Towards the Derivation of Quality Standards for Priority Substances in the Context of the Water Framework Directive

Final Report of the Study

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Identification of quality standards for priority substances in the field of water policy

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Glossary

AA-(E)QS	"Annual Average" (Environmental) Quality Standard
ACR	Acute to Chronic Ratio
ADI	Acceptable Daily Intake
BAF	Bioaccumulation Factor
BCF	Bioconcentration Factor
BMF	Biomagnification Factor
C_b	Background concentration
CMR	Carcinogenic, Mutagenic and affecting Reproduction
COMMPS	Combined Modelling Based and Monitoring Based Priority Setting Procedure
CSTÉ	Scientific Advisory Committee on Toxicity and Ecotoxicity of Chemicals of the European Commission
DIN	*Deutsche Industrie Norm* (German industry standard)
DT50	Disappearance Time in which the concentration of a substance drops to 50% of its level at T_0
EC50	Effect concentration for 50% of the individuals in a toxicity test
EPA	Environmental Protection Agency
EQS	Environmental Quality Standard
ESRA	Risk Assessment for Existing Substances
ERL	Environmental Risk Limit
EU	European Union
GLP	Good Laboratory Practice
HC_5	Hazardous concentration for 5% of the species (based on the SSD)
ISO	International Standard Organisation
INIA	Instituto Nacional de Investigación y Tecnología Agraria y Alimentaria (Spanish national institute for agricultural and food research and technique)
Kow	Octanol – water partition coefficient
Kp	Partition coefficient
LC50	Lethal concentration for 50% of the individuals in a toxicity test
LOEC	Lowest Observed Effect Concentration
log	Logarithm (base 10)
MAC-(E)QS	Maximum Admissible Concentration (Environmental) Quality Standard
MPA	Maximum Permissible Addition
MPC	Maximum Permissible Concentration
NC	Negligible Concentration
NO(A)EL	No Observed (Adverse) Effect Level
NOEC	No Observed Effect Concentration in a toxicity test
OECD	Organisation for Economic Co-operation and Development
PEC	Predicted Environmental Concentration
PNEC	Predicted No-Effect Concentration
PPP	Plant Protection Product
PPPRA	Risk Assessment for Plant Protection Products
QSAR	Quantitative Structure Activity Relationship
QT	Quality Target
RA	Risk Assessment
RAR	Risk Assessment Report
SEQ	Syst*éme d'Evaluation de la Qualite des Cours d'Eau* (system for the evaluation of quality)
SPM	Suspended Particulate Matter
SRC_{ECO}	Ecotoxicological Serious Risk Concentration
SSD	Species Sensitivity Distribution
TER	Toxicity Exposure Ratio
TGD	Technical Guidance Document
TV	Target Value
WFD	Water Framework Directive
WHO	World Health Organisation
WQS	Water Quality Standard

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0 Executive Summary

Article 16 of the Water Framework Directive (WFD, Directive 2000/60/EC) lays down the Community Strategy for the establishment of harmonised quality standards and emission controls for the priority substances and other substances posing a significant risk to, or via, the aquatic environment. In order to achieve the protection objectives of the WFD, the Commission shall (i) submit proposals for quality standards applicable to the concentrations of the priority substances in surface water, sediment or biota, and (ii) identify the appropriate cost-effective and proportionate level and combination of product and process controls for both point and diffuse sources. Proposals for environmental quality standards and emission controls for point sources shall be submitted within 2 years of the inclusion of the substance concerned on the list of priority substances (European Parliament and Council Decision No. 2455/2001/EC), i.e. in December 2003.

This study is part of the preparatory work of the Commission and its overall objectives are:

- The development and description of a concept which enables the European Commission to submit proposals for quality standards applicable to the concentrations of the priority substances of the Water Framework Directive (2000/60/EC) and those substances not on the priority list but regulated in the "daughter directives" of Directive 76/464/EEC (on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community) in water, sediment and biota, as required by Articles 16(7) and 16(10) of the Water Framework Directive. [1]
- Elaboration of proposals for quality standards for the priority substances of the Water Framework Directive and recommended values for other substances of concern (see footnote 1) with regard to surface water, sediment, biota, and human health as objectives of protection.

Concept Development

The concept for the derivation of quality standards proposed in this report was presented 3 times (March and October 2001, March 2002) to the Expert Advisory Forum on Priority Substances (EAF) at different stages of its development. Furthermore, an Expert Group on Quality Standards met on 23 January 2002 to discuss specific elements of the proposed methodology. Comments received upon the different discussion rounds have been taken into account, where appropriate. The proposed approach was finally endorsed by the EAF at its meeting in March 2002.

In order to develop a scientifically sound and practicable concept and to derive most appropriate quality standards ensuring a good chemical status[2] of the Communities' surface waters, it is necessary to assess and evaluate all three compartments (i.e. water, sediment, biota) in parallel. The starting point for the development of the concept to derive quality stan-

[1] The working list of substances comprising the WFD priority substances, a selection of substances regulated in the “daughter directives” to Directive 76/464/EEC and other substances of concern is in Annex 1 to this report.

[2] The WFD aims at the achievement of a good status for surface waters and groundwater bodies (Article 4(1)). The basic idea behind "good status" is that water bodies may be affected by human activity only to the extent that the ecological functions and the community structure of the water body in question are not fundamentally changed, i.e. the long-lasting continuance of populations of naturally occurring species should be ensured by the quality standards to be set.

dards were the provisions set out in Annex V, section 1.2.6 (Procedure for the Setting of Chemical Quality Standards by Member States) of the Water Framework Directive. However, while the provisions of Annex V may suffice as general scheme to derive quality standards for organic substances in the water body, they do not deal with specific problems arising from the inclusion of sediment quality, protection of top predators from secondary poisoning and human health as objectives of protection, nor do they account for the peculiarities that must be considered if quality standards for metals or for transitional, coastal and territorial marine waters are to be set. Therefore, it was deemed indispensable to take further approaches for effects assessment and quality standard setting into account.

To this end, the EU and Member States methods for the purpose of deriving water quality standards as well as other provisions such as the EU-concepts on risk assessment for new notified and existing substances (Directive 93/67/EEC and Regulation (EC) No 1488/94, as laid down in the Technical Guidance Document) or for plant protection products (Directives 91/414/EEC and 97/57/EC) as well as latest developments in science have been evaluated with regard to their suitability and pertinence to achieve the objectives pursued with the quality standards under the Water Framework Directive. The evaluated methods are described in sections 4 and 5 of this report.

All approaches for quality standard setting or risk assessment are in so far very similar as the application of assessment factors depending on the quality and quantity of available toxicity data is a common core element. As an alternative to the assessment factor approach, the use of statistical extrapolation methods (species sensitivity distribution) is applied in the Netherlands and is further an option that can be used in the context of the EU risk assessments.

As no fundamental differences in the national approaches for quality standard setting or the EU methods for risk assessment could be found, it was decided to built the proposal for a common EU method for quality standard setting as far as possible on the elements used for effect assessment in the EU risk assessment frameworks. The reasons for this decision are:

- to keep the ecological effects assessment methodology on EU-level as consistent as possible;
- to use, as far as possible, elements for the set up of the quality standard derivation methodological framework that are already accepted and agreed by Member States and introduced on Member State level.

The methodological framework proposed in section 8 of this report for the derivation of quality standards is intended to concomitantly protect freshwater and marine ecosystems from adverse effects as well as human beings from all impacts on health by drinking water uptake or ingestion of food originating from aquatic environments. To this end, for the entire set of objectives of protection, i.e. the pelagic and benthic communities (≈ water and sediment) in freshwater or saltwater ecosystems, the top predators of these ecosystems and human health, it is assessed by means of pre-defined trigger criteria (see table 8.1 for triggers) whether a substance may pose a certain objective at risk. For those objectives for which a possible risk (≈ exceeded trigger-value) is identified, specific quality standards are derived. In a subsequent step the lowest of the standards derived for the individual protection objectives is selected as the overall quality standard (however, if deemed justified, distinct quality standards are derived for freshwater and saltwater, respectively).

Thus, a quality standard derived by this approach takes all relevant protection objectives into account. Moreover, all direct and indirect exposure routes in aquatic systems like exposure in the water body via water and sediment or via bioaccumulation as well as possible expo-

sure via drinking water uptake are accounted for. Further, all relevant modes of toxicity are considered, e.g. for ecosystems direct and indirect toxicity (≈ after bioaccumulation) and for man oral toxicity as well as carcinogenicity, mutagenicity and adverse effects on reproduction (CMR). In addition, effects on endocrine regulation in animals or man are accounted for, if relevant.

Therefore, a quality standard derived by the described conceptual framework is not merely a threshold level ensuring the protection of only a particular protection objective (like, for instance, a Predicted No Effect Concentration for the protection of the pelagic community), but is an overall stand alone value that encompasses the consideration of direct ecotoxicological effects in different habitats (water, sediment), indirect ecotoxicological effects occurring after bioaccumulation in biota (secondary poisoning of top predators) and effects on human health by oral uptake of water and food, including long-term toxicity and CMR mechanisms.

For the purpose of this study it was deemed pertinent to derive two kinds of quality standards referring to (i) the annual average concentration and (ii) to short-term concentration peaks. To this end, a QS has been calculated which is referring to the annual "average" concentration (AA-QS) and, in addition, the so-called maximum admissible concentration QS (MAC-QS) referring to short-term transient exposure. The MAC-QS must not be exceeded any time. In conjunction, the AA-QS and the MAC-QS are intended to protect the structure and function of the addressed aquatic ecosystems from significant alterations by the impact of chemical substances. As yet no decision has been taken whether the long-term quality standard should refer to the annual arithmetic mean or to the 90-percentile of monitored concentrations, it is also not possible to draw a final conclusion on the possible pertinence of the MAC-QS.

Elaboration of Proposals for Quality Standards

The elaboration of quality standards for the substances on the working list with the proposed methodological framework required the collation of data on physico-chemical as well as (eco)toxicological properties of the substances concerned. Where available, (consolidated draft) risk assessments according to Council Regulation (EEC) No. 793/93 or Council Directive 91/414/EEC have been preferably used as sources of reliable data, as the data of these reports were already subjected to an extensive peer review and evaluation process. If Predicted No Effect Concentrations (PNECs) were already established in the risk assessments (which was the case for fourteen substances or substance groups on the working list – see Annex 3), these PNECs have been used for the derivation of quality standards. For the 22 substances or substance groups for which such risk assessment reports were not available, the acquisition of the required data was based on a questionnaire which was disseminated via the focal points of the Expert Advisory Forum to the competent authorities of Member States and Accession Countries, industry associations (such as CEFIC, ECPA, EUROCHLOR and EUROMETAUX) or other environmental NGOs. In this inquiry the addressees were asked, for those substances on the working list for which no EU risk assessment reports are available, to submit data considered by themselves as relevant and reliable to the consultant. Handling and evaluation of these data as well as selection for quality standard derivation is described in section 9 of this report. Principally, only data that are considered as reliable have been used for the derivation of the standards, irrespective of the source of the data.

All data considered as relevant for the derivation of quality standards have been drawn together for each substance or substance group in individual EQS data sheets (see Annex 4). Further, all information sources used as well as the calculations performed and the consid-

erations undertaken to derive the quality standards are comprehensively documented in these data sheets. An overview on the proposed overall quality standards for inland waters as well as transitional, coastal and territorial waters is given in table 10.1.

Conclusions

The elaboration of quality standards with the developed methodological framework clearly showed that the proposed approach is applicable for the derivation of specific quality standards addressing the particular objectives of protection as well as for the identification of the overall quality standard that finally may be imposed to safeguard the entire set of objectives of protection.

Also, with regard to the effort required to work with the concept, it can be considered as economic. This is attributable to the fact that despite the comprehensive consideration of all relevant routes of exposure and objectives of protection the different quality standards for the specific objectives are normally only derived if certain pre-defined trigger values are exceeded. This avoids the assessment of irrelevant exposure routes and the calculation of unnecessary standards.

Problems encountered during the elaboration of the standards were in general not attributable to the suggested methodological framework but mostly to the limited availability of data or to the limitations of the available data.

All proposed quality standards should be considered as preliminary and it is recommended to subject them to a peer review step. In this review step attempts should be made to fill data gaps and to assess uncertainties identified and to derive with the proposed methodological framework those quality standards that could not be established in this study because information was lacking or was not reliable.

1 Background

In 1997 the Commission proposed a European Parliament and Council Directive establishing a framework for a Community action in the field of water policy (Water Framework Directive, hereafter referred to as WFD). Following the co-decision procedure, the Directive was finally adopted by the Council and the European Parliament in October 2000 (Directive 2000/60/EC)[1].

Article 16 of Directive 2000/60/EC contains a legal framework and a clear methodological basis for the prioritisation of substances presenting a "significant risk to or via the aquatic environment, including such risks to water used for the abstraction of drinking water".

Based on the provisions laid down in Article 16 the Commission initiated expert discussions on the development of a generally accepted prioritisation mechanism. During three rounds of expert discussions from February 1998 to April 1999, the **co**mbined **m**onitoring-based and **m**odelling-based **p**riority **s**etting procedure (COMMPS)[2] was developed in collaboration with the Fraunhofer-Institute and was applied in the selection process of priority substances. Based on the outcome of that study and the comments that the Commission received from all stakeholders, a proposal was prepared which included 32 substances or groups of substances. This proposal was adopted by the Commission for a European Parliament and Council Decision establishing the list of priority substances in the field of water policy in February 2000[3] (*COM(2000) 47 final*).

As a result of the final negotiations in the conciliation of the Water Framework Directive the before mentioned proposal *COM(2000) 47 final* had to be amended since Paragraph 3 was introduced in Article 16 as a new element in order to achieve an even higher level of protection relating to substances with an outstanding concern for the fresh water, coastal and marine environment (so called priority hazardous substances; i.e. priority substances with a very high hazard profile). Paragraph 3 requires the Commission to "identify the priority hazardous substances, and, in doing so, to take into account the selection of substances of concern undertaken in the relevant Community legislation regarding hazardous substances or relevant international agreements".

A draft Working Document describing a procedure in accordance with Article 16(3) WFD for the identification of priority hazardous substances was elaborated by the Commission Services and discussed with an ad-hoc group of experts from Member States, industry, environmental NGOs and other stakeholders in consultation meetings. Comments and information received from the experts were considered in the revision of the Working Document. Based on the revised Working Document[4] the amended proposal for a Decision of the European Parliament and of the Council establishing the list of priority substances in the field of water policy was presented on 16 January 2001 (COM(2001) 17 final)[5]. In this amendment of proposal *COM(2000) 47 final*, 11 of the 32 substances or groups of substances proposed as priority substances are selected as "priority hazardous substances" based on their intrinsic hazardous properties (i.e. toxic, persistent and liable to bio-accumulate or any other properties which give rise to an equivalent level of concern). 11 substances or groups of substances are earmarked as "priority substances under review" since the available knowledge is considered as currently not sufficient to finally decide as to whether they should be selected as "priority hazardous substances". The remaining 10 priority substances do not meet the criteria to qualify as "hazardous"(see Annex 1 of this report for information on the classification of the individual priority substances).

The distinction between priority substances and priority hazardous substances triggers the proposals of controls and measures which have to be taken in accordance with Article 16 of the Water Framework Directive. Whereas, according to paragraph 6 of Article 16, for the

priority substances Commission proposals for a progressive reduction of discharges, emission and losses of the respective substances are required, the controls proposed for the priority hazardous substances shall aim at the cessation or phasing out of discharges, emissions and losses no longer than 20 years after the adoption of these proposals by the European Parliament and the Council. Even before the adoption, the Commission started the follow-up work.

In its First Reading on 15 May 2001, the European Parliament introduced 20 amendments to the Commission Proposal. However, the list of priority substances itself was mainly endorsed with only some minor changes. In its meeting on 7 June 2001, the Environment Council agreed unanimously to adopt the list of priority substances under the Water Framework Directive as amended by the European Parliament in First Reading. In relation to the Amended Proposal of the Commission, the final list of the European Parliament and Council Decision modified the status of the substances simazine, diuron and isoproturon, which are now classified as "priority substances under review". Furthermore, fluoroanthene is now listed as an individual priority substance of its own and no longer grouped under PAH which increased the total number of substances to 33. The final adoption of the decision was done on 22 November and the list was published in the Official Journal at 15 December 2001 as Decision 2455/2001/EC [48].

In order to achieve the protection objectives of the Water Framework Directive, Article 16 lays also down the Community Strategy for the establishment of harmonised quality standards and emission controls for the priority substances and other substances posing a significant risk to, or via, the aquatic environment: To this end, the Commission shall (i) submit proposals for quality standards applicable to the concentrations of the priority substances in surface water, sediment or biota, and (ii) identify the appropriate cost-effective and proportionate level and combination of product and process controls for both point and diffuse sources. Proposals for environmental quality standards and emission controls for point sources shall be submitted within 2 years of the inclusion of the substance concerned on the list of priority substances, i.e. in December 2003.

This study is part of the preparatory work of the Commission.

2 Objectives of the Study

It is the overall objective of this study to prepare a concept which enables the Commission to submit proposals for quality standards applicable to the concentrations of the priority substances and those substances not on the priority list but regulated in the "daughter directives"[10-14] of Directive 76/464/EEC[7] in water, sediment and biota, as required by Articles 16(7) and 16(10) of the Water Framework Directive.

The WFD aims at the achievement of a good status for surface waters and groundwater bodies (Article 4(1)). The basic idea behind "good status" is that water bodies may be affected by human activity only to the extent that the ecological functions and the community structure of the water body in question are not fundamentally changed, i.e. the spectrum and abundance of species may only differ slightly from undisturbed natural conditions. Thus, the protection of species is a relevant assessment endpoint but there is a common understanding that the ecological risk assessment aims not at individuals but at the protection of populations. In general, the long-lasting continuance of populations of naturally occurring species should be ensured by the quality standards to be set.

In order to develop a scientifically sound and practicable concept and to derive most appropriate quality standards ensuring a good chemical status of the Communities' surface waters, all three compartments (i.e. water, sediment, biota) shall be assessed and evaluated in parallel. The "Procedure for the Setting of Chemical Quality Standards by Member States" as set out in Annex V of the Water Framework Directive[1] must be considered as starting point in the development of the method for deriving quality objectives. Other provisions such as methods and concepts laid down in the TGD [6] or in Directives 91/414/EEC [15] and 98/8/EC [20] for environmental and human health risk assessment in the European Union for new and existing substances, plant protection products, or biocides, respectively, are also taken into account as well as existing concepts to derive quality objectives or latest developments in science related to that topic, as far as concrete details were available by March 2002.

In order to achieve these objectives, several thematic work packages had to be dealt with:

- Description and evaluation of existing concepts for the derivation of quality standards for water, sediment and biota in the Member States and the Accession Countries.
- Development of a conceptual framework for the derivation of quality standards for surface waters, sediment and biota.
- Acquisition and collation of data referring to ecotoxicological effects and bioaccumulation in the freshwater and marine environment and to human health aspects (= consideration of consumer exposure via ingestion of water and water organisms).
- Assessment of data quality and data reliability.
- Elaboration of proposals for quality standards for the priority substances (Annex X WFD [1]) and recommended values for other substances of concern (mainly List I substances of the "Daughter Directives" of 76/464/EEC [7] not on the priority list) with regard to surface water, sediment, biota, and human health as objectives of protection.

3 Working list of Substances

The substances or groups of substances on the working list (see Annex 1) were agreed with the Commission Services. The working list comprises all priority substances according to the "Proposal for a European Parliament and Council Decision establishing the list of priority substances in the field of water policy"[3] and those substances not on the priority list but regulated in the "daughter directives"[10-14] of Directive 76/464/EEC[7] as required by Articles 16(7) and 16(10) of the Water Framework Directive. For these substances quality standards shall be proposed.

Furthermore, some other substances (polychlorinated biphenyls, dioxins/furans) have been added for various reasons. Dioxins/Furans and PCBs were added because they are suspected to pose a significant risk to the marine environment and being a case of intensive historic pollution.

As for the "priority hazardous substances" on the list of priority substances[5] the controls proposed according to Article 16(6) WFD shall aim at the cessation or phasing out of discharges, emissions and losses no longer than 20 years after the adoption of these proposals by the European Parliament and the Council, it might – at first glance - not appear necessary to derive quality standards for these substances. However, according to Article 16(7) WFD, quality standards have to be derived for all priority substances including the priority hazardous substances. Moreover, the setting of such effect based standards also for the priority hazardous substances offers the opportunity to get an indication of the risk these substances currently pose to the aquatic environment or to human health (comparison of quality standards with current concentration levels). Based on this information it will be possible to adjust the extent of measures and controls to be imposed as well as the time frame in which the reduction of releases should be achieved as appropriate. Furthermore, it will be easier to monitor and evaluate the progress in phasing out emissions, discharges and losses with commonly agreed quality standards.

Annex 1 contains the working list of substances indicating their status (e.g. priority substance, priority hazardous substance, substance from list I of 76/464/EEC, other substance of concern). An updated overview on quality standards and objectives in place in Member States, Accession Countries and various other relevant bodies is also included.

PART A: Overview and Evaluation of Methods Used to Derive Quality Standards

4 Overview on Methods and Procedures Used to Derive Quality Standards in Member States

4.1 France

The second law on water of 3 January 1992 has launched the revision of French water quality objectives, which are now to be defined in the framework of each *Schéma Directeur d'Amenagement et de Gestion des Eaux* (one SDAGE for each of the 6 major hydrogeological basins in France) [21]. A new methodology has been developed to evaluate the quality of water bodies, the system for the evaluation of quality (SEQ, syst*éme d'evaluation de la qualite des cours d'eau*). SEQ exists or will exist for different water categories: rivers, groundwater, lakes (under development), and coastal and transitional waters (under development). SEQ is from June 1999 to December 2001 in a transit phase but will be the national tool to assess river quality from January 2002 on.

In the global river quality assessment of the SEQ, different aspects are distinguished [22]:

- The quality of the water itself, assessed by a system called water-SEQ
- The quality of the physical environment (river hydromorphology and hydrology), called Phys-SEQ
- The biological quality (fulfilment of habitat function), assessed by surveys of benthic invertebrates, fish or plants, called bio-SEQ
- The suitability of the river and its water to support its biological function and different uses, which can be affected by water quality, the biological river quality, or the quality of the physical environment. The uses considered are: drinking water supply, drinking water for animals, irrigation, fish farming, and recreation.

The water quality is a central element in the river quality assessment as water quality influences the biological quality and determines the possible water uses and functions.

In the water-SEQ, the water quality is described by water quality indicators, grouping together individual parameters, which correspond to particular water quality issues of concern (e.g. individual monitored substances in case of the micropollutant indexes). Indicators are, for example:

- organic and oxidizeable matter
- salinity
- acidity
- nitrogen compounds
- phosphorous compounds
- mineral micropollutants
- metals (content in mosses)
- pesticides
- organic micropollutants
- micro-organisms
- phytoplankton

For each indicator the quality is represented in two ways: by a quality index ranging from 0 (for the worst quality) to 100 (for best quality), and by 5 quality classes which are assigned to the quality index scale, dividing it in 5 intervals representing 20 points each. The 5 classes

denominate the water quality with the same terms as used in the WFD: "bad" (0-20 points), "poor" (21-40), "moderate" (41-60), "good" (60-80), and "very good" (80-100).

In the calculation of the indexes and quality classes for each indicator, the relative importance of individual parameters as well as the frequency of sampling is taken into account. The final result for each indicator corresponds to the worst quality observed in at least 10% of the samples [22] (i.e. equivalent to the 90-percentile of the data).

The water's suitability to support its biological function and the other various uses of the river(water) is determined individually for each use or function by specific requirements defined for each water quality indicator. The water quality indicator resulting in the poorest suitability for the considered use or function is decisive for the suitability. Again, the suitability of water quality to support the habitat function or a specific use is expressed in 5 classes ranging from "very suitable" to "totally unsuitable".

In the following, an overview is given on the assignment of suitability classes for the biological function of water with regard to micropollutants.

Suitability classes and threshold levels to assess the biological quality of rivers

5 suitability classes have been defined for the biological quality, based on general adverse effects on aquatic ecosystems [23] (table 4.1).

