exposure and the substance is not readily biodegradable.
- The testing strategy, figure 2, indicates when such further tests would be necessary.
- Test according to the new test method EC C.18 or the corresponding OECD guideline 106, or if adsorption to sewage sludge is of concern a test for example, US-EPA guideline OPPTS 835.1110 Activated sludge sorption isotherm (US-EPA 1998a); or draft OECD aerobic or anaerobic transformation in water/sediment systems.

Result

In 2 different sediments:

→ Kd values for active substance and metabolites

→ DT_{50} values for active substance and metabolites

7.1.4.1 Field study on accumulation in the sediment

- If non-extractable residues are formed exceeding 70% of the initial dose in the water/sediment study (7.1.2.2.2) or if the mineralization rate in the water/sediment system is less than 5% in 100 days, then a field study on accumulation in the sediment should be done.
- There is currently no standardised test guideline available.

Result

→ DT_{50} (field)

→ estimated concentration sediment residues

→ possibility of accumulation of active substance, metabolites and residue

1.2.2. Data requirements for the product

Product data are only required if there are indications that composition or method of application of the product affect degradation and transformation or mobility and adsorption properties of the active substance to such an extent that the conclusions of the risk assessment change considerably.

1.3. Risk assessment

The risk assessment methodology has been elaborated in Chapter 6 Ecotoxicology.
The assessment of fate and behaviour in water has been elaborated in the following documents:
Technical Guidance document [4] (TGD):

- Part 2, chapter 2 Environmental Exposure Assessment
- Chapter 2.2: Measured data
- Chapter 2.3.4: Characterisation of the environmental compartments.
- Chapter 2.3.5: Partition coefficients
- Chapter 2.3.6: Abiotic and biotic degradation rates
- Chapter 2.3.7: Elimination processes prior to the release to the environment
- Chapter 2.3.8: Calculation of PECs
- Chapter 2.5: Decision on environmental concentration used for risk characterisation
- Chapter 6.2: Refinement of PEC
- Chapter 6.2.1 Aquatic compartment
- Appendix VIII Environmental risk assessment for metals and metal compounds
- Appendix XI Environmental risk assessment for ionising substances

TNsG on data requirements [3]:

- Chapter 2, part C: (it is indicated per product type which compartments and which behaviour data are important).
- Chapter 7 p. 94: Testing strategy on degradation.
- Chapter 7.1: Fate and Behaviour in Water

Research into the behaviour of an active substance in water is important for a correct estimation of the concentration of such an active substance in surface water.
This estimated concentration, the PEC (Predicted Environmental Concentration), is an important parameter for risk estimation for aquatic organisms (see Chapter 6 Ecotoxicology).

The most important substance-related parameters for model estimation of the PEC are:

Core data

- DT_{50} for photolysis rate in water at 20°C (days);
- DT_{50} for hydrolysis rate in water at 20°C (days);
- DT_{50} for biodegradation rate in STP at 20°C (days);
- K_{oc} or K_p for soil/sediment (L/kg);
- Saturated vapour pressure (Pa);
- Solubility in water (mg/L);
- Molar mass (g/mol).

Additional data (depending on emission route or PEC/PNEC ratio >1 or preliminary risk assessment; the PNEC is derived in Chapter 6 Ecotoxicology).

- DT_{50} for degradation rate in water at 20°C (days);
- DT_{50} for degradation rate in sediment at 20°C (days);
- K_p for suspended organic matter (L/kg).

Besides on the substance properties, the level of the PEC depends on the following factors:

- Method of application and use;
- Dosage;
- Application frequency (single, repeated, continuous);
- Period between successive applications (days);
- Emission route (to STP, directly to water, soil or air);
- For some product types leaching of the active substance from products is relevant.

The PEC is usually calculated with the EUSES model, based on the TGD [4], where dependent on product type and use, an Emission Scenario is used for determination of the emission routes and calculation of the emission amounts. The emission scenario documents for the different product types are discussed in Appendix A of the environmental section.