Table 4.1: Suitability classes and description of predicted effects on aquatic ecosystems [23]

Suitability Class	Predicted effects on aquatic ecosystem
5 very unsuitable	Very large risk of lethal effects for many species of the ecosystem; major reduction of abundance and diversity of species; loss of species or only tolerant species present
4 unsuitable	Risk of significant lethal effects for the most sensitive species of the ecosystem, resulting in a reduction of abundance and diversity of species; tolerant species are dominating
3 average	Probable risk of adverse chronic, sub-lethal effects for sensitive species, combined with possible risk for less sensitive species; the effects may result in a reduced number of offspring produced in the affected populations and a possible reduction in abundance and, perhaps, a reduction in species diversity
2 suitable	Possible risk of adverse chronic sub-lethal effects for the most sensitive species of the ecosystem; the effects may result in a reduced number of offspring produced in the affected populations and a possible reduction in abundance and, perhaps, a reduction in species diversity
1 very suitable	Negligible risk of adverse effects for all species

Calculation of threshold levels for micropollutants [23]

Four quality threshold levels are calculated for each micropollutant corresponding to the suitability classes given in table 4.1. This has been done so far for about 130 organic and inorganic micropollutants. For the time being, there is no legal obligation not to exceed a threshold level. The official use of the thresholds is to serve as reference in the assessment of river quality and in the set-up of action plans. The threshold levels are usually compared to the 90-percentile of the levels in water. In case of suspended particulate matter, the 50-percentile is compared to the threshold levels.

The thresholds are based on toxicity data as specified in Table 4.2 and can only be calculated if a minimum set of toxicity data, consisting of organisms from 3 trophic levels (algae/plants, invertebrates, fish), is available. Preferably, the toxicity data should have been obtained with standardised and adopted test protocols (first quality data).

If toxicity data are not available for the 3 trophic levels, only provisional threshold levels can be derived. However, if toxicity data for species expected to be particularly sensitive to the substance concerned (e.g. specific mode of action) are missing, threshold levels are not being proposed. If only toxicity data for less than two trophic levels are available, threshold levels are not derived.

For some substances, in particular metals such as arsenic, chromium, copper, nickel and zinc, it is discussed to apply lower than the standard safety factors (cf. table 4.2) in view of the very low acute to chronic toxicity ratios. Also, lower safety factors may be applied when toxicity data of target species are used for the calculation of threshold levels.

For those metals, for which toxicity is depending on water hardness, toxicity data obtained in water of a "mean" hardness are used to calculate the threshold levels. The corresponding thresholds for very soft and very hard water are derived by extrapolation. Threshold levels are normally given for 3 hardness classes (0-50, 50-200 and >200 mg $CaCO_3$ equivalent per litre).

Table 4.2: Threshold levels and related suitability lasses [23]

Suitability Class	Threshold Level	Calculation of Threshold Level
1		
	1	Lowest reliable chronic concentration without effect divided by a safety factor of 10 (NOEC/10) or lowest reliable acute L(E)C50 value divided by a safety factor of 1000
2		
	2	Lowest reliable chronic NOEC without application of a safety factor, or lowest reliable acute L(E)C50 value divided by a safety factor of 100
3		
	3	Lowest reliable acute L(E)C50 without application of a safety factor
4		
	4	Geometric mean of the lowest reliable acute L(E)C50 values of species from 3 trophic levels (algae/plants, invertebrates, fish)
5		

Calculation of threshold levels for sediment and suspended matter [23]

Threshold levels for sediment and suspended matter are only calculated for substances with logKow >3. So far, only the two first threshold levels (i.e. 1 and 2) could be calculated since data required to derive the other threshold levels are lacking.

The threshold levels for sediment are derived by two methods, either by the weight of evidence approach (WEA), or by the equilibrium partitioning method (EP). If the WEA is used, the first threshold level (1) corresponds in general to the threshold effect level (TEL) to which a safety coefficient is applied if the TEL is to close to threshold 2, which is normally the probable effect level (PEL). For substances for which a TEL cannot be determined, the EP method is used in order to derive threshold level 1 which includes the application of a safety

factor of 10. Threshold level 2 corresponds to the value derived by the use of the EP method without applying a safety factor. The threshold levels derived by the application of the WEA approach or the EP method are considered as provisional, given the inherent uncertainties of both methods.

For suspended matter, the threshold levels 1 and 2 are extrapolated on the basis of the respective values for sediment. For organic substances the thresholds are multiplied by a factor of 2 and for metals by a factor of 1.5.

Threshold levels to assess the suitability of a river for drinking water supply use

The threshold levels for the drinking water supply use of a river are based on existing regulation (Council Directive 80/778/EEC), or if not defined there, the WHO's norms on quality of drinking water, the US-EPA recommendations, the British regulation (supply water quality regulation) or the SNARL (suggested no adverse response levels divided by a security factor of 10) are taken into account.

The overall first quality class for micropollutants (i.e. the "very good / good " level) is the more stringent level of either the first quality class for the biological function or the first quality class for the drinking water supply use.

4.2 Germany

In Germany, "water quality targets" for inland surface waters have been developed by the Joint Water Commission of the Federal States (*LAWA*) in collaboration with the Federal Environmental Agency [24]. The general approach and the procedures used are described in detail in [25 & 26]. Furthermore legally binding Environmental Quality Objectives have been derived for 99 substances of Council Directive 76/464 EEC (list II) on the basis of the water quality target concept [27].

The German quality targets are considered for the assessment of the actual quality of surface waters and the effectiveness of measures imposed to reduce pollution, respectively. They are no legally binding limit values. Nevertheless, water quality targets, which are exceeded result in measures to reduce the levels of the respective pollutants (i.e. by enforcement of action programmes).

The quality targets refer to individual assets to be protected, such as:

- aquatic communities
- fishery
- drinking-water abstraction
- irrigation of agricultural land
- suspended particulate matter and sediments

Quality targets are derived for hazardous substances as defined in the German Water Management Act (substances raising concern because of their (eco)toxicity, persistency, liability to accumulate, their carcinogenic or mutagenic potential as well as their potential to affect reproduction) or for substances for which quality targets must be derived in order to comply with international agreements. The quality targets are normally effects based. However, limit values as, e.g., given in the drinking-water ordinance or in the ordinance on maximum permissible pollutant levels in food are considered[25].

A quality target is normally referring to the total (i.e. sum of dissolved and adsorbed) concentration of a substance and expressed as the concentration not to be exceeded by the 90-percentile of the levels monitored in water[25]. For metals, the quality targets refer to the 50-percentile[3] [26]. Quality targets for substances with a partition coefficient exceeding 1000 l/kg are preferably expressed as levels in suspended particulate matter. To this end, the quality target for suspended particulate matter (QT_{SPM} [µg/kg]) is calculated using the total concentration of the substance concerned in water (C_{total} [µg/l]), its partition coefficient water – susp. sediment (k_{ws} [l/kg]), and the concentration of suspended particulate matter (SPM) in water (C_{SPM}). 25mg/l is used as default for C_{SPM} as this figure is the approximate average value in larger rivers in Germany.

QT_{SPM} [µg/kg] = C_{total} [µg/l] * k_{ws} [l/kg] * (10^{-6} [kg/mg] * C_{SPM}^{-1} [mg/l])$^{-1}$

4.2.1 Derivation of quality targets for the asset "aquatic communities"

Objective of the quality targets referring to the asset "aquatic communities" is to ensure the preservation or the restoration of indigenous, self-reproducing and self-regulating natural aquatic communities [25].

Organic Chemicals [25]

Toxicity tests with representative examples of the four main trophic levels of aquatic life (bacteria, green algae, small crustaceans and fish) provide the basis for the development of water quality targets (Table 4.3). The tests must be conducted according to validated test guidelines (e.g. EU, OECD, ISO, DIN) or according to test routines comparable with these guidelines.

Generally, the lowest toxicity test result (NOEC or equivalent value) for the most sensitive species is multiplied by assessment factors (F_1 and F_2) in order to account for uncertainties in the extrapolation from test results with few species under laboratory conditions to real water bodies. F_1 is usually 0.1 and F_2 is always 0.1.

Usually, if reliable NOEC data are available for all 4 trophic levels, the lowest NOEC is multiplied by F_1 ($NOEC_{min}$ * 0.1) in order to derive the quality target. However, if additional reliable data from more realistic tests (e.g. field studies, microcosm studies) are available, it may be decided on a case by case basis to use a higher figure than 0.1 for F_1.

If NOEC data are only available for 2 or 3 trophic levels, only a tentative quality target can be derived. To this end, acute toxicity data (LC50, EC50) for the trophic levels for which no NOEC data are available are multiplied by 0.1 (as long as for at least one multicellular organism the substance specific acute/chronic ratio is known and not >10. If the acute/chronic ratio is >10 a case specific decision as to whether it is possible to derive a quality target is required). After multiplication of the acute toxicity data with the factor 0.1 the resulting figures are pooled with the available NOEC data and the tentative quality target is derived by multiplying the lowest figure with the factor F_1. As soon as NOEC data are available for all 4 trophic levels the tentative quality target is revised and replaced by a regular quality target.

If NOEC data are not available for at least 2 trophic levels no quality targets should be derived for the substance concerned.

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[3] The quality targets for metals are only based on the 50-percentile of concentrations monitored in surface water for the assets "aquatic communities" and "suspended particulate matter and sediments". For the other assets the 90-percentile is used.

If there is evidence for additional risks or uncertainties that must be considered in the derivation of a quality target, the factor F2 is additionally applied ($QT = NOEC_{min} * F_1 * F_2$). For example, F2 may be applied in the derivation of the quality target if:

- validated toxicity tests show a sensitivity for aquatic organisms other than those usually used for the derivation of the quality targets
- there is evidence that the substance concerned is transformed to hazardous metabolites in the aquatic environment (and no quality targets have been set for the metabolites).

Table 4.3 Data requirements and procedure to derive a quality target for the asset "aquatic communities"

Data requirements			
Trophic level	**Example for representative species**	**Example for acceptable test**	**Endpoint used**
destruents	bacteria	test over several cell generations (16 hours)	NOEC; values <EC10 are considered equivalent to NOEC #
primary producers	green alga	test over several cell generations (72 hours)	NOEC; values <EC20 are considered equivalent to NOEC #
primary consumers	daphnia	test on reproduction (21 days)	NOEC #
secondary consumers	fish	test over 28 days including reproduction; early life stage test; test over 14 days (alternatively, if before mentioned tests not available	NOEC #
Procedures to Derive Quality Targets			
a Standard procedure (NOECs or equivalent values for representatives of 4 trophic levels available)	$QT = NOEC_{min} * F_1$ Multiplication of the lowest NOEC with F_1		$F_1 = 0.1$ (standard) $F_1 > 0.1$ (if results from more realistic toxicity studies are available, size of F_1 decided case by case)
b NOECs only available for 2 or 3 trophic levels, acute data available for all 4 trophic levels	tentative $QT = VAL_{min} * F_1$ Multiplication of acute toxicity data with factor 0.1 for those trophic levels for which NOECs not available. Pooling of the transformed acute data with the available NOECs. Selection of the lowest value (VAL_{min}) from the data pool.		
c Evidence for additional uncertainty or risk	$QT = NOEC_{min} * F_1 * F_2$ Introduction of an additional factor F_2		$F_2 = 0.1$

In case NOEC data are not available acute toxicity test results (LC50, EC50 etc.) may be used under certain conditions to derive a tentative quality target (see main text and b) under "Procedures to Derive QT"

Metals [26]

In principle, quality targets for metals are derived by the same approach as described for the organic chemicals. However, as metals are naturally occurring substances, the natural background levels had to be considered in deriving the quality targets for metals. Bioavailability was a further issue since usually only a part of the total metal concentration in natural waters is bioavailable. However, as on the one hand not all of the metal in the dissolved fraction (filtration of sample with filter <0.45 µm) is bioavailable (colloids, sequestration) and

on the other hand organisms may also take up metals from the particle bound fraction, it was decided to compare toxicity test results of metals with the total metal content in water samples and not with the dissolved fraction only.

For those metals, for which quality targets were to derive (Cd, Cr, Cu, Hg, Ni, Pb, Zn), it turned out that the NOECs of the most sensitive species in laboratory tests are in the range of the estimated aquatic background levels of these metals in Germany (total concentrations). Therefore, the quality targets have not been based on the NOECs of the most sensitive species but were pragmatically set at twice the level of the upper limit of the background concentration range in suspended particulate matter (SPM) of the metal concerned (Table 4.4). In contrast to the organic substances, the metal quality targets for the asset "aquatic communities" are referring to the 50-percentile of metal concentrations in SPM. This modification is intended to take into account better chemical analysis of metals in SPM in comparison with total metal contents in water samples, spatial and temporal variations in background levels as well as the fact that only a fraction of the total metal level might be bioavailable. It is thought that compliance with the quality targets derived by this approach will ensure that the performance of aquatic communities is normally not impaired.

The assessment of compliance with the metal quality targets is normally based on the quality targets for suspended particulate matter and respective monitoring data. The quality targets for water may only be used for this purpose if monitoring data for suspended particulate matter are not available.

Table 4.4: NOECs, metal background ranges and quality targets for the asset "aquatic communities" [36]

	Water			**Suspended particulate matter**	
	NOEC of most sensitive species	background range [1]	quality target [1) 2)]	background range	quality target
	µg/l	C_{total} µg/l	C_{total} µg/l	mg/kg	mg/kg
Cadmium	0.08	0.009 – 0.036	0.072	0.15 – 0.6	1.2
Lead	0.2	0.4 – 1.7	3.4	12.5 – 50	100
Mercury	inorg. < 0.23 org. < 0.04	0.005 – 0.02	0.04	0.1 – 0.4	0.8
Nickel	0.2	0.6 – 2.2	4.4	15 – 60	120
Copper	0.2	0.5 – 2.0	4	10 – 40	80
Chromium	Cr^{6+}: 2 Cr^{3+}: 10	1.3 - 5	10	40 - 160	320
Zinc	0.2	1.8 - 7	14	50 - 200	400

1) Values are referring to waters with a suspended particulate matter concentration of 25 mg/l

2) QT is only used alternatively, if monitoring data for suspended particulate matter are not available

4.2.2 Derivation of quality targets for other protected assets

Asset "suspended particulate matter and sediments"

Due to the lack of generally accepted methods of assessment, water-ecology quality targets for the protection of organisms inhabiting sediment have not yet been developed. The derived quality targets refer to the application of sediment spoil on agricultural land. To this end, the soil limit values given in the German Sewage Sludge Ordinance have been adopted as quality targets. [24]

Quality targets referring to the asset "suspended particulate matter and sediments" are only derived for substances with a partition coefficient ≥1000 l/kg. [25]

Asset "fishery "

Water quality targets are derived on the basis of the prevailing maximum levels for foodstuffs from aquatic sources, taking bioconcentration factors into account [24]. Quality targets are not derived for substances with BCF <100 [25].

QT_F [µg/l] = ML_{fw} [µg/kg] / BCF [l/kg] [25]

with:
QT_F quality target "fishery"
MLfw maximum level for seafood based on fresh weight
BCF bioconcentration factor

Asset "drinking water supply"

The legally binding standards of Council Directive 75/440/EEC [17] concerning the quality required of surface water intended for the abstraction of drinking water have been adopted as quality targets. In the case of substances for which this Directive contains inadequate provision (e.g. for plant protection products) the threshold values provided for in Council Directive 80/778/EEC [37] relating to the quality of water intended for human consumption have been laid down as quality targets. [24]

Asset "irrigation of agricultural land"

Legally binding requirements for irrigation water have been adopted as quality targets. Where legally binding requirements do not exist, quality targets for the protection of crops, soil and groundwater can be derived on the basis of proposals of the competent authorities. Adherence to quality targets for drinking water supply is considered to generally ensure the use of water for irrigation. [24]

4.2.3 Derivation of Environmental Quality Objectives for list II substances of Council Directive 76/464/EEC

Based on the requirements of Council Directive 76/464/EEC on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community [7], in 2000 the Federal Environmental Agency in co-operation with the competent authorities of the German federal states (*Länder*) have derived water quality objectives that have been

adopted in *Länder* ordinances on reducing water pollution by means of programs and quality objectives applicable to certain hazardous substances. At the moment there are discussions on whether to apply these quality objectives as environmental standards in line with the water framework directive, unless they need to be regulated with respect to their chemical status on an EU-wide basis.

The quality objectives of the Dangerous Substances Directive 76/464/EEC focus on the protected assets "aquatic communities" and "human health" For precautionary reasons, in each case the more sensitive asset was used as a baseline when deriving the quality objective. The technical requirements for deriving quality objectives are oriented along the lines of nationally approved standards (e.g. the framework of the Chemicals Act) and internationally agreed guidelines (within the OECD context and the EC risk assessment and authorisation provisions for existing substances and pesticides) for the assessment of substances. That way, they also correspond to the requirements of the EC Water Framework Directive. By including the asset of "human health" it is ensured that, for instance, the supply with drinking water according to Article 7 WFD is also subject of protection. In addition, by including bioaccumulation, fishery is protected, as demanded by the Water Framework Directive with regard to determining environmental quality standards in the member states.

The quality objectives stipulate concentrations for water quality or SPM (suspended particulate matter). As stipulated by the Dangerous Substances Directive and the Water Framework Directive, compliance of these quality objectives is being monitored, using the average level as reference for the year under examination.

The quality objectives in table A1-2 are based on assessments of aquatic ecotoxicity. While acknowledging the asset "drinking water supply", two rules have been applied that, from a precautionary point of view, lead to upper limit values:

1. If the ecotoxicity requirements for pesticides exceed 0.1 µg/l for each substance, these limit values will be fixed at 0.1 µg/l.
2. If the ecotoxicity requirements for all remaining dangerous substances alien to nature exceed 10 µg/l for each substance, the limit values will be fixed at 10 µg/l.

4.3 The Netherlands

The description of the approach followed in the Netherlands to derive environmental quality standards referring to the aquatic environment is mainly based on the "Guidance Document on deriving Environmental Risk Limits" [28]. Here, it is only referred to the chapters relevant for the setting of Environmental Quality Standards in the context of the Water Framework Directive (i.e. the assessment of environmental effects in water bodies and sediment, secondary poisoning by food ingestion, and the calculation of environmental risk limits). The general Dutch approach is that first Environmental Risk Limits (ERLs) are derived, which are scientifically underpinned advisory values. Then, in a subsequent steep, the Dutch government sets Environmental Quality Standards based on these advisory values.

The methodology for deriving the scientifically underpinned ERLs is the responsibility of the National Institute of Public Health and The Environment (RIVM). Deriving ERLs for plant protection products and biocides is the responsibility of the Dutch Board for the Authorisation of Pesticides. The procedure of deriving ERLs for plant protection products and biocides is harmonised with the general protocol for deriving ERLs for other substances. Further, in principle, other certified parties such as the National Institute for Inland Water Management

and Wastewater Treatment (RIZA) and the National Institute for Coastal and Marine Management (RIKZ) can derive ERLs. Any party should derive ERLs in accordance with the procedures laid down in the Guidance Document on deriving Environmental Risk Limits and be guided by RIVM [28]. ERLs always need to be verified by the Environmental Quality Standards Advisory Group.

ERLs are derived for several environmental compartments (usually water, sediment, soil, groundwater, air), based on observed or expected effects on species inhabiting these compartments, including effects from food chain exposure of predators (secondary poisoning). ERLs for soil and sediment may be derived from the ERL for water when no sufficient toxicity data for soil or sediment dwelling organisms are available, using the equilibrium partitioning method.

ERLs for soil and sediment are calculated for a standardised soil (10% organic matter, 25% clay). ERLs for water are reported for dissolved and total concentrations (including a standard amount of suspended matter – 30 mg/l) and, if found significantly different, differentiated to freshwater and saltwater.

Three types of ERLs are usually derived:

- the Negligible Concentration (NC)
- the Maximum Permissible Concentration (MPC)
- the Ecotoxicological Serious Risk Concentration (SRC_{ECO})

These ERLs have been derived for a large number of substances and serve as scientific advisory values to set environmental quality standards (EQS) by the government for various policy purposes. The term EQS is used to designate all legally and non-legally binding standards that are used in Dutch environmental policy. Based on the different types of ERLs, different EQS may be derived (Target Value, Maximum Permissible Concentration, or Intervention Value). Table 4.5 shows the relationship between the 3 different types of ERLs and EQS, respectively. For the setting of EQS, the Dutch government can take into consideration the advice of consulting parties [28].

The Maximum Permissible Concentration (MPC) is the standard at which no adverse effect is expected, or, in the case of carcinogenic substances, a probability of fatality of 10^{-6} can be predicted. The Target Value (TV) is the standard at which the environmental impact is expected to be negligible. In deriving the MPC and the TV, no account is taken of economic considerations. Both standards, MPC and TV, place an obligation on decision makers to comply with the standards within certain time frames in the case of emission control [29]. The Intervention Values for soil, groundwater and sediment (clean up or remediation) are based on the lowest value of two underlying ERLs: one based on ecotoxicological data, the other based on human toxicological data and a human exposure model. When setting the Intervention Value, additional socio-economic factors can be taken into account [28].

The Dutch EQS/ERL refer to standardised monitoring data in order to increase the comparability. These standards have the following definitions:

- water samples are calibrated to a defined, standard water sample, containing 30 mg/l suspended solids
- a standard sample of sediments contains 10% organic matter and 25% lutum (particles < 16 um)
- a standard sample of suspended matter contains 20% organic matter and 40% lutum

After standardisation, the 90-percentile value from the monitoring data (per parameter, per location, per year) is calculated and compared to the EQS/ERL.

For some parameters relevant to the eutrophication problem (phosphate, nitrogen, chlorophyll and sight) an exception is made. For these parameters the summer-average value is used. An other exception is the parameter thermotolerant colibacteria for which the 80-percentile value must be used. All other parameters use the 90-percentile (or the 10-percentile when suitable; e.g. the parameters oxygen and pH).

Table 4.5: ERLs and the related EQSs that are set by the Dutch government for the protection of ecosystems in the Netherlands [28]

NC *Negligible Concentration* *MPC* *Maximum Permissible Concentration* SRC_{eco} *Serious Risk Concentration for the ecosystem*		
Description	**ERL**	**EQS**
The NC represents a value causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account possible combination toxicity.	NC (for air, water, soil, groundwater and sediment)	Target Value (for air, water, soil, groundwater and sediment)
A concentration of a substance in air, water, soil or sediment that should protect all species in ecosystems from adverse effects of that substance. A cut-off value is set at the fifth percentile if a species sensitivity distribution of NOECs is used. This is the Hazardous Concentration for 5% of the species, the HC_5^{NOEC} .	MPC (for air, water, soil, groundwater and sediment)	MPC (for air, water, sediment and soil)
A concentration of a substance in the water, soil, sediment or groundwater at which functions in these compartments will be seriously affected or are threatened to be negatively affected. This is assumed to occur when 50% of the species and/or 50% of the microbial and enzymatic processes are possibly affected.	SRC_{ECO} (for water, soil, groundwater and sediment)	Intervention Value (for soil, sediment and groundwater)

4.3.1 Calculation of Environmental Risk Limits (ERLs)

The extrapolation methods that are used for deriving the ERLs are the “refined effect assessment” (section 4.3.1.1) and the “preliminary effect assessment” (4.3.1.2). The former method, based on species sensitivity distributions, is preferred over the latter and applied if chronic toxicity data for four or more different taxonomic groups are available. The latter method is applied if chronic toxicity data for less than four different taxonomic groups or only acute data are available.

For naturally occurring substances such as metals the “added risk approach” is applied, taking background concentrations into account (section 4.3.1.3). For both organic substances and metals that potentially accumulate through the food chain, ERLs are derived

combining direct toxicity and secondary poisoning (4.3.1.4). The equilibrium partitioning method is applied to derive ERLs from aquatic toxicity data in case insufficient data are available for sediment or soil (4.3.1.5).

When independently derived ERLs for water, soil and sediment are available, these are harmonised by applying the equilibrium partitioning method (section 4.3.1.6).

4.3.1.1 Refined Effect Assessment

Species sensitivities to toxic compounds differ since living organisms represent a vast array of diversity in terms of physiology, morphology, behaviour and spatial distribution. The basic assumption of the refined effect assessment or statistical extrapolation method is that the log of the sensitivities of a set of species in a community can be described by a distribution, usually a parametric distribution function such as the normal or logistic distribution. The available ecotoxicological data are seen as a sample from this distribution and are used to estimate the parameters of the Species Sensitivity Distribution (SSD). The variance in sensitivity among the test species and the mean are used to calculate a concentration that can be used as an environmental risk limit (ERL). Specific percentiles of the SSD are chosen to determine ERLs such as the Maximum Permissible Concentration (MPC) or the Ecotoxicological Serious Risk Concentration (SRC_{ECO}) (fig. 4.1). The Negligible Concentration (NC) is not based on a specific percentile but is based on a safety factor for combination toxicity. The NC is derived from the MPC by dividing it by a factor of 100.

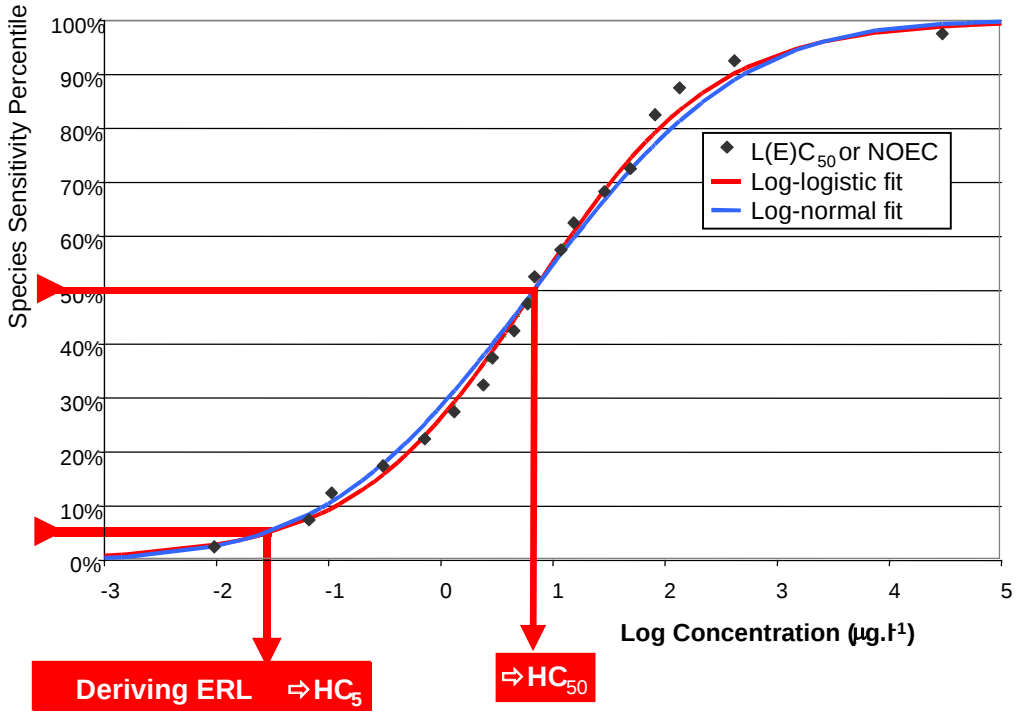


Figure 4.1: Species Sensitivity Distributions (SSDs) used to derive ERLs [NL1]. Dots are input data, the lines are the fitted SSDs.

The method is applied provided at least four chronic NOEC values of species of different taxonomic groups are available. For aquatic species, freshwater and marine data are com-

bined if there are no differences in sensitivity between these groups. This is tested with an unpaired, two-sided T-test (significance level alpha = 0.05) and with prior check of differences in variance. If differences in variance are detected, the T-test is performed with a Welch correction for differences in variance. When there is a statistically significant difference, distributions for freshwater and marine species are estimated separately. If prior knowledge about sensitive species or taxonomic groups (specific mode of toxicant action) is available, a statistical analysis should be performed for conformation or rejection of the different sensitivities of the groups.

The final NOEC data set is tested for derivations from a Gaussian distribution using the Kolmogorov-Smirnov test. However, it is acknowledged that this test has limited validity if the sample contains less than a dozen values. If the sample size is smaller it can at best be shown that the data are not inconsistent with a Gaussian population which, however, does not exclude the possibility of a non-Gaussian population. If a data set consists of less than four values, it is impossible to test for normal distribution.

Until mid-2000, the statistical extrapolation method of Aldenberg and Slob [30] was used. This method, based on the log-logistic fit is now replaced in favour of the method of Aldenberg and Jaworska [31]. The difference between the methods is that the use of the logistic distribution of log-transformed NOEC data is now replaced by a normal distribution of log-NOEC data. The differences between these two distributions are small and are mainly noticeable in the tails of the distribution (fig. 4.1). The advantage of using the normal distribution is that normal distribution theory provides the methods to calculate confidence intervals.

Based on the selected NOEC values the ERLs can be derived from the SSD. The MPC is estimated from the 5-percentile of the SSD, the HC_5 (hazardous concentration for 5% of the species), and the SRC_{ECO} is estimated from the 50-percentile or median, the HC_{50}. Since with the method of Aldenberg and Jaworska it is now possible to routinely calculate confidence intervals, the 90% confidence intervals of the HC_5 and the HC_{50} are reported as well.

The HC_5 and HC_{50} are calculated as:

$$\log HC_p = X_m - k * s$$

with:

HC_p = hazardous concentration for p% of the species, with HC_5 for the MPC and HC_{50} for SRC_{ECO}

X_m = mean of log-transformed NOEC data

k = extrapolation constant depending on protection level and sample size (according to Aldenberg and Jaworska [31], Annex 6 in [28])

s = standard deviation of log-transformed data

The extrapolation constant k is taken from Aldenberg and Jaworska [31]. 3 values are given for k. The HC_5 and the HC_{50} are calculated with the median estimate for k whereas the confidence limits are calculated using the upper and lower estimates of k.

The end result of the refined effect assessment using SSDs is a MPC and a SRC_{ECO} with reported 90% confidence intervals, and a NC derived from the MPC.

4.3.1.2 Preliminary Effect Assessment

If chronic NOEC values are available for less than 4 taxonomic groups, preliminary effect assessment is applied. In this case, assessment factors are applied to the selected chronic or acute toxicity data. The derivation of the MPC and the SRC_{ECO} are different in terms of the

assessment factors applied and the use of the available data (the NC is derived from the MPC by division with a factor of 100, as in the refined effects assessment).

Derivation of the MPC

Normally, the assessment factors given in the TGD [6] for deriving the Predicted No-Effect Concentration (PNEC), which is similar to the MPC, are used to derive the MPC (see table 5.1). However, some modifications have been introduced, e.g.:

- A classification of species in taxonomic groups is used instead of the original classification in trophic levels, because this classification is used throughout the derivation methods for MPCs.
- If several toxicity data for one species, based on the same toxicological endpoint, is available, the geometric mean is used instead of the arithmetic mean.
- As for more hydrophobic substances (log Kow >3) short-term toxicity may not be representative since the time span of an acute test may be too short to reach a toxic internal level, the completeness of the TGD base set is not demanded and – in line with a respective recommendation given in the TGD - an assessment factor of 100 may be applied to a chronic test (not to an alga test, if this is the only chronic test available).

In case the number of available ecotoxicological data does not meet the conditions for application of the TGD assessment factors (i.e. incompleteness of base set – the short-term acute tests for algae, daphnia, and fish), the modified EPA assessment factors are used (table 4.6). Besides the different application of assessment factors, the possibility of using quantitative structure activity relationships (QSAR) within the validity domain of the QSARs is a further difference to the TGD-method.

Table 4.6: Modified EPA assessment factors for aquatic organisms [28]

available data	**additional criteria**	**MPC based on**	**assessment factor**
L(E)C50 or QSAR estimate	$L(E)C50_{min}/1000 < NOEC_{min}/10$	$L(E)50_{min}$	1000
L(E)C50 or QSAR estimate for minimal algae/crustaceans/fish	$L(E)C50_{min}/100 < NOEC_{min}/10$	$L(E)50_{min}$	100
NOEC or QSAR estimate *)	$L(E)C50_{min}/1000$ (100) $< NOEC_{min}/10$	$L(E)50_{min}$	100/1000
	$L(E)C50_{min}$/ 1000 (100) $\geq NOEC_{min}/10$	$NOEC_{min}$	10
NOEC or QSAR estimate for minimal algae/crustaceans/fish		$NOEC_{min}$	10

*) The value based on NOECs is compared to the extrapolated value based on acute L(E)C50 toxicity values. The assessment factor for L(E)C50s is 100 for ≥3 L(E)C50s, 1000 for <3 L(E)C50s.

Derivation of SRC_{ECO}

The factors and conditions used for deriving a SRC_{ECO} in the preliminary effect assessment are shown in table 4.7. In principle, a motivated acute to chronic ratio (ACR) is applied to compare acute L(E)C50s with chronic NOECs. If no specific information is available, an ACR of 10 is used. In other cases, the ACR can be derived using existing databases or ACR data specific for a substance.

Table 4.7: Assessment factors used to derive the SRC_{ECO} for the aquatic compartment [28]

available data	additional criteria	SRC_{ECO} based on	assessment factor
only L(E)C50s and no NOECs		geometric mean of L(E)C50s	10 *)
NOECs available	geometric mean of L(E)C50s/10 < geometric mean of NOECs	geometric mean of L(E)C50s	10 *)
	geometric mean of L(E)C50s/10 > geometric mean of NOECs	geometric mean of NOECs	1

*) an ACR of 10 is used, unless a better estimate is available

4.3.1.3 The Added Risk Approach

The added risk approach is used to take natural background concentrations into account when calculating MPCs for naturally occurring substances. The approach starts with calculating a maximum permissible addition (MPA) on the basis of data from laboratory toxicity tests (with added amounts of toxicants as compared to the control groups). This MPA is considered to be the maximum concentration to be added to the background concentration (Cb), without causing deleterious effects. Hence, the MPC is the sum of the Cb and the MPA:

$$MPC = C_b + MPA$$

The MPA is calculated using a similar approach as the MPC for substances having no natural background concentrations (cf. section 4.3.1).

The Negligible Concentration (NC) is defined as the background concentration (C_b) plus the Negligible Addition (NA):

$$NC = C_b + NA, \text{ where } NA = MPA/100$$

The background concentration and the MPA are independently derived values. The background concentration is based on monitoring data from relatively pristine areas and the MPA is the MPC derived on the basis of the selected toxicity data minus C_b.

With regard to metals, it is assumed that the amount added to the test medium is fully bioavailable, i.e. the bioavailability of the added metal in laboratory tests is considered 100%. To which extent the background concentration of a metal is bioavailable in the real world is not relevant since any potential adverse or positive effect of the background concentration is considered not deleterious, because of its contribution to the biodiversity of ecosystems.

4.3.1.4 Secondary Poisoning

Species higher in the food chain are not only exposed to hazardous substances via environmental media such as water, air, sediment or soil but may additionally or mainly be exposed to toxic substances via their food (secondary poisoning). Secondary poisoning is considered if a substance is potentially bioaccumulating (e.g. log Kow > 3, low metabolisation and/or excretion rate). In this case data on oral toxicity in birds and mammals as well as bioconcentration/bioaccumulation factors are required.

The following steps are employed to assess toxicity data for birds and mammals with respect to secondary poisoning:

NOECs (as mg/kg food[4]) are converted to mg/l water by dividing the NOEC by the bioconcentration factor and multiplying with a correction factor for caloric content of fish or mussel and laboratory feed.

$$NOEC\ [mg/l] = \frac{NOEC_{predator}\ [mg/kg]}{BCF\ [l/kg]} * F_c$$

with:
BCF = the relevant BCF for fish or mussel
F_c = 0.32 for fish, and 0.20 for mussel

The lowest of the two NOEC values (via fish or via mussel BCFs) per test species is selected.

Until 2000, secondary poisoning was assessed by calculating an MPC for secondary poisoning and comparing it to that for direct exposure. Usually the lowest MPC of the different MPCs calculated was taken as the respective MPC.

This approach has been replaced by an alternative method where data for direct exposure and secondary poisoning are combined since the conceptual idea for deriving ERLs is the protection of all species in the ecosystem. To this end, NOECs for food exposure are recalculated to a concentration in water. The MPC is then derived from the combined data set.

In the context of the refined effect assessment, three different HC5 values are reported if secondary poisoning is assessed: one for the combined data set, one for secondary poisoning based on the bird and mammal toxicity data, and one for the direct toxicity data only. The HC5 for the combined data set is the recommended MPC, the other HC5 values are reported for the sake of comparison. MPCs can also be based on preliminary effect assessment, depending on the number and quality of data.

4.3.1.5 Equilibrium Partitioning

MPCs for sediment can be derived indirectly from the MPC_{water} by the equilibrium partitioning method if experimental data for sediment dwelling organisms are lacking.

In principle, the same approach is followed as in the risk assessment for existing substances [6].

It is assumed that:

- bioavailability, bioaccumulation and toxicity are closely related to the pore water concentrations
- sensitivities of aquatic organisms are comparable with sensitivities of organisms living in sediment
- equilibrium exists between the chemical sorbed to the particulate sediment organic carbon and the pore water, and that these concentrations are related by a partition coefficient (Koc). (For metals, empirical partition coefficients are used since metal concentration in pore water depends on additional variables. Also the assumption is that there is a

[4] if NOECs (NOELs) are reported as dose per kg body weight per day, these values are converted to food concentrations using conversion factors based on the inverse of the daily food intake.

steady-state, i.e. not necessarily equilibrium, between the particulate sediment and the pore water, and thus not (purely) related to the sediment organic carbon)

The Environmental Risk Limit for standard sediment using the equilibrium partitioning method is derived as follows:

$$ERL_{sed.ep}\ [mg/kg] = ERL_{water}\ [mg/l] * Kp_{SPM}\ [l/kg]$$

with:
$ERL_{sed.ep}$ = ERL for sediment species using the equilibrium partitioning method
ERL_{water} = ERL for aquatic species
Kp_{SPM} = partition coefficient for the standard sediment

As species may take up substances from their food or directly from the sediment, there may be reasons not to apply the equilibrium partitioning method.

4.3.1.6 Harmonisation of ERLs

As substances in the environment distribute over the different environmental compartments driven by fugacity or concentration gradients, independently derived ERLs for water, soil and sediment are harmonised (Figure 4.2).

This is achieved by calculating the ERLs for sediment or soil from the ERL for water with the equilibrium partitioning method (4.3.1.5). To determine the final harmonised ERL, the following guidelines are used:

1) If insufficient data for soil or sediment is available (e.g. no NOEC data available) the ERL is derived from the ERL water, using the equilibrium partitioning method. If the ERL for surface water is based on a relatively large data set containing chronic data on several taxonomic groups while the ERL for soil or sediment is only based on a limited data set, the ERL based on the equilibrium partitioning may, on a case by case basis, be given more weight and be chosen as ERL for soil or sediment.
2) If statistical extrapolation can be applied to terrestrial or benthic data, the ERL is derived directly and no comparison with equilibrium partitioning derived ERLs is made.
3) If condition 2 does not apply (i.e. no refined effect assessment), in principle the lowest value of the independently derived ERLs for sediment (or soil) and the ERL resulting from application of the equilibrium partitioning method is taken as the harmonised ERL.

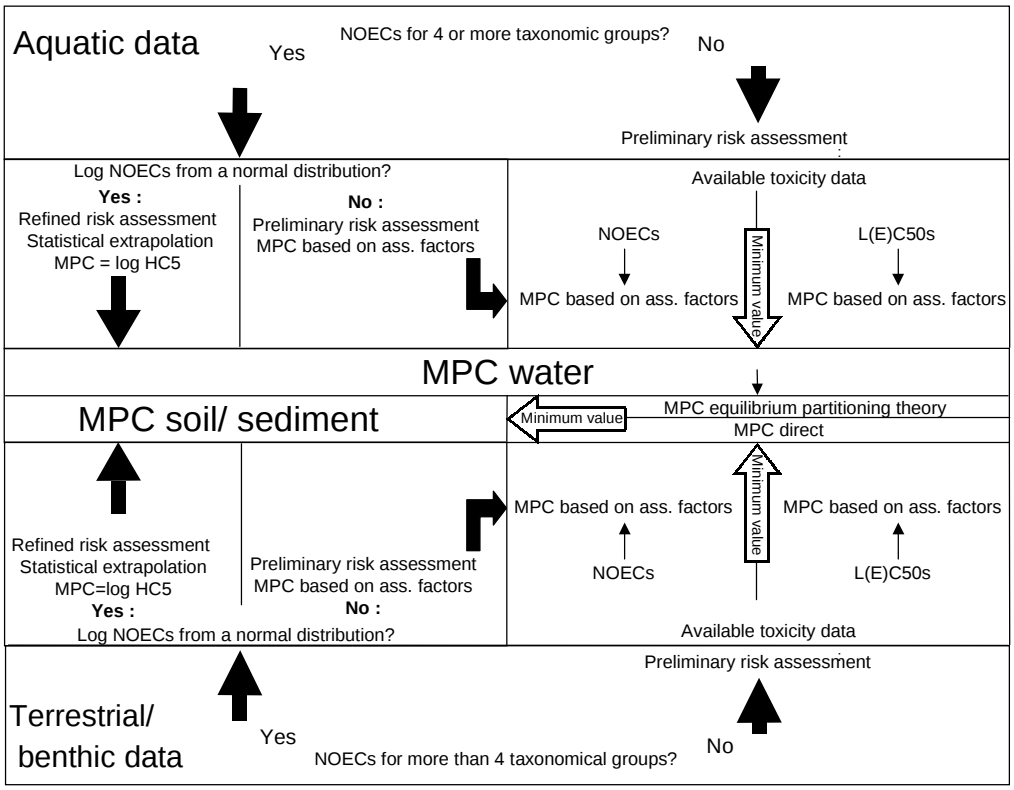


Figure 4.2: Diagram of the derivation and final harmonisation of the MPC [NL1]. The "minimum value rule (arrows)" only applies if the preliminary risk assessment for soil or sediment is applied.

4.4 United Kingdom

The description of the approach followed in the UK to derive water quality standards is based on a document entitled "Deriving Environmental Quality Standards" forwarded by the Water Quality Division of the UK Department of the Environment, Transport and the Regions (DETR, now DEFRA) to the Commission Services in September 2000 [60].

An Environmental Quality Standard (EQS) is defined as a concentration of a given substance, which should not be exceeded in receiving waters in order to protect the use of the water. The EQS is derived not to have detrimental effects on the aquatic environment and to protect all aquatic species.

The Regulatory Authorities require EQSs to be set as operational standards for certain substances to ensure that concentrations observed in the environment are below those causing environmental effects, to assess the likely impact of pollution incidents and for use in calculating discharge consents. EQSs are enforced through the regulatory authorities (Environment Agency in England and Wales, SEPA in Scotland and DOENI in Northern Ireland).

There are two ways of expressing an EQS:

a) as an **annual average concentration** (AA). An AA EQS is the highest concentration to which aquatic ecosystems can be continuously exposed without any likely adverse effects. In other words, this is equivalent to an ecosystem no-effect-concentration.

b) as a **maximum allowable concentration** (MAC). A MAC EQS is the highest transient concentration that would be expected not to cause adverse effects. This is a concentration not to be exceeded, designed to protect against short-term episodic events.

4.4.1 The Derivation of EQSs

The approach used to derive EQSs is illustrated in the flow diagram (Fig. 4.3). It is based upon the collation and critical assessment of the data available for the substance, the identification of the lowest reliable and relevant adverse effects concentration and the application of appropriate extrapolation factors. Where available, AAs are derived from the most sensitive chronic toxicity data and MACs from the most sensitive acute toxicity data.

Depending on the quantity, quality and relevance of the available data, EQSs may be set as EQSs or ‘tentative’ standards. ‘Tentative’ standards are generally proposed if the minimum aquatic toxicity data set is not available or if toxicity data for the target species are missing. In addition, the standards proposed for the protection of freshwater life may be proposed as ‘tentative’ standards for the protection of saltwater life if insufficient data are available for saltwater species to propose separate standards and there is no reason to suggest that saltwater species would be of greater sensitivity. Where data are extremely sparse, no standards may be suggested. Where tentative or no EQSs are recommended proposals are made on what tests are required to fill the missing data gaps.

Depending on the behaviour and speciation of the substance (e.g. solubility, adsorption to sediment) EQSs may be expressed as either ‘total’ concentration (i.e. unfiltered samples) or ‘dissolved’ concentrations (i.e. filtered samples or settled samples).

Preliminary EQSs, based on laboratory data, are compared with field data (when available) to assess their suitability for protecting natural populations. EQSs may be reviewed and subsequently refined on the basis of any anomalies.

Additional Considerations

Modelling: When limited data are available in a particular area, Quantitative Structure-Activity Relationships (QSARs) or models may be used to predict a substance's physico-chemical properties and aquatic toxicity. However, presently, the derived data are considered only in support of existing laboratory or field data.

Combined toxicity: The combined toxicity of mixtures of substances (e.g. additivity, synergy, antagonism) is difficult to account for in the derivation of EQSs. However, for structurally similar substances with similar modes of toxic action, combined EQSs are sometimes recommended (e.g. total trichlorobenzenes or total atrazine and simazine).

Procedure for Agreeing Standards

Detailed reports are prepared assessing all the available data for the substance. Based on the assessment, draft recommendations for appropriate EQSs are made. These are considered and revised if necessary by an independent Scientific Steering Group comprising representatives from DETR (now DEFRA), the regulators and industry. The agreed standards are subsequently submitted for public consultation before a decision is taken by Ministers as to whether the standards should be the subject of regulations.

4.4.2 Data requirements

All available data from public literature, commercial databases and unpublished sources (e.g. manufacturer's data) are collated. Before an EQS can be derived for a particular substance sufficient data of appropriate quality must be available. The data available for a substance are critically assessed in terms of their reliability and relevance for the derivation of the EQSs. Special emphasis is placed on the assessment of the experimental procedures and test species used for the toxicity test, the toxicity endpoints, and whether a dose-response relationship was established. The data are classified into primary data obtained from reliable and relevant tests, and secondary data for which inadequate test details are available. The primary data are used to derive the EQS with the secondary data providing supporting information.

In order to derive EQSs for fresh and saltwaters, ideally data, both acute and chronic, should be available for the following taxa:

- Algae and/or macrophytes
- Arthropods (e.g. crustaceans, freshwater insects)
- Non-arthropods (e.g. molluscs)
- Fish

In particular, when assessing chemicals designed for a specific purpose it is important to assess whether toxicity data are available for the target species (e.g. insects for insecticides). Other taxa for which data are available can also be taken into account where appropriate.