1.3.1. Estimation of exposure concentrations in surface water

Exposure concentrations in water are estimated with EUSES (based on TGD Part 2, 2003) [4] and/or emission scenario documents (ESDs) with selection of the emission routes and estimation of the emission amounts, directly or indirectly via an STP to surface water.
For biocides with an emission to water, calculation of a $PEC_{localwater}$ is based on a standard environment during an emission episode, taking into account dilution, sorption and - if relevant - sedimentation, volatilisation and degradation (section 2.3.8.3).

The following degradation rates / half life values in surface water are derived on the basis of the results of the ready and inherent tests:

Table 1 First order rate constants and half life values for biodegradation in surface water based on biodegradation screening tests[a] [4]

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

Notes Table 1:

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 above. The half-life of 150 days reflects a present "best expert judgement".

The PEC estimation follows a tiered approach in several steps, where depending on the results of the first step -if appropriate- more accurate calculations are carried out in the subsequent steps, on the basis of supplementary data.

- Step 1 uses basic data for phototransformation, hydrolysis and biodegradation, where depending on the removal in the STP and distribution over the compartments a PECwater is calculated.
- Step 2. If an exceedance of the risk for aquatic organisms is found, or if direct emission to surface water is expected, a supplementary simulation study should be submitted for STP or surface water, respectively.
- In case of direct emission on surface water or in case of exceedance of the PECwater/PNEC ratio 1 (the PNEC is derived in Chapter 6 Ecotoxicology), the behaviour of active substances with a partitioning coefficient Kp >2000 should be investigated in a water/sediment study. The surface water study can be skipped in that case.

Only application phase, use phase, and waste phase are taken into account in the evaluation of biocides. Emissions occurring during production and formulation of the biocide are not taken into account in the assessment (in deviation from the modelling of the PEC for existing and new substances according to the TGD).

1.3.2. Use measured data

For relevant environmental compartments information of representative measured concentrations or monitoring data, e.g. concentrations in waste water or in the environment can be used (in the TNsG on data requirements (Chapter 2, 7.1)).

The following remark is made in the TNsG on Annex I inclusion (chapter 3.3 Cumulative Exposure): “When using measured concentrations in exposure assessment it is not necessary to differentiate the sources of exposure in detail as long as it can be verified that at a general level the *measurements are representative for the exposure situation in question*. There is for example no need to differentiate in detail between primary and secondary exposure or differentiate if there are some minor non-biocidal emission sources involved. The measured data should therefore typically represent cumulative exposure from concentrations of natural origin and releases from all biocidal uses. When it comes to cumulative exposure of a substance used also outside the scope of the BPD (for example in plant protection products) and may be regulated with another directive, there is currently still a need for a common EU decision on how to handle such cases. Exclusion of other than only biocidal uses from the assessment causes difficulties when using monitoring data or comparing measured residue data with Maximum Residue Limits and should not be attempted.
For later evaluations the need for a revision of the cumulative exposure assessment should be considered. The influence of the level of use of authorised products should also be taken into account.”

If appropriate, suitable measured data can be used to adjust calculated PEC values (TGD, Sections 2.2.1 and 2.5) [4]. The availability of suitable measured data does, however, not mean that PEC calculations are not required.

The TGD describes the following procedure for evaluation of measured data:
- “reliable and representative data should be selected by evaluation of the sampling and analytical methods employed and the geographic and time scales of the measurement campaigns (Section 2.2.1);
- the data should be assigned to local or regional scenarios by taking into account the sources of exposure and the environmental fate of the substance (Section 2.2.2);

- the measured data should be compared to the corresponding calculated PEC. For naturally occurring substances background concentrations have to be taken into account. For risk characterisation, a representative PEC should be decided upon based on measured data and a calculated PEC (Section 2.5)."

Selection of adequately measured data (section 2.2.1 of the TGD)
The following aspects are relevant for determining whether the measured data are suitable for use:
Quality of the measuring techniques used:

- The techniques used for sampling, transport and storage, and preparation for analysis and analysis of the samples is relevant for evaluation of the quality of the measured concentration. Measured concentrations that are not representative in an adequate sampling programme or are of insufficient quality are not used.
- The limit of quantification (LOQ) of the analytical method must be suitable for use in the risk assessment.
- The comparability of measured data must evaluated. Concentrations in water can, e.g., be total concentrations or dissolved concentrations, depending on the sampling and preparation method used. Sediment concentrations are dependent on organic carbon content and particle size (i.e. largest particles are removed by sieving).

All measurements below the LOQ are a specific problem and should be considered on a case by case basis. A possible approach is to use a value of LOQ/2 to calculate an average or standard deviation. Because this method does strongly affect the outcome, other approaches can also be followed (e.g., on the assumption that there is a comparable distribution below the LOQ and above the LOQ). Purpose is to obtain the largest possible amount of usable exposure information from a dataset.
Improper use of a dataset for risk assessment should be avoided. The table below is recommended to gain more insight into these aspects, where the criteria should be considered flexibly. The most important aspects are checking the analytical quality and the representativeness of the sample. The percentage mistakes is higher at concentrations close to the LOQ of an analytical method than at higher concentrations.

Table 2 Quality criteria for evaluation of measured data (OECD, 2000k)(after; TGD, 2003 [4])

	Study category	
	1	**2**
What has been analysed?	X	X
Analytical method	X	X
Unit specified (normalised to e.g. organic carbon, lipid etc.)	X	X
Limit of quantitation (+ interfering substances)	X	X
Blank concentration	X	
Recovery of standard additions (spikes)	X	
Accuracy (connected to the analytical method and the matrix	X	
Reproducibility (e.g. 95% confidence interval) and standard deviation)	X	
Sample collection (frequency related to emission pattern or seasonal variation)	X	
One shot or mean (treatment of the data)	X	X
Location (representative for use or time of use)	X	X
Date dd/mm/yy (for trend modelling and analysis)	X	X a)
Compartment characteristics (lipid-, organic carbon content, and particle size)	X	
Sampling frequency and pattern	X	X
Proximity of discharge points (detailed information on distance of other sources)	X	X
Discharge emission pattern and volume (continuous discharge, or discontinuous emission showing variations in both volume and concentration with time)	X b)	X b)
Flow and dilution or application rate	X b)	X b)
Explanation of value assigned to non-detects if used in a mean	X	X

1: Valid without restriction - may be used for measured PEC

2: Valid with restrictions - May be used to support Exposure Assessment (data interpretation difficult)

a) Minimum is knowledge of year

b) for local scale

If a substance is used in materials (e.g. in polymers), the substance in the matrix of small particles of the material can reach the environment by, e.g., erosion or attrition) (see 2.3.3.5). In such cases it is important to know whether the analytical methodology used is suitable to determine the fraction of the substance in the particles. The availability for analysis is expected to be reduced by different materials, and/or large particles. Depending on the method of use, particles reach STP sludge/agricultural soil, sediments of waters in sewage overflows, industrial/urban soils and indoor dust.

Selection of representative data for the environmental compartment

Two aspects are important:

1) Reliability of the measured data. This is also determined by the number of samples, distance between the sampling points, and sampling frequency.
2) Whether the sampling location is representative of the local or regional scenario. It should be investigated whether sporadic measurements are concerned or whether the substance is measured at the same location over a certain period.

Concentrations occurring due to incidental emissions after an incident or caused by dis-functioning must not be used for exposure assessment.

Identified outliers should be discussed and explained. The data should be analysed critically to find out whether the high values are caused by an increase or new emission, a recent change in emission pattern, or a newly discovered presence in a certain compartment. It should be investigated whether the analytical method was adequate.

In case many data are available, a statistical method can be used to determine outliers (see TGD pp. 19-20). For a PEC regional it is recommended to use the average of the 90-percentile of individual locations within a region (note that the number of measurements per location can differ).