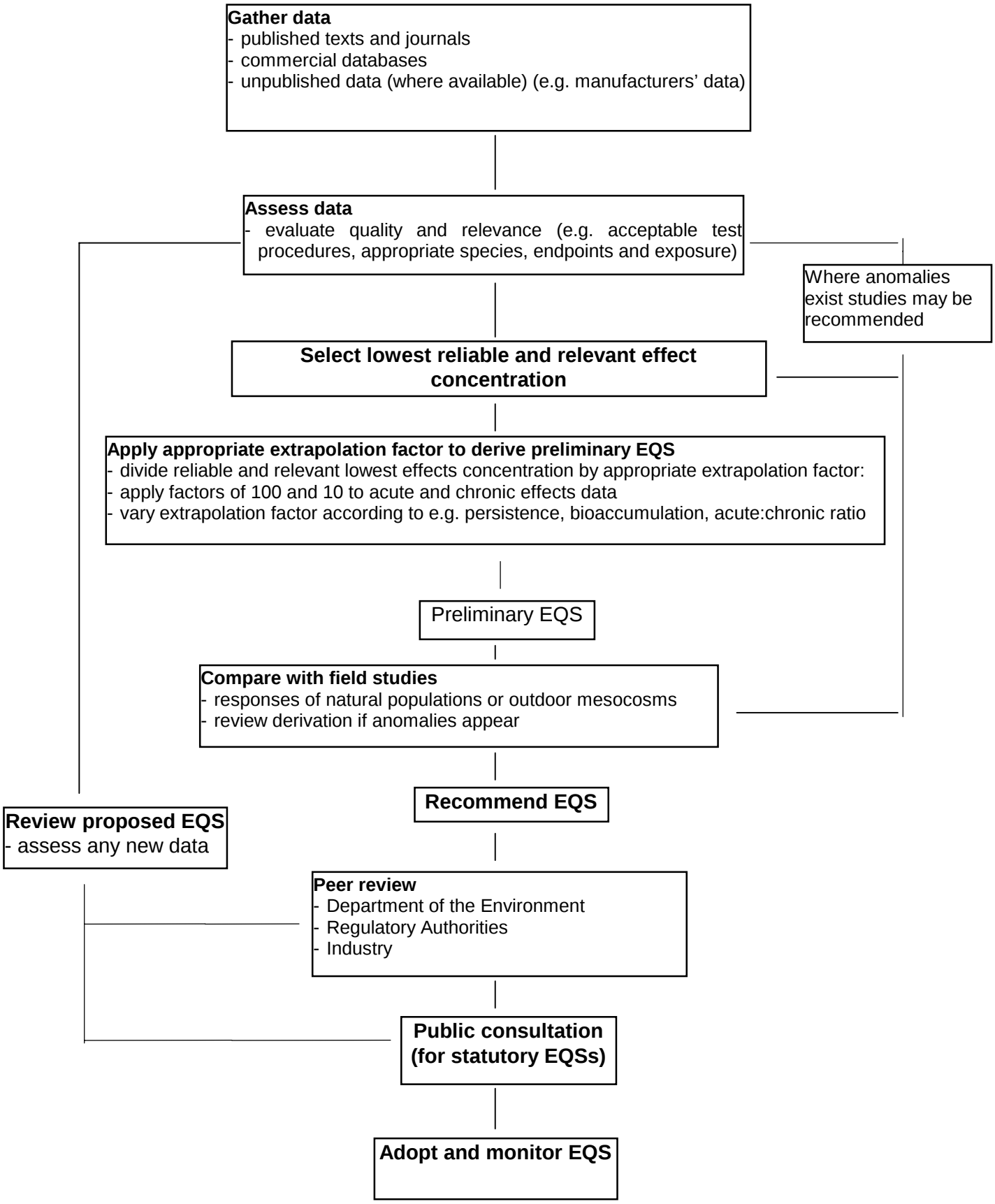


Figure 4.3 The Derivation of Environmental Quality Standards in the UK

4.4.3 The use of extrapolation factors

The primary purpose of EQS-setting is to predict the no-effect-concentration by extrapolating from laboratory and field (where available) toxicity data. EQS values are generally based on the lowest relevant and reliable adverse effect concentration in the toxicity data set, a concentration which is then subject to an extrapolation procedure.

The use of safety/ application factors based on experimental data is considered best current practice for this extrapolation (statistical methods of doubtful validity are also available). The purpose of this is *inter alia* to account for the uncertainty involved in extrapolating from one species to others, from short to long exposure times, from acute to chronic effects, from chronic to ecosystem effects, and from effects in one eco-system to those in another.

Deriving an EQS therefore requires the use of expert judgement, and it is considered important to use the database as a whole as the basis for this judgement. Fixed safety factors which have to be applied to a data set of a certain quality have not been set, such factors may be modified either up or down in particular cases (figure 4.4). However, some broad guidance about extrapolation factors is available.

An important moderating influence is the amount of available toxicity data, particularly the species range which it represents, and the environmental fate and behaviour of the substance. Clearly, extrapolation factors can be reduced if the toxicity data set is large, if toxicity data are available for the group which is expected to show the greatest sensitivity, if acute effects-to-no-acute effects ratios are small, or if acute-to-chronic ratios are small. Equally, it might be necessary to add an additional factor for a highly bioaccumulating substance.

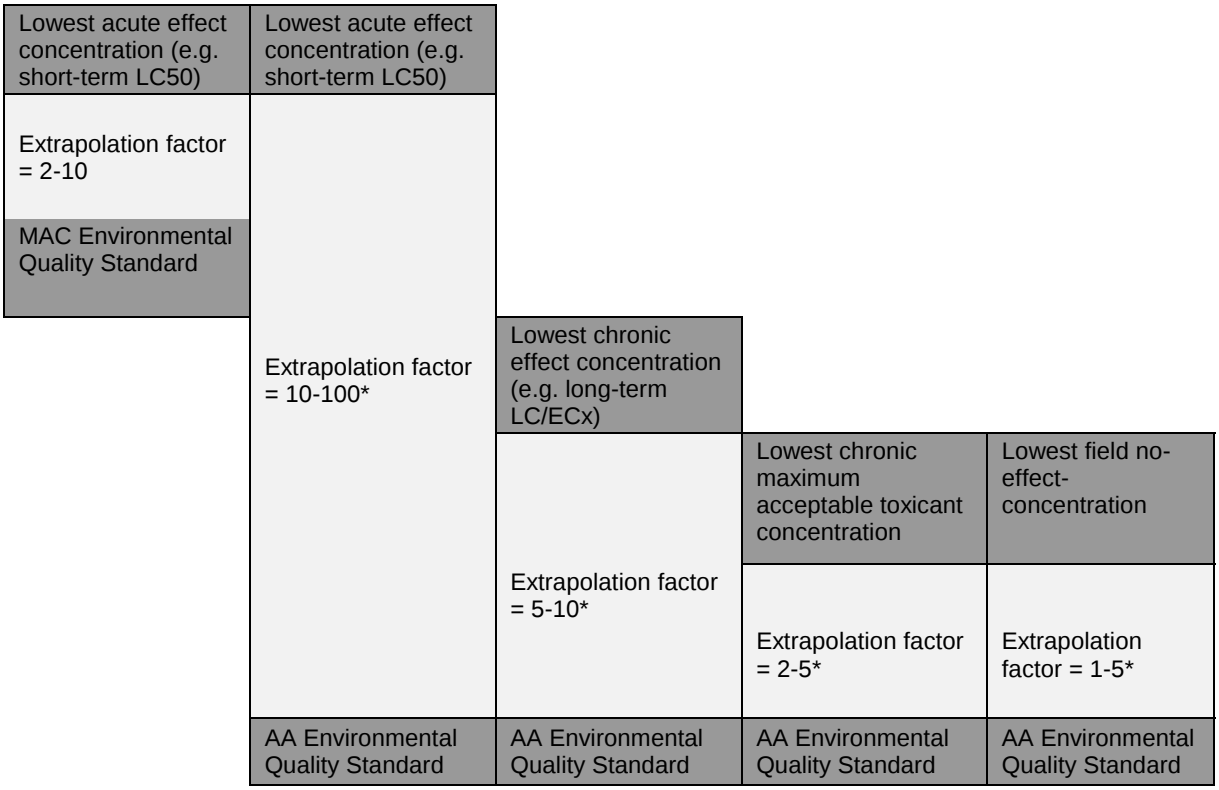
When predicting no-effect-concentrations for new chemicals with relatively limited acute toxicity (i.e. short-term LC50) databases, a conservative extrapolation factor is usually taken to be between 200 and 1000. However, as described earlier, an adequate data set for EQS-setting will consist of acute toxicity information on plants/algae, crustaceans, insects, other invertebrates, and fish. In recognition of this, when predicting the annual average (AA) EQS an acute effects-to-no-effects-concentration factor of 10-100 is usually considered adequate to account for all the uncertainties mentioned above. When predicting the maximum allowable concentration (MAC) EQS, a factor of 2-10 is usually applied to the lowest acute effects concentration.

If adequate chronic data are available for sensitive species, they should be used in preference to acute data, although the latter should be used to support the derivation of the EQSs. Chronic or sub-chronic no-observed-effects-concentrations (NOECs), when used for the risk assessment of new chemicals, are usually subject to a factor of about 10 to derive a no-effects-concentration. However, chronic NOECs are often well below the chronic threshold concentration, so for AA EQSs, it is deemed that the no-effects-concentration is more robustly derived from a chronic EC50 or a maximum acceptable toxicant concentration (MATC - the geometric mean of the chronic NOEC and the chronic lowest-observed-effect-concentration, or LOEC). Subject to expert judgement, the factor used on a chronic EC50 is approximately 5-10, while that used on an MATC is about 2-5.

If reliable no-effect-concentrations are available from field studies, it may only be necessary to apply a very small extrapolation factor (1-5) to account for differences between ecosystems (figure 4.4).

Figure 4.4: Extrapolation of Environmental Quality Standards in the UK from reliable and relevant acute and chronic toxicity data

These are not fixed extrapolation factors, but are varied by expert judgement according to the properties of the chemical and its toxicity profile.



* Note: If substance is highly bioaccumulative, a higher extrapolation factor may be used.

4.5 Denmark

The text presented in this section is adapted from Annex 1 of the Danish comments on documents presented at EAF(2) on priority substances [61].

The calculation of quality standards for water (WQS) in Denmark is generally the responsibility of the county authorities. According to the Danish Statutory Order no. 921 of 9th October 1996 companies and organisations that wish to discharge wastewater into surface waters must apply for a discharge permit from the county authorities

When giving this permit a basic provision is that installation of best available technique (BAT) shall be required. Furthermore, the county authorities shall apply the combined approach (similar to the provisions of the WFD) and shall consider whether or not the WQS can be met for the substances to be discharged. If concentrations in the outlet exceed the WQSs after an "initial dilution" or outside a well defined, designated area around the mixing zone , more stringent requirements needs to be set in order to grant a discharge permit.

The statutory order contains WQS for a number of substances, mostly the EU List I substances and the List I candidates.

If a WQS is not set at a national level for a given substance then the county authority must calculate a WQS. The respective method is laid down in a guideline referring to Statutory Order 921 and in the report "Miljøproject 250" (both in Danish), and is shortly outlined below.

Only QS for water have so far been calculated. The method used for the last about 5 years follows the recommendation of CSTE [9]. In certain cases the Danish Environmental Protection Agency (DK-EPA) has conducted calculations of WQS in order to provide for less different standards nationwide.

Current practice is, as mentioned, based on the recommendations of CSTE, but in certain cases inspired by the risk assessment TGD. The basis thus is the use of assessment factors according to the following table:

a)	Few LC(EC)50 values	1000
b)	Many LC(EC)50 values	100
c)	Sufficient number of long-term NOECs	10

Usually an assessment factor (AF) greater than 1000 is not applied. However, at the b) and c) levels of data availability the AF may be increased if the substance is considered as liable to bioaccumulation and not readily degradable or persistent, or if behavioural effects like e.g. avoidance have been observed. Also carcinogenic properties and other health effects (e.g. reprotoxicity) may influence the AF. Furthermore tainting of fish and shellfish may not occur.

If a certain species shows a marked greater sensibility (judged valid) than the other species, say a factor of 1000, then the WQS as usual will be based on the most sensitive species, but the AF will be lowered (usually by a factor of 10). The rationale for this is that it seems quite certain that the species in question is among the most sensitive thus lowering the uncertainty of the assessment. The latter is an inspiration from the RAR-practice.

With naturally occurring substances DK has recently adopted the "added risk approach" for naturally occurring substances (e.g. copper, formaldehyde and iodine). For copper, however, upper limits in freshwater and saltwater have been set.

The DK strategy for collection of data is to use data from the risk assessment report (or draft) if such a report exists. If a RAR is not available the practice is to follow the strategy outlined in 'Environmental Hazardous Classification – data collection and interpretation guide (2^{nd} edition)' (TemaNord, 1995: 581, Nordic Council of Ministers) . In general all values are used except if they are actually invalidated.

Concerning the use of SSD the Danish EPA has in some cases used the Wagner & Løkke method supporting the AF-method. The SSD has been used both with NOEC- and LC(EC)50-values. When using LC(EC)50-values a supplementary AF of 10 has been applied. It should be stressed, however, that the acute/chronic ratio varies, and that an AF extrapolation should only be used in cases where long-term NOEC or EC10 values are not found and cannot be requested.

Normally the Danish authorities round down the WQS value to the nearest order of magnitude because of the inherent uncertainties.

For a few substances calculations of a WQS has been carried our both according to the CSTE method and the WFD method (RA) for a comparison. For several substances this leads to the same result, some get a more stringent result with the WFD method and a few a less stringent result.

4.6 Spain

The text presented in this section is adapted from section II.2 of the Spanish comments on the EAF(2) meeting documents and describes the procedures followed to establish Water Quality Objectives in Spain [62]. These WQOs are published in the Official State Bulletin (B.O.E. number 147 20/Jun/00, R.D. 995/2000).

4.6.1 QS Setting Procedure for Organic Chemicals

It is evident from Council Directive 76/464/EEC that WQOs should be founded principally on toxicity, persistence and bioaccumulation of the substance. For the majority of List 1 chemicals, the Scientific Advisory Committee has tended to emphasise on toxicity data with information on persistence and bioaccumulation acting as modifying factors (cf. section 5.4).

In Spain two main methodologies were considered:

1) Deterministic estimation following the procedure described by the CSTE
2) Probabilistic models (i.e., US EPA, 1985)

The deterministic model proposed by the CSTE was finally selected as the basic methodology for the derivation of WQOs for organic chemicals. It comprises the evaluation of available toxicity data and the selection of those corresponding to the most sensitive organism. The water quality objective is then established by applying several safety factors (described in point 5. below) in order to obtain a margin of safety (MOS) for the protection of structure and function of aquatic ecosystems. The selected margin of safety is applied to the lower end of the toxicity range, and then rounded to orders of magnitude. Expert judgement is required for the selection of the lower end of the toxicity range (i.e., detection of relevant data, out-layers, aggregation of data for the same species) and for the rounding process.

The general procedure for the derivation of the Spanish WQOs is as follows:

1. *Toxicity data compilation:* Published data were obtained from all kinds of data sources. Information on ambient concentration levels as well as environmental levels related to point source contamination in various compartments of aquatic ecosystems should be available. The toxicity endpoints relevant for the aquatic environment, i.e. acute, subacute, and chronic effects, including reproduction, should be reported for flora, microbial systems, and fauna. On-line databases (EPA, IUCLID, POLTOX, MEDLINE, AGRIS, CAB, etc.) and other WQO published were the principal data sources.

2. *Taxonomic groups and species more relevant and/or sensitive:* All taxonomic groups must be represented in the data set. With regard to the aquatic environment ecotoxicological data for algae, invertebrates and fish are required. Data on other taxonomic groups were considered if available.

3. *Physical-chemical properties of the pollutant:* There are several inherent pollutant properties that can affect its toxicity. Knowledge on speciation capacity, toxicokinetic properties and the relationship between toxicity and water quality parameters (pH, hardness, chloride concentration, etc.) is required.

4. *Data selection and classification:* The compiled toxicity data must be selected and classified according to their end-point ($L(E)C_{50}$, NOEC, etc.) and quality (e.g. GLP study).

5. *Safety factors:* Finally, the WQO is obtained by applying a margin of safety on the selected toxicity data. This margin is obtained aggregating the following factors:

Toxicity: margins for the acute and chronic values are considered:

1/100 of L(E)C_{50} value

1/10 of NOEC value

Additional factors: Lack of data, persistence, bioaccumulation potential and genotoxicity increase the hazard and requires additional margins:

1/10 in addition to toxicity if there is a lack of relevant species

1/10 in addition to toxicity to cover persistence and/or liability to bioaccumulate

1/10 in addition to toxicity to cover genotoxic potential

4.6.2 QS Setting Procedure for Inorganic Chemicals including Metals

The procedure proposed by the CSTE did not consider the effects of water quality parameters on the toxicity. This factor was considered essential in the derivation of the Spanish WQOs for inorganic chemicals including metals. Therefore the CSTE procedure was not directly applicable.

Four different alternatives were considered :

1. To select those water quality conditions for which the toxicity is the highest.
2. To establish the toxicity distribution curve for each relevant water quality parameter, and to select the 95 % percentile.
3. To estimate the toxicity values for different ranges of the relevant water quality parameter.
4. To study the quantitative relationship between the affecting water quality parameter and toxicity.

Each of these alternatives offers different protection levels, closeness to reality and requires different toxicological information. The differences are summarised in table 4.8.

Table 4.8: Different characteristics of the alternatives for WQO derivation for inorganic pollutants

Alternative	Level of Protection	Reality	Required Information
1	***	*	*
2	*	**	*
3	***	**	**
4	***	***	***

After studying all different possibilities, on the basis of the available information and the required protection needs, alternative 3 was selected for the derivation of WQOs for inorganic chemicals. Obviously, alternative 4 would constitute the ideal option but it was considered that the available information did not allow a scientifically sound derivation of quantitative relationships in all cases.

Two additional considerations were made. First, the need to account for natural background concentrations. Secondly, the convenience for maintaining the CSTE criteria for expressing

the WQO as orders of magnitude. It was finally decided that the WQOs should be expressed as concentrations in excess of the natural backgrounds, and that the values obtained by applying the selected margin of safety to the lower end of the toxicity range will be used directly, and therefore the values will not be rounded (or rounded down) to the closer order of magnitude.

The derivation of the WQO for copper may serve as example:

The toxicity of copper to aquatic organisms is well known and there is a considerable of information available covering the main taxonomic groups of fish and invertebrates. However, information about algae is poor. The Cu toxicity on aquatic organisms is related to the water hardness[5] and it is possible to establish a quantitative relationship (US EPA) between them. In figure 4.5 the graph of acute toxicity to fish *versus* water hardness is shown. In addition, the US-EPA and Canadian water quality criteria are compared with the INIA proposal for the derivation of the Spanish WQO in this figure.

A clear relationship between toxicity and hardness can be seen, but there is not a good regression function. For this reason, it was decided to fix four different WQO values for copper referring to four calcium carbonate concentration classes. Also WQO for other heavy metals (e.g. Zn, Ni, Pb) were established accounting for the water hardness range.

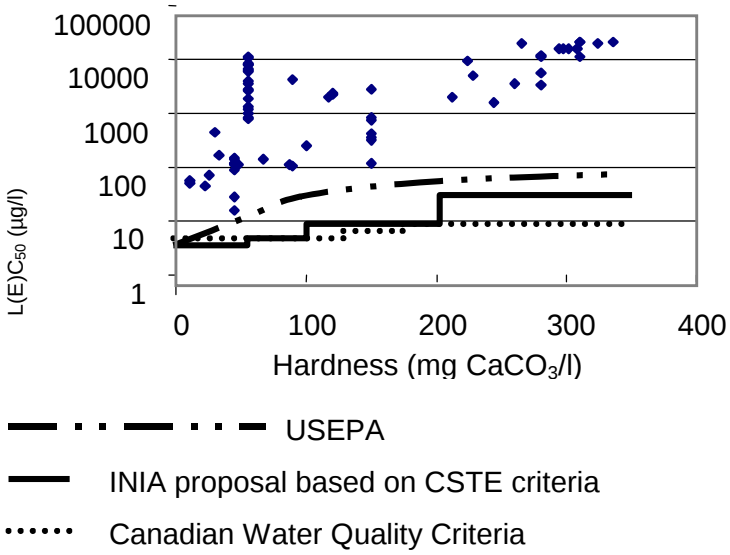


Figure 4.5: Acute copper toxicity to fish *versus* water hardness

[5] See section 8.5.3 for further information on the quality of correlations between water quality parameters and metal toxicity.

4.7 Finland

The text presented in this section was adapted from a letter received from the Finnish Environment Institute [46] and describes the procedures followed to derive quality standards in Finland.

At present quality standards referring to drinking water abstraction from the aquatic environment are set by ministerial order no. 461/2000 of the Ministry of Social Affairs and Health. These standards were taken directly from Council Directive 98/83/EEC, thus no specific methodology was applied.

In addition, there is a proposal for quality standards for disposal of dredged spoils in the marine environment. The standards derived for the polluted spoil are so called "Maximum Acceptable Risk Levels" (MAR) derived by the Dutch National Institute of Public Health and Environmental Protection (RIVM). The standards indicating levels of metals (Hg, Cd, Cr, Cu, Pb, Ni, Zn) in uncontaminated dredged material correspond to the coastal background levels. The standards indicating the levels of organic hazardous substances in uncontaminated dredge material are set to 1/100*MAR –value, except for PCDD/Fs where a newest mammalian TEF-value of WHO has been applied.

The measured concentrations of copper and lead have to be normalised with regard to clay and organic matter content before comparing to the quality standards. The measured values of organic substances have to be normalised with regard to organic matter content before comparing to the quality standards.

5 Utility of Elements Used in the EU Risk Assessment Frameworks for Quality Standard Setting

5.1 Risk Assessment for Existing Substances and New Notified Substances

The Council Regulation (EEC) No. 793/93 on the evaluation and control of existing substances [19] requires under Article 10 the real or potential risk for man and environment of priority substances to be assessed using principles which have been laid down in the Commission Regulation (EC) No. 1488/94 on risk assessment for existing substances [32].

Council Directive 67/548/EEC [16] (as amended by Directive 92/32/EEC [33]) on the approximation of the laws, regulations, administrative provisions relating to classification, packaging and labelling of dangerous substances requires the manufacturer or importer of a new substance, before placing it on the market, to notify it to the competent authority of the Member State in which it is manufactured ore into which it will be imported. Having received the notification, the competent authority is required to carry out an assessment of the risks of the substance to man and the environment in accordance with the principles set out in Commission Directive 93/67/EEC [34].

The principles for the above mentioned risk assessments are laid down in a Technical Guidance Document (TGD) [6]. Part II (chapter 3) of this document dealing with environmental risk assessment is currently under revision. Amongst other amendments and updates, the assessment of biocides is now included in the document and sections addressing exposure and effects assessment for the marine environment have been added. The latest available draft version of this revised TGD [38] has been used for drafting the following sub-sections of section 5.1. In this report, it is only referred to the sections of Part II of the revised TGD that are relevant with respect to the setting of Quality Standards in the context of the Water Framework Directive (i.e. the assessment of environmental effects in water bodies and sediment, secondary poisoning through food ingestion, and the calculation of predicted no effect concentrations).

5.1.1 General Outline

The function of the risk assessment for the aquatic environment is the overall protection of the aquatic environment. In essence, the procedure for the environmental risk assessment of a substance consists of comparing the concentration in the environmental compartments (predicted environmental concentration, PEC) with the concentration below which unacceptable effects on organisms will most likely not occur (predicted no effect concentration, PNEC). The risk assessment for food ingestion follows the same approach: From the predicted concentration in food (PEC_{oral}) a daily intake is calculated and compared with a $PNEC_{oral}$ for fish eating mammals or birds and the ADI or TDI (acceptable or tolerable daily intake) in the case of man, respectively.

Dependent of the PEC/PNEC ratio the decision whether a substance presents a risk is taken. Normally, it is assumed that there is no risk for the environmental compartment concerned if the ratio is <1. If the PEC/PNEC ratio is >1 it is recommended to analyse whether further testing/information may lead to a revision of the ratio before a final conclusion on the acceptability of the risk is reached. If it is not possible to conduct a quantitative risk assess-

ment, either because the PEC or PNEC or both cannot be derived, a qualitative evaluation is carried out of the likelihood that an adverse effect may occur.

5.1.2 Exposure Assessment

As outlined in section 2 (Environmental Exposure Assessment) of the revised chapter 3 of the TGD [38], the aquatic exposure assessment considers in principle all direct and indirect (e.g. via the atmosphere) emissions to water including sediment from all stages of the life cycle of a substance.

The predicted environmental concentration (PEC) of a substance is usually calculated for generic local (for point sources) or regional environments (point plus diffuse sources). These generic local or regional environments are no actual sites, but hypothetical sites with predefined agreed environmental characteristics, so-called "standard environments", representing European average environmental conditions or reasonable worst-case values, depending on the parameter in question. Reliable and representative monitoring data may also be used for the exposure assessment. However, the availability of adequate measured data does not imply that PEC calculations are unnecessary.

5.1.3 Calculation of the Predicted No Effect Concentration (PNEC)

This section is based on section 3.3.1 of the revised chapter 3 of the TGD [38].