In case of intermittent release scenarios, 90-percentile values can not always be used to describe emission periods of short duration but with high emission concentration. PEClocal calculations are more realistic in such cases, and the highest value of average concentrations during emission periods should be determined.

2.2.2 Allocation of the measured data to a local or a regional scale

The measured data should be allocated to a local or regional scale in order to define the nature of the environmental concentration that is derived. This allows a comparison with the corresponding calculated PEC to be made to determine which PEC should be used in the risk characterisation (Section 2.5).

Evaluation of the geographical relation between emission sources and sampling site
If there is no spatial proximity between the sampling site and point sources of emission (e.g. from rural regions), the data represent a regional concentration (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 already included.

Use of calculated PEC or measured PEC for risk assessment

Where PEC values from measured as well as calculated data are available, these are compared. A critical evaluation should be carried out in case the measured and calculated values are not of the same order of magnitude.
The following cases are possible:

- Calculated PEC ≈ PEC based on measured values
  The result indicates that the most important emission sources have been taken into account. The most reliable value is used in the risk assessment.
- Calculated PEC > PEC based on measured values
  Indicates that possibly relevant removal processes have not been taken into account in the calculated PEC or that the used model is not suitable for simulation of the actual situation. The measured values, however, can also be unreliable or only representative of background values of the PEC regional.

In case the measured PEC has been derived from a sufficient number of representative samples, this value can replace the calculated PEC value. If it can, however, not be demonstrated that the scenario is an unrealistic worst-case, the calculated PEC is preferred.

- Calculated PEC < PEC based on measured values
  This may be caused by certain emission sources not being taken into account in the calculation of the PEC, or by the used models not being suitable.
  But degradation of the substances may also be overestimated. Alternatives are leakage, recent changes of use patterns, or the fact that emission reducing measures are not yet visible in the samples.

Other causes may be:
- cross-border influx;
- presence of other sources;
- the substance is a metabolite of a different substance;
- delayed remobilisation from a source in different environmental compartments;
- there are other uses of the active substance that are not covered by the present evaluation or that are beyond the scope of the Biocides Directive.

If the measured values meet the procedure of critical statistical and geographical evaluation, these data are considered as very reliable and they then replace the calculated PEC.

1.4. Approval

According to the Directive of the European Parliament and the Council of 16 February 1998 concerning the placing of biocides on the market (98/8/EG) it should be investigated whether biocides have, when approved, no unacceptable effect on the environment and in particular the health humans and animals (consideration 8) if used properly for the envisaged purpose, in the light of the current scientific and technical knowledge.

Article 5, 1, b ii), iii) and iv) stipulates that Member States may only authorise a biocide if the product, when used consistent with the authorisation and taking into account:
- all conditions under which the biocide is normally used,
- the way in which material treated with the product can be used,
- the consequences of use and removal,

ii) has no unacceptable effects on the target organisms, such as unacceptable resistance or cross-resistance or unnecessary suffering and pain for vertebrates,

(iii) has no unacceptable effects itself or as a result of its residues, on human or animal health, directly or indirectly (e.g. through drinking water, food or feed, indoor air or consequences in the place of work) or on surface water and groundwater,

(iv) has no unacceptable effect itself, or as a result of its residues, on the environment having particular regard to the following considerations:
- its fate and distribution in the environment; particularly contamination of surface waters (including estuarian and seawater), groundwater and drinking water,
- its impact on non-target organisms;

1.4.1. Evaluation

The Common Principles (Annex VI to 98/8) present the starting points for evaluation as regards the effects on the environment.
These concern the relevant parts of the introductory principles, the common principles, and the specific principles for the effects on the environment.
The specific principles for Behaviour in surface water and sediment are in the text below printed in a grey frame. This text, including numbering, is the verbatim text of Annex VI to Directive 98/8/EC.