A PNEC is regarded as a concentration below which an unacceptable effect will most likely not occur. Two assumptions are made concerning the aquatic environment which allow to extrapolate from single-species toxicity data to ecosystem effects:

- ecosystem sensitivity depends on the most sensitive species
- protecting ecosystem structure protects community function

Consequences of these two assumptions are that by identifying the species most sensitive to the toxic effects of a chemical in the laboratory, extrapolation can subsequently be based on the data from that species. Furthermore, the functioning of the ecosystem in which that species exists can be considered as protected since it is generally accepted that protection of the most sensitive species should protect structure, and hence function.

Two approaches, the assessment factor method or a suitable statistical extrapolation method, may be used to calculate the PNEC, depending on the quantity and quality of available effects data.

5.1.3.1 PNEC Calculation Using Assessment Factors

For most substances, the data available to predict ecosystem effects are very limited and it is, therefore, required to use empirically derived assessment factors. The intention of the application of such factors is to predict a concentration below which an unacceptable effect will most likely not occur. The assessment factors reflect the degree of uncertainty in extrapolation from laboratory toxicity test data for a limited number of species to the "real" environment, arising e.g. from intra- and inter-laboratory variation of toxicity data, intra- and inter-species biological variance, short-term to long-term toxicity extrapolation, and laboratory data to field impact extrapolation.

The size of the assessment factor depends on the confidence with which a PNEC can be derived from the available data. This confidence increases if data are available on the toxic-

ity to organisms at a number of trophic levels, taxonomic groups and with lifestyles representing various feeding strategies. Thus lower assessment factors can be used with larger and more relevant data-sets (table 5.1).

Table 5.1: Assessment factors to derive a PNEC (adaptation from table 16 of [38])

Data set	**Assessment factor**
At least one short-term $L(E)C_{50}$ from each of three trophic levels of the base set (fish, Daphnia, algae)	1000[(a)]
One long-term NOEC (either fish or Daphnia)	100[(b)]
Two long-term NOECs from species representing two trophic levels (fish and/or Daphnia and/or algae)	50[(c)]
Long-term NOECs from at least three species (normally fish, Daphnia and algae) representing three trophic levels	10[(d)]
Species sensitivity distribution (SSD) method	5-1 to be fully justified case by case[(e)]
Field data or model ecosystems	Reviewed on a case by case basis[(f)]

Notes:

(a) The assessment factor 1000 is a conservative and protective factor. For a given substance there may be evidence that the factor 1000 is to high or to low. In these circumstances it may be necessary to vary this factor, leading to a raised or lowered assessment factor depending on the available evidence. However, variation from a factor of 1000 should not be regarded as normal and should be fully supported by accompanying evidence. Except for substances with intermittent releases under no circumstances should a factor lower than 100 be used in deriving a PNEC from short-term toxicity data.

(b) AF 100 applies to a single long-term NOEC (fish or daphnia) if this NOEC was generated for the trophic level showing the lowest short-term L(E)C50. If the available NOEC is from a species which does not have the lowest L(E)C50, it cannot be regarded as protective of the other more sensitive species. Therefore the effects assessment is based on the short-term data with an AF of 1000. However, the resulting PNEC based on short-term data may not be higher than the PNEC based on the available NOEC.

AF 100 applies also to the lowest of 2 NOECs covering different trophic levels when such NOECs have not been generated from that showing the lowest L(E)C50. This should however not apply in cases where the acutely most sensitive species has an $L(E)C_{50}$ value lower than the lowest NOEC value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest $L(E)C_{50}$ of the short-term tests.

(c) AF 50 applies to the lowest of 2 NOECs covering different trophic levels when such NOECs have been generated covering that level showing the lowest L(E)C50.

AF 50 applies also to the lowest of 3 NOECs covering different trophic levels when such NOECs have not been generated from that level showing the lowest L(E)C50. This should however not apply in cases where the acutely most sensitive species has an $L(E)C_{50}$ value lower than the lowest NOEC value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest $L(E)C_{50}$ of the short-term tests.

(d) AF 10 will normally only be applied when long-term toxicity NOECs are available from at least 3 species across 3 trophic levels. A factor of 10 cannot be decreased on the basis of laboratory studies.

It may sometimes be possible to determine with high probability that the most sensitive species has been examined, i.e. that a further long-term NOEC from a different taxonomic group would not be lower than the data already available (particularly important if the substance does not have a potential to bioaccumulate). In those circumstances, a factor of 10 applied to the lowest NOEC from only two species would also be appropriate. If it is not possible to make this judgement, then an AF of 50 should be applied.

(e) Basic considerations and minimum requirements as outlined in section 3.3.1.2 (of [38],.see also section 5.3.1.2 of this report)

(f) The AF to be used on mesocosm studies or (semi) field data will need to be reviewed on a case by case basis.

Assessment factors applied for long-term tests are small as the uncertainty of the extrapolation from laboratory data to the natural environment is reduced. For this reason long-term data are preferred to short-term data. However, since aquatic organisms are exposed for a short period to compounds with an intermittent release pattern short-term L(E)C50 values are used to derive a PNEC for these compounds.

5.1.3.2 PNEC Calculation Using Statistical Extrapolation Methods

According to section 3.3.1.2 of the draft revised chapter 3 of the TGD [38] the effects assessment performed with the assessment factor method can be supported by a suitable statistical extrapolation method if the data basis on Species Sensitivity Distributions (SSDs) is sufficient for its application. The main underlying assumptions of the statistical extrapolation methods are:

- The distribution of species sensitivities follows a theoretical distribution function;
- The group of species tested in the laboratory is a random sample of this distribution.

In general, the method works as described in section 4.3.1.1 of this report: Long-term toxicity data are log transformed and fitted according the distribution function and a prescribed percentile of that distribution is used as cut-off criterion (see figure 4.1 for illustration).

In the framework of the EU Existing Substances programme a workshop on the use of statistical extrapolation for the derivation of PNEC values in case of data-rich substances was held in January 2001 in London [39]. Objective of this Workshop was to discuss how statistical extrapolation techniques might be used in the risk assessment process for the environment. In particular, the primary emphasis was on how they might be used to derive PNECs in the assessments of metals and their compounds currently being carried out under the Existing Substances Risk Assessment Programme. The outcome of the workshop formed the basis for a further discussion on the more general application of extrapolation methods based on species sensitivity distributions (SSDs) in the context of the TGD revision.

The workshop recommended to include statistical extrapolation in the derivation of PNEC values, provided two basic conditions are fulfilled:

1. The methods should be applied on chronic/long-term data.
2. NOEC values below the 5^{th} percentile of the SSD need to be discussed in the risk assessment report. For example, if all such NOECs are from one trophic level, then this could be an indication that a particular sensitive group exists, implying that some of the underlying assumptions for applying the statistical extrapolation method may not be met.

Several motivations for introducing the usage of SSDs into the PNEC derivation were expressed by the delegates to the workshop, e.g.:

- The method helps to reduce the uncertainties in the PNEC estimation; it is therefore an integral part of the uncertainty management of the effects assessment.
- The SSD approach makes use of all the available data when deriving a PNEC.
- The PNEC value based on the statistical extrapolation method produces a higher PNEC than that derived using the ”standard” TGD approach, with both approaches relying on empirical evidence for their validity.
- The SSD approach does not ‘punish’ substances with larger databases.

The approach of statistical extrapolation is still under debate and needs further validation [38]. Among the most common drawbacks, the reasons put forward are: the lack of transparency by using this method compared to the standard approach, the question of representativeness of the selected test species, the comparability of different endpoints, the arbitrary choice of a specific percentile and a statistical confidence level etc.

The major recommendations made at the workshop [39] and included in the draft revised TGD [38] are the following:

- **General requirements for input data** (chronic NOEC values, preferably of full life-cycle or multi-generation studies): at least 10 values and preferably more than 15 values, for different species covering at least 8 taxonomic groups (as given in table 8.3 of this report for the pelagic community in freshwater).

  As internationally standardised test guidelines for long-term tests are not yet available for some of the taxa mentioned in table 8.3, the applicability of existing test data and the fulfilment of the above requirements need to be assessed on a case-by-case basis. There is a need to evaluate additional information in order to assess how relevant and representative the list of taxonomic groups is to the risk assessment scenario being investigated.

  The acute toxicity database of the substance can be used to assist in evaluating the representativeness and the sensitivity of particular species. It can also identify acutely sensitive species which may be missing from the NOEC database. It should not be used directly in the determination of the PNEC value. [39]

  It is important to consider any available knowledge on the mode of action of the chemical, in order to evaluate the need to include possible other (sensitive) taxonomic groups or exclude possible over-representation of certain taxonomic groups.

  A similar approach can be considered for the sediment compartment, the soil compartment and the marine environment (no specific proposals are given).

- **Multiple data for one species:** For comparable data on the same toxicological endpoint for a particular species, the geometric mean value should be used as input. In case the toxicity is highly dependent on environmental parameters, then in addition the full data set could be used or several calculations could be performed on the basis of grouped data, for example for different pH ranges.

- **Distribution function:** the log-normal distribution is considered a pragmatic choice because of its mathematical properties (methods exist that allow for most in-depth analysis of various uncertainties; methods mentioned: Wagner & Løkke (1991) and Aldenberg & Jaworska (2000)). However, different distributions like e.g. log-logistic or others may be used, if suitable.

  If the data do not fit any distribution, the left tail of the distribution (the lowest effect concentrations) should be analysed more carefully. If a subgroup of species can be identified as particularly sensitive and if the number of data on this subgroup is sufficient, the distribution can be fit to this subgroup. In case of lack of fit, the SSD method should not be used.

- **Level of protection and calculation of the PNEC:** The use of the 5th percentile value[6] of the SSD is recommended as intermediate value in the determination of the PNEC. A 50% confidence interval (c.i.) associated with this concentration should also be derived.

  The PNEC is calculated as:

$$PNEC = \frac{\text{5-percentile SSD (50\% c.i.)}}{AF}$$

  AF is an appropriate assessment factor, reflecting the further uncertainties identified. AF should be between 5 and 1, to be judged on a case by case basis (criteria to determine AF: e.g. quality of the database and the end-points covered; diversity and representativeness of the taxonomic groups; statistical uncertainties around the 5th percentile estimate; outcome of comparisons between field and mesocosm studies and the 5th percentile in order to evaluate the laboratory to field extrapolation).

  A full justification should be given for the method used to determine the PNEC

- **Further recommendations:** The deterministic PNEC should be derived applying the "standard" Assessment Factor Approach on the same database. If mesocosm studies are available, they should also be evaluated and a PNEC derived following the TGD according to the standard method (deterministic approach). The various estimates of PNEC should be compared and discussed and the final choice of a PNEC be based on this comparison.

5.1.3.3 PNEC Calculation for Sediment (section 3.5 of [38])

For most chemicals the number of toxicity data on sediment organisms is limited. Therefore, the equilibrium partitioning method is recommended as a screening approach to compensate for this lack of toxicity data. Results from this screening can be used as a trigger for determining whether whole-sediment tests with benthic organisms should be conducted.

If results from whole-sediment tests with benthic organisms are available the $PNEC_{sed}$ has to be derived from these tests using assessment factors.

Statistical extrapolation methods for calculation of PNEC for sediment organisms could be used when sufficient data are available (cf. 3.3.1.2. of [38]). Further guidance needs to be developed in future.

Calculation of $PNEC_{sediment}$ Using the Equilibrium Partitioning Approach

As toxicity data for benthic organisms are normally lacking for many substances, the $PNEC_{sediment}$ may be calculated using the equilibrium partitioning method. This method uses the $PNEC_{water}$ for aquatic organisms and the suspended particulate matter / water partitioning coefficient ($Kp_{SPM\text{-}water}$). It is assumed that sediment dwelling organisms and water column organisms are equally sensitive to the substance concerned.

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[6] Note that in many cases and reports the result of the statistical extrapolation method is referred to as the Hazardous Concentration for x percent of the species (HCx). It was felt by the participants of the workshop that the use of this terminology should be avoided since it can be and has been misinterpreted as if 5% of the species will be sacrificed with each substance that is brought onto the market. Therefore the term HC5 is avoided in the report of the "London Workshop" and replaced by the 5th percentile value which is the statistical cut-off value of the species sensitivity distribution (SSD) [39].

$$PNEC_{sed}\ [mg.kg^{-1}] = \frac{Kp_{SPM\text{-}water}\ [l.l^{-1}]}{bulk\ density_{SPM}\ [kg.l^{-1}]} * PNEC_{water}\ [mg.l^{-1}]$$

The formula only considers uptake via the water phase. However, uptake may also occur via ingestion of sediment. This may become important for chemicals with a log Pow > 3. Thus, for these compounds the total uptake may be underestimated. However, evidence exists that the additional uptake via sediment ingestion remains low for chemicals with a log Pow up to 5. For compounds with a log Pow > 5 it is recommended to correct the equilibrium partitioning method for uptake via sediment ingestion by increasing the $PEC_{sediment}$ by a factor of 10. It should be borne in mind that this approach is considered only as a screening to assess the level of risk to sediment dwelling organisms.

Calculation of $PNEC_{sediment}$ Using Assessment Factors

If valid results from whole-sediment tests with benthic organisms are available (cf. section 3.5.4 of [38]) the $PNEC_{sed}$ has to be derived from these tests using assessment factors. Results from long-term tests with sub-lethal endpoints such as reproduction, growth, emergence, sediment avoidance and burrowing activity are regarded as most relevant due to the generally long-term exposure of benthic organisms to sediment-bound substances. Consequently, if results from short-term tests with sediment-dwelling organisms are only available (at least one) an assessment factor of 1000 is applied to the lowest value. In addition, the $PNEC_{sed}$ should also be calculated from the $PNEC_{water}$ using the equilibrium-partitioning method. A reduction in the size of the assessment factor should only be accepted if results form long-term tests with sediment-dwelling organisms are available.

The $PNEC_{sediment}$ is derived from the lowest available NOEC/EC_{10} obtained in long-term tests by application of the assessment factors given in table 5.2.

Table 5.2: Assessment factors to derive a $PNEC_{sediment}$ (table 19 of [38])

Available test result	**Assessment factor**
One long-term test (NOEC or EC10)	100
Two long-term tests (NOEC or EC10) with species representing different living and feeding conditions	50
Three long-term tests (NOEC or EC10) with species representing different living and feeding conditions	10

5.1.3.4 PNEC Calculation for Substances with Intermittent Release (section 3.3.2 of [38])

For substances subject to intermittent release (i.e. infrequent release only recurring less than once per month and for no more than 24 hours) exposure may be of only short duration. At least for dynamic systems like rivers the likelihood of long-term effects arising from such exposure is low. In extrapolating to a PNEC, therefore, generally only short-term effects may need to be considered. Normally an assessment factor of 100 be applied to the lowest L(E)C50 of at least 3 short-term tests of three trophic levels is considered appropriate to derive a PNEC for such situations. For substances with a potential to bioaccumulate the low-

ered assessment factor of 100 may not always be justified. For substances with a known non-specific mode of action inter-species variations may be low and therefore a factor lower than 100 appropriate. In no case should a factor lower than 10 be applied to a short-term L(E)C50 value.

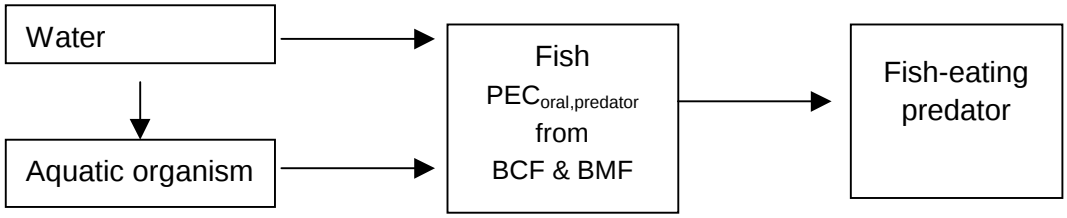
5.1.4 Secondary Poisoning of Top Predators Through Food Ingestion

Guidance related to the assessment of secondary poisoning is given in section 3.8.3 of [38].

Accumulation of hydrophobic chemicals through the food chains may result in toxic concentrations in predatory birds or mammals ingesting biota containing the chemical (≈secondary poisoning). The assessment of the potential of a substance for secondary poisoning is based on a comparison of the (predicted) concentration in the food of the top-predator (PEC_{oral} predatory bird/mammal) and the (predicted) no-effect concentration for oral intake ($PNEC_{oral}$) which is based on studies with laboratory animals. 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.

For substances with a log Kow < 4.5 the primary uptake route is direct uptake from the water phase. In the absence of data on other uptake routes, it is assumed that the direct uptake accounts for 100% of the intake. For substances with a log Kow ≥ 4.5, other uptake routes such as intake of contaminated food leading to secondary poisoning may become increasingly important.

On this basis, possible effects are estimated on birds and mammals in the environment via uptake through the food-chain water → aquatic organisms → fish → fish-eating mammal or fish-eating bird.



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.

5.1.4.1 Calculation of the Predicted Environmental Concentration in Food (PEC_{oral})

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

$$PEC_{oral,\ predator} = PEC_{water} * BCF_{prey\ (fish)} * BMF_{fish}$$

Note that $PEC_{oral,\ predator}$ could also be calculated for other relevant species that are part of the food of predators.

The BMF should ideally be based on measured data. However, the availability of such data is at present very limited and therefore, the default values given in table 5.3 are proposed in

[38] (proposal based on published data, see section 4.4.3 of [38] for details). When measured BCF values are available, these should form the basis for deciding on the size of the BMF.

Table 5.3: Default BMF values for organic substances (table 21 of [38])

log Kow of substance	BCF (fish)	BMF
<4.5	< 2000	1
4.5 - <5	2000-5000	3
5 – 8	> 5000	10
>8 – 9	2000-5000	3
>9	< 2000	1

5.1.4.2 Calculation of the Predicted No-Effect Concentration ($PNEC_{oral}$)

Only toxicity studies reporting on dietary and oral exposure are relevant as the pathway for secondary poisoning is referring exclusively to the uptake through the food chain. Secondary poisoning effects on bird and mammal populations rarely become manifest in short-term studies. Therefore, results from long-term studies are strongly preferred, such as NOECs for mortality, reproduction or growth.

As toxicity data for wildlife birds and mammals are normally not available, it will - in most instances - be necessary to extrapolate threshold levels for wildlife species from toxicity data of laboratory test species assuming that interspecies correlations exist.

The results of the relevant mammalian or avian tests may be expressed as concentration in food ($mg.kg_{food}^{-1}$) or as dose (mg.kg body weight.day^{-1}) causing no effect. For the assessment of secondary poisoning, the results always have to be expressed as the concentration in food. In case toxicity data are given as NOAEL only, these NOAELs can be converted to NOECs with the formulae given in section 3.8.3.5 of [38].

$$NOEC_{oral\_uptake} = NOAEL_{oral} * CONV$$

with:
CONV: conversion factor from NOAEL to NOEC (conversion factors for several mammalian species [ranging from 8.3 to 40] and one bird species [8] are given in table 22 of [38])

The $PNEC_{oral}$ is then derived from the toxicity data (food basis) applying an assessment factor.

$$PNEC_{oral} = TOX_{oral} / AF_{oral}$$

The AF_{oral} (table 5.4) takes into account interspecies variation, acute/subchronic to chronic extrapolation and laboratory data to field impact extrapolation. In addition, some specific considerations with regard to predators are considered (cf. section 3.8.3.5 of [38]).

If a NOEC for both birds and mammals is given, the lower of the resulting PNECs is used in the risk assessment.

When the BCF of a substance is known, the PEC_{water} can be used to calculate the PEC in food (PEC_{oral}). This concentration is compared with the $PNEC_{oral}$.

If the above described assessment is performed for fish as food source only, it has to be kept in mind that save levels for fish eating predators do not necessarily exclude risks for

predators feeding on other aquatic organisms (e.g. mussels or worms). Therefore it is emphasised in [38] that the proposed methodology gives only an indication that secondary poisoning is a critical process in the aquatic risk characterisation of a chemical. For a more detailed analysis of secondary poisoning, it may be required to take several further factors into account (cf. section 3.8.3.6 of [38]).

Table 5.4: Assessment factors for extrapolation of mammalian and bird toxicity data [38]

TOX_{oral}	Duration of test	AF_{oral}
$LC_{50\ bird}$	5 days	3000
$NOEC_{bird}$	chronic	30
$NOEC_{mammal,\ food,chr}$	28 days 90 days chronic	300 90 30

5.1.5 Risk Assessment for Metals

Guidance with respect to the environmental risk assessment for metals and metal compounds is given in Appendix VIII of the TGD [6] (this appendix has not been amended in the TGD revision):

As there are a number of fundamental differences between metals and organic chemicals, these must be taken into account when assessing the risks:

- Metals are a class of substances of natural origin. Consequently natural background concentrations and the exposure due to these background concentrations should be taken into account. Natural background concentrations may vary within the aquatic environment from site to site by several orders of magnitude. In certain regions clearly elevated natural background concentrations can be encountered. Also, due to natural dynamic processes like weathering, natural background concentrations may change over time. Therefore, it is evident that it is impossible to attribute single values to natural background concentrations of specific metals within a certain compartment.
- Metals are taken up by organisms. For essential metals, biota will keep their intracellular levels relatively constant within a certain range of varying external concentrations, in order to satisfy their need requirements for the essential element. This may lead to high BCF values if concentrations in the environment (or BCF studies) are very low.
- The availability of metals for uptake by organism under field conditions is limited, will vary from site to site and is highly dependent on the speciation of the metals and environmental conditions such as e.g. pH, alkalinity, hardness, and presence of complexing agents. Hence it is of utmost importance that both PEC and PNEC are based on similar levels of availability in both exposure and effect assessment.
- Calculated PNECs for essential metals should not be lower than natural background concentrations.

The risk assessment for metals is currently discussed and further developed in the course of the ongoing risk assessments for zinc [40], cadmium [41] and their compounds, respectively.

As for both metals many toxicity data for a range of aquatic species are available, the use of statistical extrapolation is recommended by the authors of the draft risk assessment reports.

For both metals the PNEC for the aquatic compartment is calculated with statistical extrapolation methods using the species sensitivity distribution to derive a PNEC (see section 5.1.3.2 of this report for further details). Furthermore, the PNECs derived refer to the dissolved fraction of the metals and may therefore only be compared to monitoring data referring to the dissolved fraction.

As regards the consideration of environmental parameters such as e.g. water hardness, pH and dissolved organic carbon which may influence metal toxicity, it is concluded in the draft zinc risk assessment that – for the time being - there is a too poor, inconsistent and partially contradicting data base to derive PNEC values dependent on these parameters. Also, in the draft risk assessment for cadmium oxide such parameters are not considered for the derivation of the generic $PNEC_{water}$. However, for the relationship between water hardness and long cadmium toxicity a regression equation could be established, indicating that dissolved Cd is more toxic at lower water hardness. The authors of the draft risk assessment report consider a correction of the PNEC for water hardness as useful for local risk characterisation.

Natural background concentrations have been accounted for in the draft zinc risk assessment by implementation of the "added risk approach" as described in sections 4.3.1.3 and 8.6.1 of this report.

5.1.6 Risk Assessment for the Marine Environment

In the current TGD on risk assessment for existing substances and new notified substances [6], the risk assessment for the aquatic environment basically deals with freshwater systems only. However, in the TDG revision process, a rationale for marine risk assessment is has been elaborated (section 4 of [38]).

PEC estimations are be based on generic local and regional marine standard environments. However, for substances with PTB-properties (persistent, liable to bioaccumulate and toxic) which are likely to be transported to the open sea PEC estimates and risk characterisation based on the PEC/PNEC ratio will not be performed as this approach is not deemed appropriate to protect open sea ecosystems. For PTB-substances likely to reach the open sea the further evaluation in the risk assessment process will focus primarily on identifying sources, major emissions and pathways to the marine environment in order to establish the most appropriate and effective measures to reduce the releases which lead to contamination of the marine environment.

Impact assessment of substances entering estuarine and marine waters should ideally be based upon data generated using relevant saltwater species. However, usually there are no or only few data on the efffects of a particular chemical on estuarine or marine organisms available. Therefore it may be necessary to use freshwater data instead of data for estuarine or marine species.