36. The risk assessment shall take account of any adverse effects arising in any of the three environmental compartments — air, soil and water (including sediment) — and of the biota following the use of the biocidal product.
37. The hazard identification shall address the properties and potential adverse effects of the active substance and any substances of concern present in the biocidal product. If this results in the biocidal product being classified according to the requirements of this Directive then dose (concentration) — response (effect) assessment, exposure assessment and risk characterisation shall be required.
38. In those cases where the test appropriate to hazard identification in relation to a particular potential effect of an active substance or a substance of concern present in a biocidal product has been conducted but the results have not led to classification of the biocidal product then risk characterisation in relation to that effect shall not be necessary unless there are other reasonable grounds for concern. Such grounds may derive from the properties and effects of any active substance or substance of concern in the biocidal product, in particular:
    - any indications of bioaccumulation potential,
    - the persistence characteristics,
    - the shape of the toxicity/time curve in ecotoxicity testing,
    - indications of other adverse effects on the basis of toxicity studies (e.g. classification as a mutagen),
    - data on structurally analogous substances,
    - endocrine effects.
39. A dose (concentration) — response (effect) assessment shall be carried out in order to predict the concentration below which adverse effects in the environmental compartment of concern are not expected to occur. This shall be carried out for the active substance and for any substance of concern present in the biocidal product. This concentration is known as the predicted no-effect concentration (PNEC). However, in some cases, it may not be possible to establish a PNEC and a qualitative estimation of the dose (concentration) — response (effect) then has to be made.
40. The PNEC shall be determined from the data on effects on organisms and ecotoxicity studies submitted in accordance with requirements of Article 8 of this Directive. It shall be calculated by applying an assessment factor to the values resulting from tests on organisms, e.g. LD50 (median lethal dose), LC50 (median lethal concentration), EC50 (median effective concentration), IC50 (concentration causing 50% inhibition of a given parameter, e.g. growth), NOEL(C) (no-observed-effect level (concentration)), or LOEL(C) (lowest-observed-effect level (concentration)).

41. An assessment factor is an expression of the degree of uncertainty in extrapolation from test data on a limited number of species to the real environment. Therefore, in general, the more extensive the data and the longer the duration of the tests, the smaller is the degree of uncertainty and the size of the assessment factor.
    The specifications for the assessment factors shall be elaborated in the notes for technical guidance which, to this end, shall be based particularly on the indications given in Commission Directive 93/67/EEC of 20 July 1993 laying down the principles for assessment of risks to man and environment from substances notified in accordance with Council Directive 67/548/EEC(*).
    (*) OJ L 227, 8.9.1993, p. 9.
42. For each environmental compartment an exposure assessment shall be carried out in order to predict the concentration likely to be found of each active substance or substance of concern present in the biocidal product. This concentration is known as the predicted environmental concentration (PEC). However in some cases it may not be possible to establish a PEC and a qualitative estimate of exposure then has to be made.
43. A PEC, or where necessary a qualitative estimate of exposure, need only be determined for the environmental compartments to which emissions, discharges, disposal or distributions including any relevant contribution from material treated with biocidal products are known or are reasonably foreseeable.
44. The PEC, or qualitative estimation of exposure, shall be determined taking account of, in particular, and if appropriate:
    - adequately measured exposure data,
    - the form in which the product is marketed,
    - the type of biocidal product,
    - the application method and application rate,
    - the physico-chemical properties,
    - breakdown/transformation products,
    - likely pathways to environmental compartments and potential for adsorption/desorption and degradation,
    - the frequency and duration of exposure.

45. Where adequately measured, representative exposure data are available, special consideration shall be given to them when conducting the exposure assessment. Where calculation methods are used for the estimation of exposure levels, adequate models shall be applied. The characteristics of these models shall be as listed in paragraph 33. Where appropriate, on a case-by-case basis, relevant monitoring data from substances with analogous use and exposure patterns or analogous properties should also be considered.
46. For any given environmental compartment, the risk characterisation shall, as far as possible, entail comparison of the PEC with the PNEC so that a PEC/PNEC ratio may be derived.
47. If it has not been possible to derive a PEC/PNEC ratio, the risk characterisation shall entail a qualitative evaluation of the likelihood that an effect is occurring under the current conditions of exposure or will occur under the expected conditions of exposure.

1.4.2. Decision making

The Common Principles (Annex VI to 98/8/EC) present the starting points for decision making as regards the effects on the environment.
These concern the relevant parts of the introductory principles, the common principles, and the specific principles for the effects on the environment.
The specific principles for Behaviour in surface water and sediment are in the text below printed in a grey frame. This text, including numbering, is the verbatim text of Annex VI to Directive 98/8/EC.

78. The Member State shall not authorise a biocidal product if the risk assessment confirms that the active substance, or any substance of concern, or any degradation, or reaction product presents an unacceptable risk in any of the environmental compartments, water (including sediment), soil and air. This shall include the assessment of risks to non-target organisms in these compartments.

81. The Member State shall not authorise a biocidal product, if under the proposed conditions of use, the foreseeable concentration of the active substance or of any other substance of concern or of relevant metabolites or breakdown or reaction products in water (or its sediments) has an unacceptable impact on non-target species in the aquatic, marine or estuarine environment unless it is scientifically demonstrated that under relevant field conditions there is no unacceptable effect.

82. The Member State shall not authorise a biocidal product if, under the proposed conditions of use, the foreseeable concentration of the active substance or of any other substance of concern or of relevant metabolites or breakdown or reaction products in groundwater exceeds the lower of the following concentrations:
(a) the maximum permissible concentration laid down by Directive 80/778/EEC, or
(b) the maximum concentration as laid down following the procedure for including the active substance in Annex I, IA or IB to this Directive, on the basis of appropriate data, in particular toxicological data unless it is scientifically demonstrated that under relevant field conditions the lower concentration is not exceeded.

83. The Member State shall not authorise a biocidal product if the foreseeable concentration of the active substance or a substance of concern or of relevant metabolites, breakdown or reaction products to be expected in surface water or its sediments after use of the biocidal product under the proposed conditions of use:
- exceeds, where the surface water in or from the area of envisaged use is intended for the abstraction of drinking water, the values fixed by
- Council Directive 75/440/EEC of 16 June 1975 concerning the quality required of surface water intended for the abstraction of drinking water in the Member States(1), (1) Directive as last amended by Directive 91/692/EEC (OJ L 377, 31.12.1991, p. 48).
- Directive 80/778/EEC [a]

[a] •Replaced by Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption

or
- has an impact deemed unacceptable on non-target species
unless it is scientifically demonstrated that under relevant field conditions this concentration is not exceeded.

Other surface water limit values mentioned in the Water Framework Directive [5].

84. The proposed instructions for use of the biocidal product, including procedures for cleaning application equipment, must be such that the likelihood of accidental contamination of water or its sediments is minimised.

Chapter 5.3 of the TNsG on Annex I inclusion [6] describes the starting points as regards decision making concerning the behaviour in surface water and sediment.

The text below in grey frame is from Chapter 5.3 of the TNsG on Annex I inclusion.

The consequences or effects on non-target organisms will already have been assessed in the risk assessment. The following directives may also be relevant for limit concentrations in surface water: Directive 75/440/EEC and the Water Framework Directive 2000/60/EC.

Furthermore, an active substance should not be included in Annex I if
- it shows in the sediment of a laboratory water/sediment system a DT_{50} >6 months at 20 °C or
- during laboratory tests in aerobic sediment/water system (20-25 °C) it forms non-extractable residues in amounts exceeding 70% of the initial dose after 100 days with a mineralisation rate of less than 5% in 100 days unless it is scientifically demonstrated that under relevant field conditions there is no unacceptable accumulation in sediment.

An active substance containing a metal or a semi-metal element shall not be included in annex I if the use will cause significant accumulation above the natural background levels.