As data reviewed and current marine risk assessment practice suggest, a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota exists - at least for the usual taxa (i.e. fish, crustacea, algae). Where differences in the apparent sensitivity of freshwater and marine biota were observed for individual compounds, such differences were consistently within a factor of 10 and usually somewhat less (<1 log unit). Average differences in sensitivity for such paired species comparisons were typically within a factor of 2. Thus, the use of freshwater effects data instead of or in addition to saltwater effects data is not contra-indicated by the empirical data and the use of pooled data is therefore recom-

mended. PNEC values should be derived from the most sensitive endpoint regardless of medium.

However, for several metals and plant protection products differences larger than a factor of 10 were shown indicating that for these substances fresh water and saltwater data should not be pooled for effects assessment and PNEC calculation.

5.1.6.1 Aquatic Effects Assessment – Derivation of $PNEC_{saltwater}$

For the aquatic effects assessment and the PNEC calculation the assessment factor method is proposed, but with modified assessment factors, accounting for additional uncertainty due to peculiarities of the marine ecosystem such as, e.g., greater species diversity or limited data availability for marine species and use of freshwater toxicity data as surrogate (table 5.5).

Statistical extrapolation methods for calculation of PNEC for marine organisms could be used when sufficient data are available (cf. to section 5.1.3.2 of this report).

Table 5.5: Assessment factors proposed for use to derive $PNEC_{water}$ for saltwater [38]

Data set	Assessment factor
Lowest short-term $L(E)C_{50}$ from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10000(a)
Lowest short-term $L(E)C_{50}$ from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels, + 2 additional marine taxonomic groups (e.g. echinoderms, molluscs)	1000
One long-term NOEC (from freshwater or saltwater crustacean reproduction or fish growth studies)	1000(b)
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish)	500(c)
Lowest long-term NOECs from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels	100(d)
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish) + 1 long-term NOEC from an additional marine taxonomic group (e.g., echinoderms, molluscs)	50
Lowest long-term NOECs from three freshwater or saltwater species (normally algae land/or crustaceans and/or fish) representing three trophic levels + 2 long-term NOECs from additional marine taxonomic groups (e.g., echinoderms, molluscs)	10

NOTES

General: Evidence for varying the assessment factor should in general include a consideration of the availability of data from a wider selection of species covering additional feeding strategies/ life forms/ taxonomic groups other than those represented by the algal, crustacean and fish species (such as echinoderms or molluscs). This is especially the case, where data are available for additional taxonomic groups representative of marine species. When substantiated evidence exists that the substances may be disrupting the endocrine system of species, it should be considered whether the assessment factor would also be sufficient to protect against effects caused by such a mode of action.

(a) The use of a factor of 10000 on short-term toxicity data is a conservative and protective factor and is designed to ensure that substances with the potential to cause adverse effects are identified in the effects assessment. It assumes that each of the identified uncertainties described above makes a significant contribution to the overall uncertainty.

For any given substance there may be evidence that this is not so, or that one particular component of the uncertainty is more important than any other. In these circumstances it may be necessary to vary this factor. This variation may lead to a raised or lowered assessment factor depending on the evidence available. Except for substances with intermittent release, under no circumstances should a factor lower than 1000 be used in deriving a $PNEC_{water}$ for saltwaters from short-term toxicity data.

Evidence for varying the assessment factor could include one or more of the following:

- Evidence from structurally similar compounds which may demonstrate that a higher or lower factor may be appropriate;
- Knowledge of the mode of action as some substances by virtue of their structure, may be known to act in a non-specific manner. A lower factor may therefore be considered. Equally a known specific mode of action may lead to a raised factor.
- The availability of data from a variety of species covering the taxonomic groups of the base set species across at least three trophic levels. In such a case the assessment factors may only be lowered if multiple data points are available for the most sensitive taxonomic group (i.e. the group showing acute toxicity more than 10 times lower than for the other groups).

There are cases where there will not be a complete short-term data set even for freshwater algae, crustacean and fish species, for example for substances which are produced at < 1 t/a (notifications according to Annex VII B of Directive 92/32/EEC). In these situations, the only data may be short-term $L(E)C_{50}$ data for *Daphnia*. In these exceptional cases, the PNEC should be calculated with a factor of 10000.

(continued overleaf)

Table 5.5: (continued) Assessment factors proposed for use to derive $PNEC_{water}$ for the marine environment

(b) An assessment factor of 1000 applies where data from a wider selection of species are available covering additional taxonomic groups (such as echinoderms or molluscs) other than those represented by algal, crustacean and fish species; if at least data are available for two additional taxonomic groups representative of marine species

An assessment factor of 1000 applies to a single long-term NOEC (freshwater or saltwater crustacean or fish) if this NOEC was generated for the taxonomic group showing the lowest $L(E)C_{50}$ in the short-term algae, crustacean or fish tests.

If the only available long-term NOEC is from a species which does not have the lowest $L(E)C_{50}$ in the short-term tests, it cannot be regarded as protective of other more sensitive species using the assessment factors available. Thus, the effects assessment is based on the short-term data with an assessment factor of 10000. However, normally the lowest PNEC should prevail.

An assessment factor of 1000 applies also to the lowest of the two long-term NOECs covering two trophic levels (freshwater or saltwater algae and/or crustacean and/or fish) when such NOECs have not been generated from that showing the lowest $L(E)C_{50}$ of the short-term tests. This should not apply in cases where the acutely most sensitive species has an $L(E)C_{50}$-value lower than the lowest NOEC value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest $L(E)C_{50}$ of the short-term tests.

(c) An assessment factor of 500 applies to the lowest of two NOECs covering two trophic levels (freshwater or saltwater algae and/or crustacean and/or fish) when such NOECs have been generated covering those trophic levels showing the lowest $L(E)C_{50}$ in the short-term tests with these species. Consideration can be given to lowering this factor in the following circumstances.

It may sometimes be possible to determine with a high probability that the most sensitive species covering fish, crustacea and algae has been examined, that is that a further longer-term NOEC from third taxonomic group would not be lower than the data already available. In such circumstances an assessment factor of 100 would be justified,

A reduced assessment factor (to 100 if only one short-term test, to 50 if two short-term tests on marine species are available) applied to the lowest NOEC from only two species may be appropriate where:

- short-term tests for additional species representing marine taxonomic groups (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and;
- it has been determined with a high probability that long-term NOECs generated for these marine groups would not be lower than that already obtained. This is particularly important if the substance does not have the potential to bioaccumulate.

An assessment factor of 500 also applies to the lowest of three NOECs covering three trophic levels, when such NOECs have not been generated from the taxonomic group showing the lowest $L(E)C_{50}$ in short-term tests. This should, however, not apply in the case where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest $L(E)C_{50}$ in the short-term tests.

(d) An assessment factor of 100 will be applied when longer-term toxicity NOECs are available from three freshwater or saltwater species (algae, crustaceans and fish) across three trophic levels.

The assessment factor may be reduced to a minimum of 10 in the following situations:

- where short-term tests for additional taxonomic groups representing marine species (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and it has been determined with a high probability that long-term NOECs generated for these species would not be lower than that already obtained.
- where short-term tests for additional taxonomic groups (for example echinoderms or molluscs) have indicated that one of these is the most sensitive group and a longer-term NOEC test has been carried out for that species. This will only apply when it has been determined with a high probability that additional NOECs generated from other taxa will not be lower than the NOECs already available.

A factor of 10 cannot be decreased on the basis of laboratory studies only.

5.1.6.2 Effects assessment for marine sediment organisms

With respect to the effects assessment of marine benthic organisms, in principle the same strategy as for freshwater sediment is recommended.

Four situations can be distinguished for deriving a PNEC $_{marine\ sediment}$:

1. If only acute tests with benthic freshwater organisms are available (at least one) the risk assessment is performed both on basis of this test (assessment factor 10000, see table 5.5) and on the basis of the equilibrium partitioning method (see section 5.1.3.3 of this report). The lowest PNEC $_{marine\ sediment}$ is then used for the risk characterisation.
2. If additionally to the tests with freshwater benthic organisms an acute toxicity test is performed with a marine benthic organism, preferentially performed with an organism of the same taxa that seems to be the most sensitive in aquatic assessment, a lower assessment factor can be used test (AF 1000, see table 5.6). Also in this situation a comparison with the results obtained by application of the equilibrium partitioning method has to be made, and the lowest PNEC$_{marine\ sediment}$ is used for the risk characterisation.
3. If long-term toxicity data are available for benthic freshwater organisms the PNEC$_{marine\ sediment}$ is calculated using assessment factors for long-term tests. (AFs see table 5.7.)
4. If long-term toxicity data are available for benthic freshwater *and* a minimum of two marine organisms, and a minimum of two marine data are available, PNEC $_{marine\ sediment}$ is calculated using lower assessment factors for long-term tests (AFs see table 5.7). A PNEC$_{marine_sediment}$ obtained from such data is preferred in the risk assessment.

Table 5.6: Assessment factors for derivation of the PNEC $_{marine\ sediment}$ based on the lowest available LC_{50} from acute tests [38]

Available test results	**Assessment factor**	**PNEC**
One acute freshwater or marine test	10000	lowest of LC_{50} /10000 and equilibrium-partitioning method
Two acute test including a minimum of one marine test with an organism of a sensitive taxa	1000	lowest of LC_{50} /1000 and equilibrium-partitioning method

Table 5.7: Assessment factors for derivation of the PNEC $_{marine\ sediment}$ based on the lowest available NOEC/EC_{10} from long-term tests [38]

Available test results	**Assessment factor** [a)]
One long-term freshwater sediment test	1000
Two long-term freshwater sediment tests with species representing different living and feeding conditions	500
One long-term freshwater and one saltwater sediment test representing different living and feeding conditions	100
Three long-term sediment tests with species representing different living and feeding conditions	50
Three long-term tests with species representing different living and feeding conditions including a minimum of two tests with marine species	10

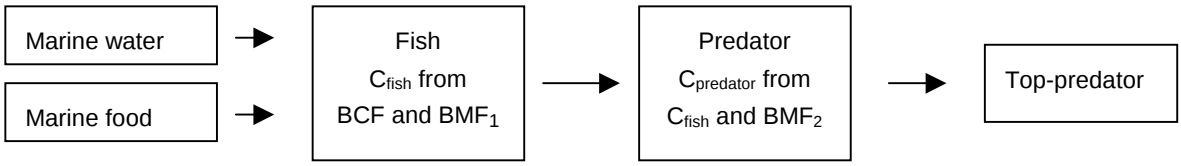
[a)] The general principles of notes (c) and (d) as applied to data on aquatic organisms (table 5.4) shall also apply to sediment data. Additionally, where there is convincing evidence that the sensitivity of marine organisms is adequately covered by that available from freshwater species, the assessment factors used for freshwater sediment data may be applied. Such evidence may include data from long-term testing of freshwater and marine aquatic organisms, and must include data on specific marine taxa.

5.1.6.3 Secondary Poisoning of top predators in the marine environment

The following explanation of the approach is based on section 4.4.3 of the revised TGD [38].

The proposed risk assessment strategy for secondary poisoning of marine top predators by food ingestion is in principle based on the same methodology as followed for the freshwater environment. Thus, a $PNEC_{oral}$ for top predators is derived as described in section 5.1.4 of this report and compared to the corresponding PEC_{oral} (i.e. the concentration in the food of the top predator).

However, accounting for the longer food chains in the marine environment, it is suggested to consider for substances[7] with log Kow >5 and <9 not only bioconcentration (uptake from water) but also biomagnification (uptake from ingestion of food) in the prey of predators (e.g. fish) and top predators (i.e. predators). Thus the calculation of the PEC of a chemical in the food of predators and top predators is performed as follows:



$PEC_{oral,\ predator} = PEC_{seawater} * BCF_{prey\ (fish)} * BMF1_{\ prey\ (fish)}$ (≈ concentration in fish)

$PEC_{oral,\ top\ predator} = PEC_{oral,\ predator} * BMF2_{\ prey\ (predator)} = PEC_{water} * BCF_{fish} * BMF1_{fish} * BMF2_{predator}$
(≈ concentration in predator)

1. *Risks to marine fish:* No specific calculation needs to be performed for estimating the risk to marine fish as this is covered by the risk assessment for aquatic organisms.
2. *Risks to marine predators:* The risk to marine predators is calculated as the ratio between the concentration in their food (marine fish) and the no-effect concentration for oral intake ($PNEC_{oral,\ predator}$). The concentration in the marine fish (C_{fish}) is obtained from bioconcentration of the substance from the aqueous phase and (for very hydrophobic substances) as a result of bioaccumulation from the food the fish. Therefore, both a bioconcentration factor (BCF) and a biomagnification factor (BMF_1) are used to calculate C_{fish}. Note that for the BCF_{fish} also information for other organisms such as mussels may be considered.
3. *Risks to marine top-predators:* The risk to marine top-predators is calculated as the ratio between the concentration in their food (marine predators) and the no-effect concentration for oral intake ($PNEC_{oral,\ top\text{-}predator}$). Since very hydrophobic substances may biomagnify in the tissue and organs of the predator, for the calculation of the internal concentration of the predator an additional biomagnification factor (BMF_2) must be applied. Note that no additional BMF factor for the top-predator itself is required since the comparison between PEC_{oral} and $PNEC_{oral}$ is not based on internal concentrations but on intake rates.

[7] Except metal ions, hydrolytically unstable substances and large molecules, as for these compounds the Kow does not represent a suitable indicator for estimating bioconcentration.

Ideally, the biomagnification factors used should be based on measured values. However, as measured BMF data may not be available in many instances, default values for BMF1 and BMF2 are proposed based on published data (table 5.8, see section 4.4.3 of [38] for details). If a BCF for fish is available, that should be used as a trigger instead of log Kow. The BCF triggers recommended are less conservative than the log Kow triggers because they more realistically take the potential for metabolism in biota (i.e. fish) into account.

Table 5.8: Default BMF values for organic substances with different log K_{ow} or BCF in fish [38]

log K_{ow} of substance	**BCF (fish)**	**BMF_1**	**BMF_2**
< 4.5	< 2000	1	1
4.5 - < 5	2000-5000	2	2
5 – 8	> 5000	10	10
> 8 - 9	2000 – 5000	3	3
> 9	< 2000	1	1

5.2 Risk Assessment for Plant Protection Products

Plant protection products (PPP) are preparations that contain one or more active substances intended to protect agricultural plants against harmful organisms (e.g. fungicides, insecticides) or against the competition of undesired plants (herbicides) or to influence life processes of plants (growth regulators). Due to the use pattern of PPP (application in open agricultural systems) and the inherent properties of their active substances capable of interfering with biological systems they may have the potential - beside the intended effects - to adversely affect human health, non-target organisms or the environment. These potential hazards may arise from the active substances or (and) metabolites and breakdown products thereof. Direct or indirect exposure of the environment as well as man may occur via various exposure routes, e.g. by pesticide vapour, spraydrift during application, run-off from treated areas after storm events (into adjacent surface waters or terrestrial non-target areas), leaching to groundwater, and residues in food or drinking-water.

Because of the given hazard potential and in order to ensure a high level of protection of human and animal health and the environment, PPP and active ingredients have to be authorized prior to marketing and use in the EU and its Member States. The placing on the market of plant protection products is regulated by Council Directive 91/414/EEC [15] and several successive amendments to it.

The authorization procedure comprises a tiered risk assessment taking account of the risks posed by a pesticide to man, non-target animals, aquatic ecosystems, soil function, and groundwater. The detailed evaluation and decision making criteria are laid down in Annex VI to the Directive, the so called “Uniform Principles Directive”, which is established by Council Directive 97/57/EC [8]. Further guidance regarding the assessment of aquatic ecotoxicology in the frame of Directive 91/414/EEC is given in a working document elaborated by the Commission Services in co-operation with the Member States [35]. Here, only the elements of the risk assessment according to Directive 91/414/EEC that are relevant with respect to the

derivation of quality standards in the context of the Water Framework Directive are referred to.[8]

5.2.1 Risk Assessment for the Aquatic Environment

The risk assessment for the aquatic environment is based on an exposure assessment resulting in predicted environmental concentrations (PEC) which are compared with the results of toxicity tests of a range of aquatic organisms of different taxonomic groups and trophic levels (fish, daphnia, algae). The toxicity exposure ratios (TER) resulting from the division of the respective toxicity test results by the calculated short-term or long-term PECs should not fall below any of the triggers given in table 5.9 in order to permit the authorization of a PPP, unless it can be clearly established that under field conditions no unacceptable impact on the viability of the exposed species occurs. The TER trigger values are not intended as simple regulatory cut-off criteria but – at the initial stage of the risk assessment – should only be used as indicator that a refined risk assessment is necessary. Refined assessments should pay full attention to the specific details of the proposed use, utilise fate and behaviour data, assess bioavailability, consider all available toxicity data (e.g. results from microcosm or mesocosm studies), the potential for recovery to occur and the effects of risk mitigation measures such as the stipulation of buffer zones. Some mitigating factors may not numerically influence the TER values, in which case a more qualitative approach is necessary to fully take these factors into account when reaching regulatory conclusions. Overall, the lower the initial TER value, the greater the degree of risk mitigating factors which are required to render the risk acceptable. [35]

Table 5.9: Minimum **T**oxicity – **E**xposure **R**atios (quotient: toxicity test result / PEC) to be achieved according to the Uniform Principles Directive (97/57/EC) [8]

Species	short-term TER (based on L(E)C50s)	long-term TER (based on NOECs)
Fish	100	10
Daphnia	100	10
Algae	10	-

In order to explain the concept of the TER a brief summary on the ***exposure assessment*** is given as described in the Guidance Document on Aquatic Ecotoxicology in the frame of Directive 91/414/EEC [35]. The exposure assessment takes account of all relevant exposure routes of surface water (e.g. spray-drift, run-off, drainage), the proposed conditions of use of the PPP (agricultural plant species, mode and frequency of application(s), applied amount per application) and the physico-chemical properties of the active ingredient(s) governing their fate and partition in the environment. For the PEC calculation, a ditch of 1 m width and 0.3 m depth is defined as generic aquatic ecosystem, possible water flow is not taken into account (static water body). The distance between the ditch and the treated area is variable (range e.g. 1 – 50 m), in order to find a safe distance. The short-term PEC is calculated as initial concentration not taking into account fate and behaviour data. For the long-term PEC a time weighted average concentration (TWA) may be calculated, taking into account fate and

[8] Further working documents for guidance in the implementation of Council Directive 91/414/EEC and related issues with regard to pesticide safety (assessment) can be found under http://europa.eu.int/comm/food/fs/ph_ps/index_en.htm

behaviour data and the toxicity profile of the active substance(s) (e.g. the time to onset of effects in toxicity studies) as well as the implications of multiple applications on TWA PEC values and the potential for exposure to metabolites of the active ingredient(s).

For the ***aquatic effects assessment*** various short-term and longer term/chronic studies with the organisms given in table 5.9 are required. The types and sophistication level of studies which have to be presented is dependent on certain triggers and expert judgement [35].

For example, a long-term fish study is only required if the DT50 of the active substance or its relevant metabolite(s) in the water column is >2 days at the environmentally relevant pH range of 6-9. This study should have a 28 day exposure duration and include survival, growth and behaviour as endpoints. If the toxicity of the active ingredient is <0.1 mg/l (acute LC50), a fish early life stage test should be conducted. In special cases fish life cycle tests are required, e.g. where a substance is a known endocrine disrupter or where the BCF is >1000 and the elimination rate in the 14d depuration phase of the bioconcentration studies is <95% or the substance is stable in water or sediment (DT90 >100 days). The above mentioned chronic toxicity studies may be replaced by suitable microcosm or mesocosm studies, if those include suitable data on fish.

A long-term test with aquatic invertebrates (usually Daphnia, 21 day reproduction study) is required if the DT50 of the active substance or it s relevant metabolites in the water column is >2 days at an environmentally relevant pH in the range of 6-9. If there is evidence that the data for Daphnia are not representative for insects, a test with a species from this taxonomic group (e.g. Chironomids) should be required. Available toxicity data on other groups of aquatic invertebrates including Oligochaeta, Turbellaria or Rotifera may also be taken into account. The before mentioned chronic toxicity studies may be replaced by suitable microcosm or mesocosm studies.

For herbicides, two tests on algae species from different taxonomic groups are required. One species should belong to the green algae, the second species should be from another group such as diatoms or the blue-green algae. In addition to the algae studies, a test on aquatic plants has to be conducted (preferably with Lemna). The before mentioned chronic toxicity studies may be replaced by suitable microcosm or mesocosm studies.

A test on *sediment-dwelling organisms* should be required if, in a sediment water study, the distribution of applied radioactivity indicates significant partitioning to sediment and that this residue persists such that 10% or more of the total applied radioactivity is measured in the sediment after day 14 and the NOEC in the chronic Daphnia test (or in a comparable study with insects) is <0.1 mg/l. If there is clear evidence that the radioactivity in the sediment is related to a metabolite, the test should fully address the toxicity of that metabolite. In Annex II of Directive 91/414/EEC Chironomus sp. is specified as the test organism and survival and development (including emergence of adults) as endpoints. However, as risk assessment for sediment dwelling organisms is currently the subject of much discussion, flexibility is recommended in accepting data regarding toxicity to sediment dwelling organisms [35].

The ***potential for bioaccumulation*** of an active substance is addressed by a fish-bioconcentration study which is required for the substance concerned if log Pow >3, unless the substance is not stable in water and a significant long-term exposure due to multiple applications is not to be expected. An authorization for a PPP cannot be granted if the maximum bioconcentration factor (BCF) in predators is >1000 for active substances that are readily

biodegradable or >100 for those which are not readily biodegradable, unless it is clearly established through appropriate risk assessment that under field conditions no unacceptable impact of the viability of the exposed species occurs.

Further, ***secondary poisoning*** of birds or other non-target terrestrial vertebrates can be considered as addressed in Council Directive 91/414/EEC as, according to Annex VI (section 2.5.2.1), no authorization shall be granted if the bioconcentration factor[9] related to fat tissue of the before mentioned groups is >1.

5.2.2 Exposure assessment for groundwater

According to Annex VI, section 2.5.1.2 of Council Directive 91/414/EEC the authorization of a PPP cannot be granted if the concentration in *groundwater* is expected to exceed the lowest of the limit values set in Council Directive 98/83/EC related to the quality of water intended for human consumption (i.e. 0.1 µg/l for an individual active substance), or the maximum concentration laid down by the Commission when including the active substance in Annex I, or, when that concentration has not been laid down, the concentration corresponding to one tenth of the acceptable daily intake (ADI) of the respective substance.

5.2.3 Human health aspects

With respect to the potential hazard arising from *residues of PPP in treated plants or plant products* the following assessment steps are foreseen [45] [10]:

Based on the residue levels in or on the agricultural crop established in supervised trials under the intended use conditions and in compliance with good agricultural practice, the daily residue intake for the European population, for national populations and sub-populations (e.g. children) under normal and worst case conditions is estimated using appropriate consumer intake models. For the calculation of the consumer intake the residue levels of all commodities on or in which the occurrence of the concerned residues is probable have to be taken into account (including food products of animal origin if exposure of the animals to residues by feed is possible) as well as all authorized uses of the active substance(s) in the PPP under evaluation and in any other authorized PPP and imports of residues on or in food and feed commodities.

In cases were the calculated intake is higher as the ADI (Acceptable Daily Intake, i.e. the highest dose in toxicological tests that would produce no adverse effects over a lifetime exposure, reduced by an appropriate safety factor) the use conditions have to be modified to reduce the residue level in the crop. If this is not possible the use of that PPP on that crop cannot be authorized.

5.3 Risk Assessment for Biocides

Biocidal products are active substances and preparations containing one or more active substances, put up in the form in which they are supplied to the user, intended to destroy,

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[9] Apparently, the term bioconcentration is not used in Annex VI, section 2.5.2.1 in the same way as in the TGD for existing substances. As bioaccumulation through the food chain is addressed, the term biomagnification is more appropriate.

[10] More documents on human health related issues in the context of pesticide residues on treated plants or plant products as well as information regarding the underlying legislation can be found under: http://europa.eu.int/comm/food/fs/ph_ps/pest/index_en.htm

deter, render harmless, prevent the action of, or otherwise exert a controlling effect on any harmful organism by chemical or biological means[20].

Provisions for risk assessment and authorisation of biocidal products are laid down in Council Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market[20].

According to the provisions laid down in the Directive 98/8/EC, it is necessary in the risk assessment of active biocidal substances to cover, where appropriate, the same aspects as those covered by Council Regulation (EEC) No 793/93 on the evaluation and control of the risks of existing substances[19]. Consequently, the approaches to effects assessment for biocides are addressed and included in the revised TGD [38]. In addition, it is stated in Council Directive 98/8/EC that close co-ordination should be ensured with Directive 91/414/EEC concerning the placing of plant protection products on the market [15].

Thus, no new or other aspects in the effects assessment methodology as those already described in the context of the risk assessment for new notified and existing substances and the risk assessment for plant protection products are provided for in the Directive concerning biocides authorisation. Differences mainly occur due to other exposure scenarios which must be taken into account for biocides.

5.4 Method for QS Derivation elaborated by the Scientific Advisory Committee on Toxicity and Ecotoxicity of Chemicals of the European Commission (CSTÉ[11])

In the context of Council Directive 76/464/EEC on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community [7] the Commission asked the CSTE with regard to the substances of List I of the Directive for proposals of appropriate water quality objectives (WQOs) meeting the requirements of the Directive.

The following gives an account of the working practices that evolved in the Scientific Advisory Committee during the years 1980-1993 with respect to the establishment of WQOs [9]:

As Article 6.2 of Directive 76/464/EEC provides that WQOs should be laid down principally on the basis of the toxicity, persistence, and accumulation of the substances in living organisms and in sediments (....), taking into account the differences in characteristics between salt water and fresh water, the WQOs for List I substances have been derived on the basis of the evaluation of intrinsic hazard properties of individual chemicals and by taking into account the so-called "zero-effect evaluations". The latter have been established by referring to the best available scientific information and data related to toxicity (including mutagenicity/carcinogenicity), persistence, and bioaccumulation in living aquatic organisms, sediments, etc.

Data used to establish WQOs were the toxic parameters relevant to the aquatic environment, i.e. acute, subacute, and chronic effects, including reproduction and other sublethal effects on the aquatic ecosystems (for flora, fauna, and microbial systems), supplemented by "zero-effect" dosages. Toxicological data on terrestrial mammals, including man, were required to assess possible carcinogenic, mutagenic or teratogenic properties effective through the aquatic systems. Further, data on persistence and bioaccumulation have been considered (in practise, this was reflected in some cases in which information on persistence

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/ bioaccumulation has had a direct influence on the decision for setting a WQO-value, e.g. for some of the persistent/lipophilic organo-halogen compounds).

Taking into account the objectives of Directive 76/464/EEC it was defined by the CSTE that the WQOs:

- should be such as to permit all stages in the life of aquatic organism to be successfully completed,
- should not produce conditions that cause these organisms to avoid parts of the habitat where they would normally be present,
- should not give rise to the accumulation of substances that can be harmful to the biota (including man) whether via the food chain or otherwise, and
- should not produce conditions that alter the functioning of the ecosystem.

Thus, the WQOs should reflect the maximum amount of a chemical that may be present in the water body, without affecting the biological communities in their functional processes or otherwise give rise to unacceptable, adverse effects on the ecosystem or accumulation of substances that are harmful to biota (including man) whether via the food chain or otherwise. The WQOs could thus be lower than the no-observed effect concentration of the ecosystem (NOEC).

As ecosystem-level no-effect level data did not exist for most chemicals, practices had been developed to derive ecosystem NOEC values by extrapolation from single species toxicity data. To this end, extrapolation factors reflecting the type and amount of information available have been applied to the data as follows:

Application Factor	
1000	to the lower end of the acute L(E)C50 range, when the data available are few, or the range of organisms is narrow, bearing in mind that outlier values may be due to error or experimental conditions that deviate to much from real world conditions.
100	to the lower end of the range of acute L(E)C50 when there is an extensive database covering a (phylogenetically) wide range of test species, or to the lower end of the chronic L(E)C50, or NOEC values when few data are available.
10	to the lower end of (apparent) chronic NOEC data determined by a sufficient and representative number of tests.

Taking into account the experimental uncertainties and the variabilities mentioned above, the extrapolated figure was subsequently rounded to the nearest order of magnitude.

In deriving the WQOs, the extrapolation rules were not applied automatically as a mere mathematical exercise, but it was always kept in mind that due account must be taken of the quality of the data available. This comprised the consideration of any factors that may – directly or indirectly – contribute to the hazards of a compound, such as persistence, bioaccumulation potential, carcinogenic and mutagenic properties, and in specific cases, even avoidance reactions and other sublethal effects on populations and communities. Thus the establishment of WQOs remained a case by case consideration supported by expert judgement.

With regard to human health, exposure for man was estimated by taking into account possible exposure routes and comparing the exposure values – whenever possible – with values

set for the protection of humans (e.g. acceptable daily intake values or maximum allowable concentrations).

In borderline cases a derivation from the above described standard procedure was possible, especially if:

- identifiable uncertainties justified a special, possibly more restrictive extrapolation procedure.
- a proposed WQO should be adopted as "preliminary", in the case where the toxicity database was either insufficient or the date were questionable to the extent that the CSTE decided against recommending a firm WQO until an improved data set was available.

The WQOs were developed in a committee procedure, which included expert evaluation at several steps: namely the judgement on validity, plausibility of available data, and their weighting with respect to their being a basis for the proposed WQO. It was essential that data as well as evaluations had been discussed intensively in the CSTE prior to the recommendation of an unequivocal opinion in order that the necessary consistency be achieved.

Due to the high degree of variability of available data, an element of approximation was adopted in every finalised recommendation: The CSTE only proposed WQOs as orders of magnitude which reflected the overall judgement of the precision and reliability of information.

5.5 Comparative evaluation of the procedures used for the aquatic effects assessment in the Framework of EU Risk Assessments

The most obvious difference in the aquatic risk assessment protocols for new and existing substances (ESRA) and plant protection products (PPPRA), respectively, is the fact that for new and existing substances a single PNEC is derived which is set in relation with the corresponding PEC, whereas for plant protection products several toxicity exposure ratios must be established which are compared with corresponding predetermined TER trigger values. The calculated TER values normally must not be lower than the triggers in order to permit the authorisation of the PPP. Thus, the application of safety factors accounting for uncertainties is different although the factors itself are in most instances comparable in size.

Therefore, despite the apparent formal differences, both approaches are in principle equivalent and should - in most instances - for the same data set give the same result with regard to the acceptability of risk, because the TER ratio (toxicity / PEC) is merely the inverse expression of the PEC/PNEC ratio. Also, the strategy followed to refine the results of the risk assessments for the aquatic environment is very similar. In case the risk of a substance appears to be unacceptable in the initial stage of the risk assessment a "refined" (ESRA) or "higher tier" (PPPRA) risk assessment may be conducted utilising more sophisticated means for exposure and effects assessment such as, e.g., microcosm or mesocosm studies. (see table 5.10 for an overview and comparison of the basic principles and steps in PPPRA and ESRA).

However, with regard to the consideration of toxicity to algae, a difference exists in both risk assessment frameworks that might lead to different results in case algae are the most sensitive organisms. In the PPPRA, only acute toxicity to algae (EC50) is considered whereas in the ESRA also the no-effect level (NOEC, EC10) is taken into account, if respective data are

available. Moreover, the safety factors to account for alga toxicity are different in both RA frameworks. In the ESRA, assessment factors of 10 for NOEC/EC10 values and 100 for EC50 data are normally used (provided a "full" data set is available, cf. section 5.1.3.1) whereas the respective PPPRA TER ratio for the $EC50_{algae}$ must not fall below 10 (equivalent to AF 10 in ESRA).

Another difference in the notification process is that for plant protection products beneficial effects of the (intentional) use of a PPP are taken into account and, therefore, the risk characterisation in the PPPRA is focused on the acceptability of effects occurring after exposure. To this end, specific consideration is given to the recovery potential of small water courses (e.g. ditches) in the immediate vicinity of the treated area after transient exposure to a PPP. This might be the reason why effects on algae are not considered exactly the same way as any other effects on invertebrates or fish (many alga species have a high recovery potential and recover fast once the toxicant concentration falls below the effect level). **Thus, the philosophy and objective of the PPPRA differ to some extent from that followed by the ESRA.**

A further remarkable difference between the PPPRA and the new and existing substances RA exists with respect to data availability for the aquatic effects assessment. For the PPP RA a full data set comprising L(E)C50 and NOEC data for algae, daphnia and fish must be provided by the notifier (unless DT50s of the active ingredient(s) and of relevant metabolites are < 2 days, in this case no long-term toxicity studies are required). If the data set is not complete, no risk assessment is conducted by the competent authority. For the effects assessment of new and existing substances however, long-term data may not be available as for certain substances only the base set of data consisting of short-term effect data may be available.

Other aspects of aquatic effects assessment such as bioaccumulation and secondary poisoning are addressed in both risk assessment frameworks and the outcome of these assessments can be considered as equivalent.

Overall, it can be concluded that the procedures used for the aquatic effects assessments applied in the context of the authorisation of plant protection products or in the context of the risk assessment for new and existing substances are, in principle, equivalent. For the same environmental exposure concentration (PEC) and the same effects data set the same level of risk for the aquatic environment should be indicated by both approaches. However, the latter statement does not apply if algae are the most sensitive organisms.

Table 5.10: Overview on the basic principles and steps in the risk assessments for plant protection products and new and existing substances

	RA for new & existing substances	**RA for plant protection products**
Principle:	Calculate one PEC/PNEC ratio	Calculate several predetermined TERs (toxicity exposure ratios)
Trigger Values:	Indicator for acceptable risk: **PEC/PNEC < 1**	Indicators for acceptable risk: **short-term TER ≥ 100 (10)** [(a)] $L(E)C50_{acute}$ / PEC_{inital} ≥ 100 for the most sensitive species of the groups fish & daphnia (10 for algae) **long-term TER ≥ 10** $NOEC_{long\text{-}term}$ / $PEC_{time\ weighted\ average}$ ≥ 10 for the most sensitive species of each of the groups fish and daphnia (algae normally not considered)
Assessment Factors:	**Dependent on quality and quantity of data** available for PNEC derivation: **1000**: only short-term L(E)C50s available [(b)] **100**: only short-term L(E)C50s available, but substance is subject to intermittent release [(a)] **10**: three long-term NOECs for fish, daphnia and algae available	Normally short-term (L(E)C50s as well as long-term NOECs for representatives of at least the groups fish, daphnia and algae must be provided by the notifier. Thus, a rather extended data set is already available at the first tier of the risk assessment **Assessment factors are not applied** to the toxicity data
Example: Intermittent release of substance (as usual for PPP) PEC 5 µg/l $LC50_{fish}$: 600 µg/l $EC50_{daphnia}$: 750 µg/l $EC50_{alga}$: 900 µg/l $NOEC_{fish}$: 200 µg/l $NOEC_{daphnia}$: 100 µg/l $NOEC_{alga}$: 750 µg/l	**PNEC derivation:** for full data set lowest of 3 long-term NOECs / AF 10 PNEC = 100 µg/l /10 = 10 µg/l intermittent release lowest of 3 acute L(E)C50 / AF 100 PNEC = 600µg/l / 100 = 6 µg/l **PEC/PNEC ratio:** for full data set 5 µg/l / 10 µg/l = 0.5 intermittent release 5 µg/l / 6 µg/l = 0.83	**short-term TERs**: fish: 600 µg/l / 5 µg/l = 120 daphnia: 750 µg/l / 5 µg/l = 150 alga: 900 µg/l / 5 µg/l = 180 **long-term TERs** [(c)]: fish: 200 µg/l / 5 µg/l = 40 daphnia: 100 µg/l / 5 µg/l = 20 alga: TER normally not required, but alga NOEC must be provided in the data set
Conclusion: **There is no principal difference in the methodological approach followed for risk assessment in both the PPPRA and the ESRA, but toxicity to algae is considered differently. This might lead to different results of the RA, if algae are the most sensitive organisms**	Intermittent release: PEC/PNEC ratio of 0.83 for intermittent release is the inverse value of 1.2 = equivalent to short-term TER 120 divided by 100 (100 is the AF used to derive the $PNEC_{interm.\ release}$)	The PEC/PNEC ratio of 0.5 for the full data set is the inverse value of 2 = equivalent to long-term TER 20 divided by 10 (10 is the AF used to derive the PNEC for the full data set)
In case a substance does not pass the trigger levels:	**Refined risk assessment:** Analysis required whether further testing/information may lead to a revision of the PEC/PNEC ratio before a final conclusion on the acceptability of the risk is drawn. Data of e.g. microcosm or mesocosm studies are accepted if test design meets quality requirements.	**"Unless" clauses in the Uniform Principles – Higher Tier RA:** Refinement of exposure and effects assessment. Microcosm and mesocosm studies allowing for an exposure and effects assessment under more realistic environmental conditions may be required (subject to expert judgement).

continued overleaf

Table 5.10: (continued) Overview on the basic principles and steps in the risk assessments for plant protection products and new and existing substances

Notes:

(a) A TER trigger of "≥100" for the required short-term tests for fish and daphnia is equivalent to a PEC/PNEC trigger of "<1" for the lowest L(E)C50 of these tests divided by an assessment factor of 100. In both cases the exposure to the substance should at least be 100-fold lower than the L(E)C50 of the most sensitive species. Thus, the assessment of the short-term risk of intermittent releases (which is usually the mode of release of PPP) in the ESRA is equivalent to the assessment of the risk from short-term exposure to a PPP, as long as algae are not the most sensitive organisms.

(b) In the PPP effects assessment a TER trigger of " ≥1000" - equivalent to an assessment factor of 1000 applied in the ESRA if only acute data are available - is not necessary as according to Directive 91/414/EEC normally a full data set consisting of L(E)C50 and NOEC data for algae, daphnia and fish must be provided by the notifier.

(c) The availability of only two long-term NOECs for fish and daphnia would in the ESRA normally result in the application of an assessment factor of 50 and not of a factor of 10. But this is no real difference in the RA-strategies for PPP and existing substances. In the PPPRA the algae NOEC must be provided as supplementary information in the data set and is therefore available (even though it is normally not used).

If herbicides are to be assessed in the context of the PPP risk assessment, two tests on different algae species and one test with a higher aquatic plant are required and given due consideration. Similarly, in the TGD for the risk assessment of new and existing substances it is recommended to support the algae toxicity data available from the base set with data for a second species if the substance concerned shows a specific toxicity to algae.

6 Assessment of the EU and Member States Methods for the Purpose of Deriving EU Quality Standards

The information presented earlier regarding the concepts followed to derive quality standards in the Member States have been evaluated with regard to the:

- scientific soundness of the concept;
- effort required to implement the concept and make it operational;
- availability of data required for calculations;
- suitability of the concept to achieve the objectives pursued with the EU quality standards under the Water Framework Directive.

Overall conclusion:

The French river quality assessment system (SEQ) is a complex system. Its main objective is not to deal with quality objectives but to assess the suitability of water for various uses. However, the components of the SEQ can be used to derive quality objectives. The SEQ allows for each indicator ("alteration") to define a quality class whose "very good / good" level can be considered as a quality objective. The other approaches developed by the Member States or by the CSTE are designed to derive quality standards. They are in so far very similar as the application of assessment factors depending on the quality and quantity of available toxicity data is a common core element (those factors are, however, also used in the French SEQ for the calculation of threshold levels in order to distinguish between different suitability classes). The use of assessment factors links the national approaches or the CSTE-method with the EU risk assessment frameworks for new and existing substances and for plant protection products as well (in the PPP risk assessment, the assessment factors are integral part of predefined toxicity exposure ratios not to be exceeded).

As an alternative to the assessment factor approach, the use of statistical extrapolation methods (species sensitivity distributions) is applied in the Netherlands and is further an option that can be used in the risk assessment for new and existing substances [6]. In the TGD revision this approach has gained more weight [38].

As no fundamental differences in the national approaches or the CSTE-method for quality standard setting and the EU methods for risk assessment could be found, it was deemed most appropriate to built the proposal for a common EU method for quality standard derivation as far as possible on the elements used for effect assessment in the EU risk assessment frameworks.

The reasons for this decision are:

- To keep the ecological effects assessment methodology on EU-level as consistent as possible.
- To use, as far as possible, elements for the set up of the quality standard derivation methodological framework that are already accepted and agreed by Member States and introduced on Member State level.

Part B: Proposals for Procedures to Derive EU Quality Standards for Water, Sediment, and Biota

7 Compliance Checking for Quality Standards

Issues regarding exposure monitoring, the averaging of monitored levels or the selection of the suitable reference data for compliance checking with the quality standards are beyond the scope of this study. However, as these issues are directly related to the level of protection that can be achieved with a quality standard some considerations with regard to the averaging of monitoring data and the selection of appropriate water and sediment references are briefly given in the following sections 7.1 and 7.3. Section 7.2 deals with potential impacts on ecosystem health by transient exposure to peak concentrations and how this can be accounted for by a specific quality standard referring to short-term exposure.

7.1 Averaging of Monitored Levels

Annex V, section 1.2.6, of the WFD stipulates that the quality standards for the groups of main pollutants listed under 1.-9. in Annex VIII shall refer to a "maximum annual average concentration" tolerable for the substance concerned. However, it is not unequivocally clear whether this stipulation does also include the Priority Substances which are listed in Annex X of the WFD.

As there is no method explicitly mentioned in Annex V as to how the averaging of monitoring data shall be achieved, several options may be taken into account. For instance, the annual average concentration at a monitoring point may be calculated as arithmetic mean, as median (50-percentile), or as 90-percentile. Further options exist with respect to the consideration of monitoring data where levels above the limit of detection (LOD) but below the limit of quantification (LOQ $\approx$ determination limit) of a specific substance were found. Thus, the approach by which the monitoring data are aggregated to an annual average concentration has a direct influence on the protection level that is achieved with the quality standard (the percentage of monitored levels above the quality standard as well as the numerical distance between the quality standard and the maximum levels in the data set are dependent on the aggregation method applied). This is illustrated by the examples of frequency distributions based on monitoring data taken from the COMMPS database [2] (figures 7.1 and 7.2)[12]. The arithmetic mean, the 50-percentile and the 90-percentile are given in the histograms (where applicable, existing EU QS are given in addition). In figure 7.1 a possible effect of a different treatment of values below the limit of quantification is shown in addition.

During the meeting at 15 October 2001, the Expert Advisory Forum was invited to discuss which averaging procedure for monitoring data is deemed the most appropriate to calculate the reference concentration the quality standards are compared to. In response to this invitation several Member States and NGOs submitted their views on this topic. While numerous options for data aggregation were mentioned in the written responses (see table 7.1), the discussions related to that topic at the expert meeting on 23 January 2002 in Brussels revealed that the two preferred options are to aggregate monitoring data on an annual

[12] For the substances shown in figures 7.1 and 7.2, the COMMPS monitoring database was screened for the monitoring station with the most values above the limit of quantification. By coincidence, this was in all cases the monitoring station Schnackenburg.

basis[13] either as the 90-percentile or as the arithmetic mean. Both methods have merits and the decision which to prefer is more a political question with regard to the quality standard enforcement and compliance checking strategy to be followed than a decision between an, in scientific terms, superior or inferior approach.

Therefore, the question to which type of aggregated monitoring data the quality standards for the priority substances should refer to is left open in the context of this study. A decision will be taken by the Expert Advisory Forum or by another competent body at a later stage.

Table 7.1: Responses to the question "which averaging procedure for monitoring data is most appropriate to calculate the reference concentration for the QS?"

Most appropriate aggregation procedure	Reasoning
• annual arithmetic mean	in line with: Annex V WFD, other Directives, legal continuity
• geometric mean	best centrality estimator; for skewed data
• median	best of the options proposed in draft report
• "mean" annual average	least number of samples required to check compliance with a specified degree of confidence
• 90-percentile	the only acceptable indicator with regard to WFD objectives; no problem to include data below the determination limit
• relevant exposure period mean	annual values are insufficient to check compliance
• QS = C_{max} any time	the QS should be considered as threshold level
• arithmetic mean & 90-percentile	depending on the data available and/or the analytical method used

7.2 Exceedence of Quality Standards referring to Annual Reference Concentrations by Concentration Peaks

As described in section 7.1, quality standards shall normally refer to an annual "average" (or better: reference) concentration. This implies that for a certain percentage of time the concentration in the compartment concerned may (considerably) exceed the annual reference concentration (i.e. due to concentration peaks resulting from intermittent releases, varying concentrations due to seasonal differences in the flow regime etc). In case of substances showing a very high acute toxicity (or a narrow acute to chronic toxicity ratio) it can thus not ruled out that a quality standard referring to the annual reference concentration is insufficient to protect the aquatic ecosystem against an impact by transient concentration peaks.

In order to account for potential impacts on ecosystem health by transient exposure to peak concentrations of highly toxic chemicals, it may thus be required to establish in addition to the quality standard referring to the annual reference concentration a second quality standard setting a **maximum acceptable concentration** (MAC) which must not be exceeded any time. As partition between water, sediment and biota is normally rather slow, it is proposed to derive this MAC-QS for water only.

During the meeting on 15 October 2001 the Expert Advisory Forum was invited to discuss whether the derivation of a MAC-QS is deemed pertinent and, if yes, whether such a MAC-

[13] It was acknowledged in addition that for certain chemicals with an intermittent release pattern (e.g. plant protection products) data aggregation on a shorter than annual time scale might be sensible.

QS should be derived for all substances on the working list or only for those exceeding a certain trigger-value for toxicity. The responses by members of the EAF to these questions and the discussion related to that topic at the Expert Meeting on 23 January 2002 showed very clearly that a MAC-QS is considered as a useful tool, especially if the "annual" quality standard is referring to the arithmetic mean of monitored levels. However, in order to cover episodic exposure events, a MAC-QS was also considered necessary by many experts if the 90-percentile of the annual monitoring is chosen as the reference concentration for the long-term QS.

With regard to the question whether a MAC-QS should be derived for all substances on the working list or only for those identified by a trigger-value, no clear recommendation was given. Proposals were that MAC-QS should be derived:

- independent of a trigger-value,
- if the ratio $toxicity_{acute}$ / $toxicity_{long\text{-}term}$ < 10 or
- if the acute aquatic toxicity < 1 mg/l (or <10 mg/l or <100 mg/l)

It was therefore decided to derive an example for a MAC-QS for all substances on the working list. Based on this exercise the EAF or another competent body may later on decide for which substances MAC-QSs are deemed necessary and which trigger-value (if any) may be used.

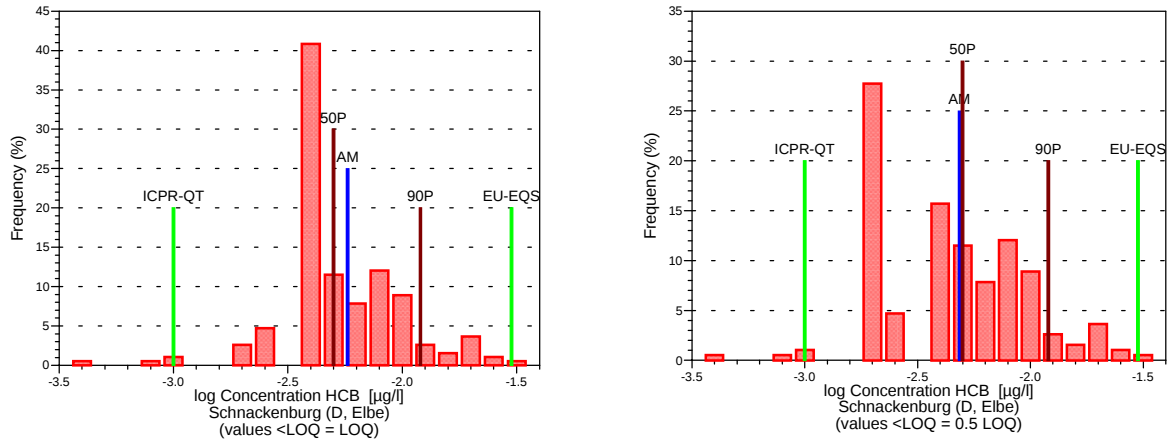
It may also be decided later whether a MAC-QS should be a **statutory standard** or more a **guidance value**, how compliance with it should be checked and what consequences the exceedance of a MAC-QS should have.