1.5. Developments

Developments
- None

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- For the EU framework it has not yet been elaborated which scenario or guideline must be met for evaluation of field accumulation.
- For the EU framework it has not yet been elaborated what is to be understood by relevant metabolites. In transformation studies metabolites are identified that are at any point in time present in a concentration >10% of the added substance.
  No relationship has been established between relevant metabolites and metabolites with a concentration >10% of the added substance. Follow-up steps have not been developed for derivation of DT50 values and/or requests for additional behaviour studies with metabolites. In addition, in the TNsG no link is made between relevant metabolites and evaluation against the persistence criterion in sediment.

2. APPENDICES

Appendix 1; Figure 1 and 2 from the TNsG on Data requirements

FIG 1. BIOCIDES BIODEGRADATION TEST STRATEGY

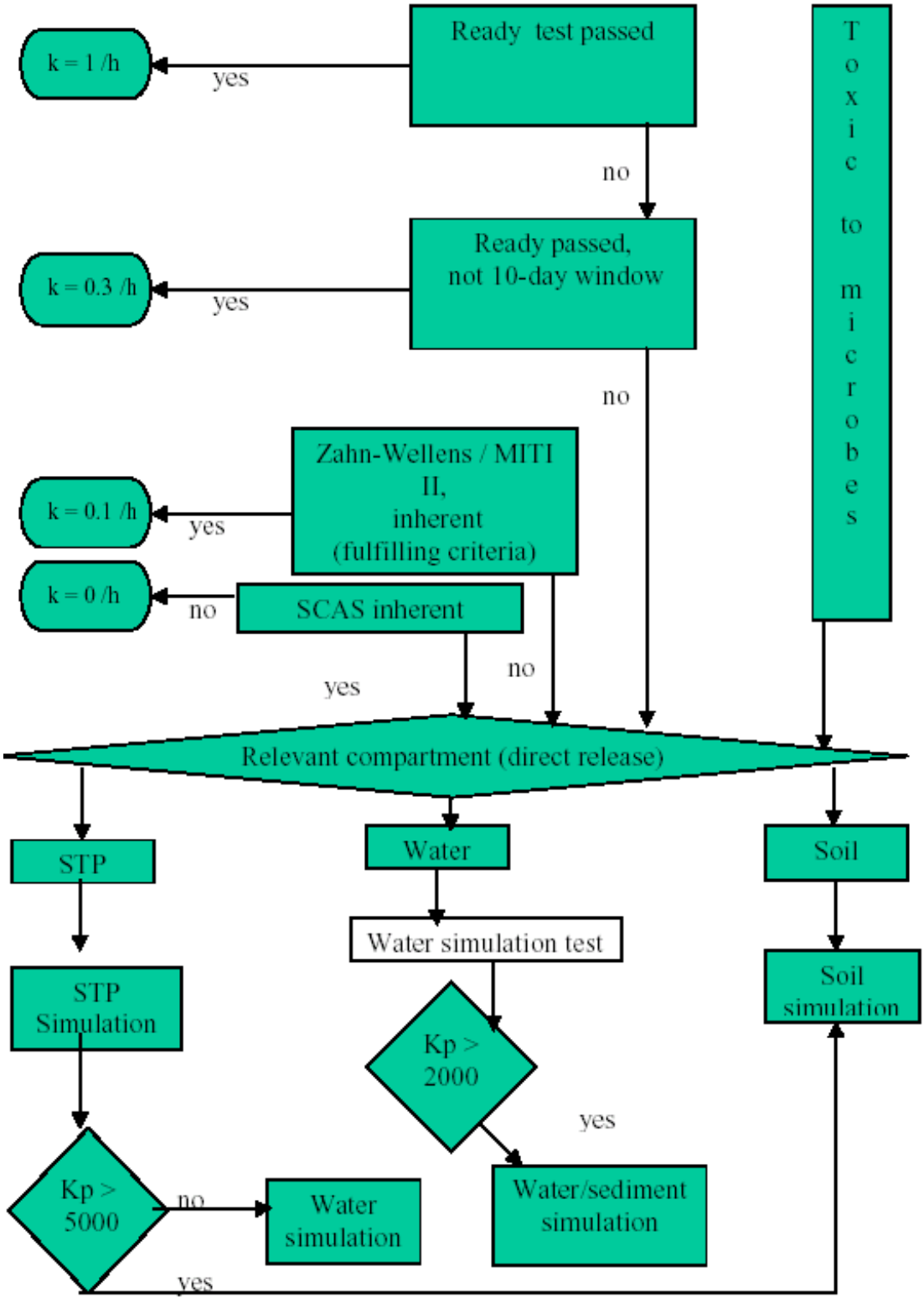
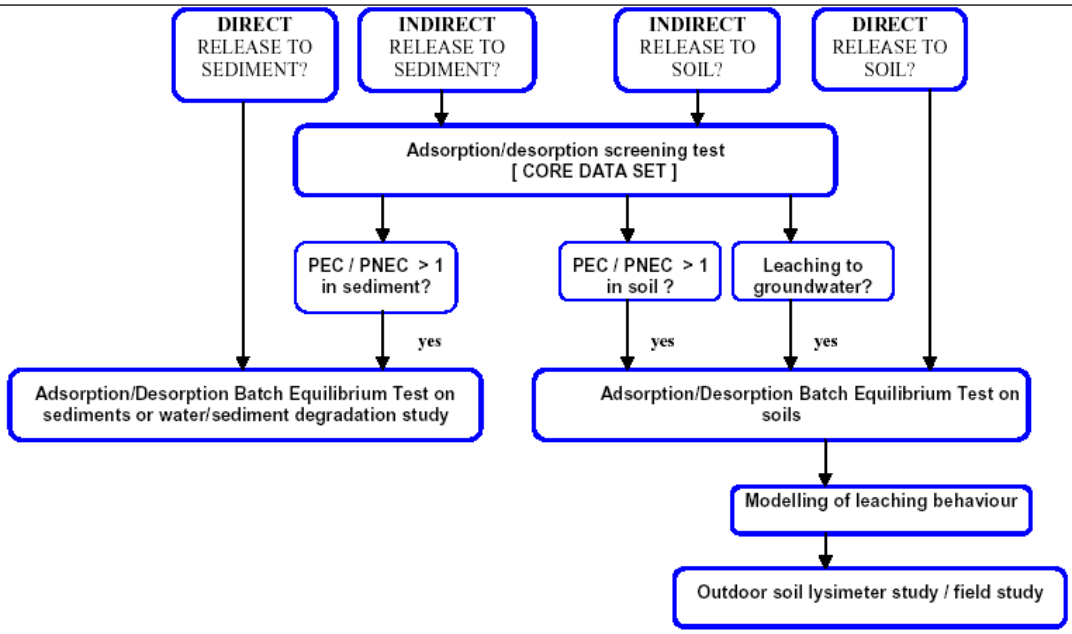


FIG 2 Testing strategy for adsorption and mobility (page 17)



Note: If necessary to characterise more accurately the partitioning behaviour of a substance in a sewage treatment plant, an adsorption/desorption equilibrium test can also be performed with activated sludge.

3. REFERENCES

1 Biocides Directive (98/8/EC).
2 http://ecb.jrc.ec.europa.eu/documents/Biocides/EMISSION_SCENARIO_DOCUMENTS/
3 TNsG on data requirements. Technical guidance document in support of Directive 98/8/EC concerning the placing of biocidal products on the market. Guidance on data requirements for active substances and biocidal products. February 2008. In the February 2008 version, Chapter 2.5 of the previous version (October 2002) has been renamed to Part C of Chapter 2. No other changes have been made with respect to the content of the Guidance Document.
4 TGD, 2003. Technical Guidance Document on Risk Assessment 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 Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market Part II
5 Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for the Community action in the field of water policy. L 327/1
6 TNsG on Annex I inclusion. 2002. Technical Notes for Guidance in Support of Directive 98/8/EC of the European Parliament and the Council Concerning the Placing of Biocidal Products on the Market. Principles and Practical Procedures for the inclusion of active substances in Annexes I, IA and IB. April 2002