With regard to the possible methodology to derive a MAC-QS, it is proposed to rely on the procedure recommended in the draft revised TGD [38] for the effects assessment of intermittent releases (section 3.3.2 of part II – environmental risk assessment). Normally, any single monitoring datum should not exceed the lowest relevant $L(E)C_{50}$ divided by an assessment factor of 100 (see table 7.2). However, there may be occasions when a higher or lower factor would be appropriate (see section 5.1.3.4 for details).

Table 7.2: Proposed method to derive a MAC-QS

• lowest L(E)C50 / 100 (standard procedure)
• in certain cases attenuation of AF to minimally 10 (acc. TGD)
• MAC-QS in no case lower than long-term AA-QS

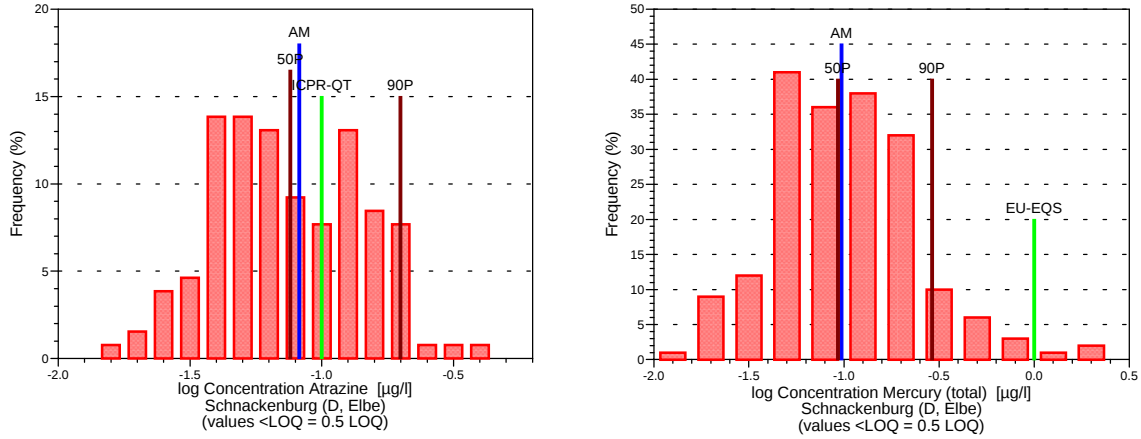
a) **b)**



	arithmetic mean (log10)	50-percentile (log10)	90-percentile (log10)
a) values <LOQ = LOQ	-2.239	-2.301	-1.921
b) values <LOQ = 0.5LOQ	-2.314	-2.301	-1.921
Quality Standards:	CD 86/280/EEC: 0.03 µg/l (log10 = -1.523) ICPR: 0.001 µg/l (log10 = -3) (Quality Target of the International Commission for the Protection of the Rhine)		

Figure 7.1: Frequency distribution of monitoring data of hexachlorobenzene at the monitoring station Schnackenburg. In contrast to the arithmetic mean, 50-percentile and 90-percentile values are not affected by different treatments of monitoring data <LOQ.

a) **b)**



	arithmetic mean (log10)	50-percentile (log10)	90-percentile (log10)
a) Atrazine (Values <LOQ = 0.5LOQ)	-1.085	-1.119	-0.701
b) Mercury (Values <LOQ = 0.5LOQ)	-1.014	-1.032	-0.538
Quality Standards:	Atrazine – ICPR: 0.1 µg/l (log10 = -1) (Quality Target of the International Commission for the Protection of the Rhine) Mercury - CD 82/176/EEC: 1µg/l (inland waters) (log10 = 0)		

Figure 7.2: Frequency Distribution of monitoring data of atrazine and mercury at the monitoring station Schnackenburg.

7.3 Selection of a Reference for Sediment Quality Standards

Although objections regarding the use of suspended particulate matter (SPM) as reference material for sediment quality standards have been raised by some delegates to the Expert Meeting of 23 January 2002 on methods for the derivation of quality standards, it is still suggested that the quality standards for sediment should refer to the substance levels monitored in SPM. Reasons are that in this case the sediment quality standard is directly linked to the present contamination level of the material that will finally sink to the ground of the water body and contribute to the build up of new sediment layers and that, moreover, this new settled material is the main food source of detrivorous benthic organisms.

It is thought that in contrast to suspended particulate matter, sediment samples taken from the ground of waters give mainly a time integrated indication of past levels of pollution (the time interval covered is dependent on the sampling depth and the intensity as well as the frequency of occurrence of torrential events) and are therefore not recommended as reference for the monitoring of current pollutant levels[14]. However, sediment samples from the ground of a water body might be suitable to assess the contamination by "historic" pollutants. Further, they might be a suitable reference for quality standards triggering the need for remediation of seriously contaminated sediments. However, the development of such "remediation standards" is beyond the scope of this study.

[14] This point was controversly discussed at the Expert Meeting of 23 January 2002 on methods for the derivation of quality standards. The opinion of some experts was that the contamination level of settled sediments cannot be considered as a time integrated indication of past levels of pollution as sediments might rather often be resuspended after torrential events.

8 Proposals for Procedures to Derive EU Quality Standards for Water, Sediment, and Biota

Quality standards established in the context of the Water Framework Directive shall ensure a sustainable functioning of aquatic ecosystems as well as the protection of human health. The procedures proposed in this section for the derivation of respective standards deal therefore only with the appropriate approach for effects assessment. Other relevant issues in the context of quality standard setting, such as, e.g., appropriate analytical methods to monitor substances or the standardisation of monitoring procedures are not addressed since they are beyond the scope of this study. Issues regarding suitable exposure reference data for compliance checking with the quality standards are addressed in section 7 of this report.

The concept for the derivation of quality standards proposed in the following sub-sections of chapter 8 was presented 3 times (March and October 2001, March 2002) to the Expert Advisory Forum on Priority Substances (EAF) at different stages of its development. In addition, an Expert Group on Setting of Quality Standards discussed several important issues in relation to the proposed methodology on its meeting of 23 January 2002. Comments received upon the different discussion rounds have been taken into account, where appropriate. The proposed approach was finally endorsed by the EAF at its meeting in March 2002.

8.1 Starting Point for the Development of Quality Standards

The starting point for the development of a concept to derive quality standards are the provisions set out in Annex V, section 1.2.6 (Procedure for the Setting of Chemical Quality Standards by Member States) of the Water Framework Directive [1]. The description of the procedural provisions given in the following is an adapted citation from Annex V, section 1.2.6, WFD:

> Environmental quality standards for the protection of aquatic biota may be set for water, sediment or biota. In deriving environmental quality standards, both acute and chronic data shall be used for the taxa which are relevant for the water body type concerned as well as any other aquatic taxa for which data are available. The "base set" of taxa that should be used are:
>
> - algae and/or macrophytes,
> - daphnia or representative organisms for saline waters,
> - fish.
>
> In setting quality standards the safety factor method as set out in Section 3.3.1 of Part II of the TGDs [6] shall be applied. The TGD method provides for safety factors which differ depending on the quantity and quality of available effects data (Table 5.1)
>
> Where data on persistence and bioaccumulation are available, these shall be taken into account in deriving the final value of the environmental quality standard. The quality standard shall refer to a maximum annual average concentration tolerable for the substance concerned.
>
> Standards thus derived should be compared with any evidence from field studies. Where anomalies appear, the derivation shall be reviewed to allow a more precise safety factor to be calculated. Further, the derived standards shall be subject to peer review and public consultation including to allow a more precise safety factor to be calculated.

While the above described provisions of Annex V may suffice as general scheme to derive quality standards for organic substances in the water body, they do not deal with specific prob-

lems arising from the inclusion of sediment quality, protection of top predators from secondary poisoning and human health as objectives of protection, nor do they account for the peculiarities that must be considered if quality standards for metals or for transitional, coastal and territorial marine waters are to be set.

Therefore, it is deemed indispensable to take further approaches for effects assessment and quality standard setting into account.

8.2 Objectives of the Proposed Approach to Derive Quality Standards

The quality standards derived with the approaches proposed in the following sub-sections of section 8 are intended to protect - on the one hand - the structure and function of aquatic ecosystems in freshwater as well as in transitional, coastal and territorial waters from any significant alterations by the impact of hazardous chemicals. According to current scientific knowledge, the objective of maintaining ecosystem function can be best achieved by protecting the community structure (i.e. species diversity, abundance and seasonal dynamics). Thus, not only toxic effects or effects on reproduction should be considered when assessing possible impacts on community structure by a chemical, but all relevant effects on the population dynamics and abundance of species must be accounted for. Hence, effects on behaviour or avoidance of the habitat should also be included in the assessment. According to current scientific knowledge community structure can be preserved by protecting the most sensitive species known. In setting a save level for sensitive species due account must be given to additional uncertainties arising from limitations of the data available.

On the other hand – the protection of human health from the occurrence of adverse effects due to the ingestion of food originating from aquatic environments or due to uptake of water is a further objective to be protected by the quality standard.

The methods proposed to derive the quality standards are therefore intended to concomitantly protect freshwater and marine ecosystems from adverse effects as well as human beings from all impacts on health by drinking water uptake or ingestion of food originating from aquatic environments. To this end, for the entire set of objectives of protection, i.e. the pelagic and benthic communities (≈ water and sediment) in freshwater or saltwater ecosystems, the top predators of these ecosystems and human health, it is assessed by means of pre-defined trigger criteria whether a substance may pose a certain objective at risk. For those objectives for which a possible risk (≈ exceeded trigger-value) is identified, quality standards are derived. In a subsequent step the lowest of the standards derived for the individual protection objectives is selected as the overall quality standard.

Thus, a quality standard derived by this approach takes all relevant protection objectives into account. Moreover, all direct and indirect exposure routes in aquatic systems like exposure in the water body via water and sediment or via bioconcentration and biomagnification (uptake of contaminated biota as food or feed) as well as possible exposure via drinking water uptake are considered[15]. Further, all relevant modes of toxicity are considered, e.g. for ecosystems direct

[15] Although persistence is mentioned in Annex V of the WFD as one of the criteria that should be taken into account, it will not be explicitly considered in the proposed approach for the derivation of quality standards. The reason for this is that persistence is an exposure related criterion and accordingly should be addressed in the derivation of emission standards. In this step it must be ensured that a build up of environmental concentrations of a substance with time can be excluded. Effect based quality standards refer to a certain threshold concentration no be exceeded in the compartment concerned (e.g. water). The mechanisms that may lead to a possible rise of the concentration in that compartment, however, cannot be adequately addressed and accounted for in the effects assessment.

and indirect toxicity (≈ after bioaccumulation) and for man oral toxicity as well as carcinogenicity, mutagenicity and adverse effects on reproduction. In addition, endocrine disruption will be taken into consideration for both aquatic communities and man, if relevant.

Therefore, a quality standard derived by the described conceptual framework is not merely a threshold level ensuring the protection of only a particular protection objective (like, for instance, a PNEC for the protection of the pelagic community), but is an overall stand alone value that encompasses the consideration of direct ecotoxicological effects in different habitats (water, sediment), indirect ecotoxicological effects occurring after bioaccumulation in biota (secondary poisoning of top predators) and effects on human health by oral uptake of water and food, including long-term toxicity and CMR mechanisms.[16]

In order to safeguard human health as well as ecosystem structure and function, it is proposed to apply for effects assessment and quality standard setting the state-of-the-art, internationally acknowledged, effects assessment procedures used in the EU-risk assessment frameworks for existing substances [6, 38] or plant protection products [8, 15, 35]. Further, elements of Member State approaches for quality standard setting or latest findings in research related to exposure or effects assessment are proposed for use, if deemed pertinent (e.g. in the QS setting procedure for metals).

The mentioned EU-risk assessment frameworks comprise only methods that have been extensively discussed and peer reviewed by experts nominated by the Member States, by industry or by other NGOs. The methods are not intended to be applied in an quasi automated manner. In the contrary, in each of the frameworks ample room for expert judgement is conceded. This is, for instance, reflected in the procedural approach taken to set up and evaluate risk assessment reports. These reports must pass several expert fora and discussion rounds before a final conclusion can be drawn.

Finally, it is notable that the proposed general approach for the derivation of quality standards in the context of the Water Framework Directive is very similar to the approach for the derivation of EU Water Quality Objectives in the context of Council Directive 76/464/EEC developed by the former CSTÉ [9] (see section 5.4), as possible impacts on aquatic ecotoxicity, human health effects and bioaccumulation potential are accounted for in setting the standards. However, as effects assessment methodology has been considerably refined in the last decade, it is deemed appropriate to use today's state of the art methods in the present exercise.

This proposed approach was discussed and endorsed by the Expert Advisory Forum on Priority Substances. Comments have been taken into account, where appropriate. Some open issues of the discussion are mentioned in the respective sections.

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[16] Quality Standards derived by the proposed methodological framework do not account explicitly for a possible combined action of pollutant mixtures. Nonetheless, it is assumed that the safety factors applied in the effects assessment do cover the possible occurrence of combined action of pollutants in most instances to a great extent. For the time being, there is apparently no consolidated and validated approach to account for combined action of pollutants available that is applicable in the context of quality standard setting. Therefore, the Commission, has commissioned a research project on the regulation of mixtures of toxic chemicals in the aquatic environment, the so-called BEAM project. The results of this project should be considered in future adaptations of the proposed quality standard setting methodology to scientific progress.

8.3 General Procedures for Quality Standard Setting

According to Article 16(7) WFD the Commission shall submit proposals for quality standards applicable to concentrations in water, sediments or biota. This implies that for certain substances the setting of quality standards for all the mentioned compartments is optional. Quality standards (QS) for a specific compartment may not be required if – based on the current scientific knowledge - there is no indication that a given substance poses this compartment at risk. For instance, a quality standard for sediment may not be necessary if there is no indication that the substance concerned accumulates in the sediment. Similarly, quality standards for concentrations in biota may not be required if there is no indication for bioaccumulation, biomagnification (secondary poisoning of top predators), or risk to human health by consumption of food originating from aquatic environments.

In terms of working economy it is therefore intended to derive a quality standard for each substance on the working list (cf. section 3) only for the **water phase** by default. This quality standard will usually be given in a mass per volume unit (e.g. µg/l). However, for hydrophobic or strongly adsorbing substances it is suggested to additionally express the quality standard referring to water as concentration in suspended particulate matter (µg/kg) if this appears meaningful, e.g. for analytical reasons[17].

If deemed justified, distinct QS will be derived for freshwater and saltwater, respectively (e.g. for metals, plant protection products and tributyltin compounds; cf. sections 8.4.1.2 and 8.6 of this report). The setting of further quality standards for drinking water abstraction, biota or sediments is triggered by the criteria given in table 8.1.

It is proposed to adopt the lowest standard derived for the different **objectives of protection**[18] as overall quality standard. However, if different quality standards for the freshwater and the marine environment are derived, the lowest standards relevant for either the marine or the freshwater environment will be proposed as specific overall $QS_{marine\text{-}env}$ or $QS_{freshwater\text{-}env}$.

In order to be able to adopt the lowest quality standard as overall standard, it may be required to transform standards from mass per volume to mass per mass units (e.g. µg/l (water) to µg/kg (sediment, biota)) or vice versa using appropriate model calculations and parameters. Similarly, biota quality standards may be transformed to concentrations in water or suspended particulate matter (and be given as those) in order to avoid routine monitoring (and thus sampling) of biota for compliance checking with quality standards. The respective algorithms for transformation are given in the following sub-sections of chapter 8.

The quality standards for **sediment** should preferably be derived on the basis of toxicity tests with sediment dwelling organisms. However, as those toxicity tests with benthic organisms are not available for many of the substances on the working list, it is proposed to use the so-called equilibrium partitioning method in order to extrapolate a quality standard applicable to the concentration in sediment (for the protection of benthic life) from the quality standard derived for the protection of life in water (see section 8.4.2 for details).

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[17] Thus, for hydrophobic organic substances, the quality standard referring to water will be given for unfiltered water samples (µg/l) ("total" concentration) and for the corresponding concentration in suspended particulate matter (µg/kg) (see section 8.4.1 for transformation algorithms).

[18] Objectives of protection: Water quality to support aquatic life or to allow for drinking water abstraction, sediment quality to support benthic life, and quality of biota in order to protect humans or top predators from secondary poisoning by ingestion of food.

Although some Member States are in favour of relating the sediment standard to the settled sediment at the bottom of water bodies, it is proposed to compare the sediment quality standard for check of compliance with the level monitored in suspended particulate matter (SPM). By doing so, compliance of the level in SPM with the sediment quality standard ensures that the material that will eventually settle down and contribute as most important fraction to the build-up of new sediment layers is suitable to fully support sustainable benthic life (i.e. the contaminant level in new sediment will not exceed the no-effect threshold level). In contrast to SPM, sediment samples from the ground of a water body might be a suitable reference for quality standards triggering the need for remediation of seriously contaminated sediments. However, the development of such "remediation standards" is beyond the scope of this study.

With respect to **drinking water quality**, existing standards will be accounted for, e.g. those given in Council Directive 75/440/EEC concerning the quality required of surface water intended for the abstraction of drinking water [17] or in Council Directive 98/83/EC concerning the quality of water intended for human consumption [18]. Both directives require Member States to ensure that any measures taken in no circumstances have the effect of allowing, directly or indirectly, either any deterioration of the present quality of water intended for human consumption or any increase in the pollution of waters used for the production of drinking water (Article 7, CD 75/440/EEC and Article 4, CD 98/83/EC; see also Articles 7(2,3) and 16(1), WFD). In this sense, the "A1 values" of Council Directive 75/440/EEC referring to "simple filtration and disinfection" to produce drinking water from surface water are considered as minimum quality standard. For those priority substances for which no values are given in CD 75/440/EEC a standard for drinking water abstraction from surface water may be derived by the procedure described in section 8.4.4.

In order to derive the human health related quality standards for **biota** (consumption of food originating from aquatic environments), it is suggested to follow the guidance and models given in the context of Council Regulation (EEC) No. 793/93 [19] (i.e. in the TGD [6, 38]) and/or Council Directive 91/414/EEC [15] as far as possible (see sections 8.4.3 and 8.5). The quality standards for cadmium, lead and mercury derived by the method proposed in section 8.4.3 for levels in biota will be checked for compliance with the respective maximum levels fixed in Council Regulation (EC) No 466/2001 [43] for food originating from aquatic environments (fish, crustaceans, molluscs).

It is deemed necessary to derive two kinds of quality standards referring to (i) the **annual average concentration** and (ii) to **short-term concentration peaks**. To this end, in line with the provisions of Annex V of the WFD and the approaches followed in the "daughter directives" of Council Directive 76/464/EEC, a long-term QS is calculated. This so-called AA-QS is intended to refer to the annual "mean" concentration. In addition to the AA-QS, the so-called maximum admissible concentration QS (MAC-QS) referring to short-term transient exposure is derived. The MAC-QS is intended not to be exceeded any time.

As it was not yet decided by the Expert Advisory Forum whether the long-term quality standard should refer to the annual arithmetic mean or to the 90-percentile of monitored concentrations, it is also not possible to draw a final conclusion on the possible pertinence of the MAC-QS and to give a recommendation regarding the status it should be given (i.e. statutory standard or guidance value; for details see sections 7.1 and 7.2)

In conjunction, the AA-QS and the MAC-QS are intended to protect the structure and function of the addressed freshwater and marine ecosystems from significant alterations by the impact of chemical substances.

Table 8.2 gives an overview on the methods proposed for the derivation of quality standards for the different objectives of protection. The methods are outlined in the following sections 8.4 – 8.6.

Table 8.1a: Environmental protection objectives and triggers to derive quality standards

Water	**Sediments (suspended particulate matter)**	**Biota (secondary poisoning)**
No trigger value applies. QS are derived for <u>all</u> substances on the working list. For hydrophobic / adsorbing substances the QS referring to water are additionally given as concentration in suspended particulate matter (SPM) if this is meaningful. Trigger value: log $Kp_{SPM\text{-}water} \geq 3$	QS are derived for all substances with al log $Kp_{SPM\text{-}water} \geq 3$ The $QS_{sediment}$ refers to suspended particulate matter in order to protect the new sediment.	QS are derived for organic substances and metals with experimental BCF ≥ 100 or BMF >1. If a reliable BCF is not available, the trigger is log Pow ≥ 3 (applies only to organic substances) In order to avoid routine monitoring of biota the concentrations in animal tissue are transformed to concentrations in water or suspended particulate matter, using appropriate model estimates.

Table 8.1b: Human health related protection objectives and triggers to derive quality standards

Biota (Food consumption)	**Drinking water abstraction from surface water**
Derivation of QS for substances being: - a known or suspected carcinogen (cat. I-III, R-phrases R45 or R40) - a known or suspected mutagen (cat. I-III, R-phrases R46 or R40) - a substance known or suspected to affect reproduction (cat. I-III, R-phrases R60, R61, R62, R63 or R64) - potential to bioaccumulate (experimental BCF ≥ 100 or BMF >1 (or logPow ≥ 3, for organic substances only)) *<u>plus</u>* - harmful or (very) toxic if swallowed or in contact with skin (R-phrases R21, R22, R24, R25, R27 or R28); or - R48 (danger of serious damage to health by prolonged exposure) Check for compliance of the proposed QS with the maximum permissible levels in seafood fixed by Council Regulation (EC) No 466/2001 for Cd, Hg and Pb.	Derivation of DW * abstraction QS only if the following cases apply (see section 8.4.4 for details): 1. A "A1 value" is fixed in Directive 75/440/EEC and this value is lower than the QS for other objectives of protection: ⇒ QS = "A1 value" of CD 75/440/EEC 2. No "A1 value" is fixed in CD 75/440/EEC but a DW Standard is available in CD 98/83/EC and the DWS ** is lower than the QS for other protection objectives: ⇒ Assessment (Experts): Identification of the substance specific removal efficiency in DW processing. QS = DWS / Fraction not removable 3. No A1 value or DW Standard exists for the substance concerned: ⇒ a) Calculation of a provisional DWS b) Assessment based on expert knowledge with regard to: 1. Removal efficiency of substance in DW processing; 2. toxicological appropriateness of the provisional DWS QS = appropriate DWS / Fract. not removable

* DW = drinking water; ** DWS = drinking water standard

Table 8.2: Overview on the methods proposed for the derivation of quality standards in relation to the different objectives of protection
(AF: assessment factor ; CD: Council Directive; DW(S): drinking water (standard); ME: metals; MPA: maximum permissible addition; OC: organic chemicals; PPP: plant protection product; QS: quality standard; SPM: suspended particulate matter; SSD: species sensitivity distribution; TER: toxicity-exposure ratio; TGD: technical guidance document)

Objective of protection	Type of substance	Compartment	Method proposed	Description in section
pelagic community	OC	freshwater (unfiltered sample) (for hydrophobic substances in addition: corresponding concentration in SPM)	• TGD Assessment Factor method (freshwater AFs) • SSD method (data rich substances	8.4.1.1 8.4.1.3 & 8.6.2
pelagic community	OC	saltwater (unfiltered sample) (for hydrophobic substances in addition: corresponding concentration in SPM)	• TGD Assessment Factor method (saltwater AFs) • SSD method (data rich substances)	8.4.1.2 8.4.1.3 & 8.6.2
benthic community	OC	freshwater sediment (SPM) QS are derived if log $Kp_{sediment\text{-}water} \geq 3$ or log Pow ≥ 3	• TGD Assessment Factor method (freshwater AFs) • SSD method (data rich substances) • Equilibrium partitioning approach (if no or only insufficient data for sediment organisms are available	8.4.2.1 8.4.1.3 & 8.6.2 8.4.2.1
benthic community	OC	marine sediment (SPM) QS are derived if log $Kp_{sediment\text{-}water} \geq 3$ or log Pow ≥ 3	• TGD Assessment Factor method (AFs for marine sediment) • SSD method (data rich substances) • Equilibrium partitioning approach (if no or only insufficient data for sediment organisms are available)	8.4.2.2 8.4.1.3 & 8.6.2 8.4.2.2
pelagic community	PPP	freshwater (unfiltered sample) (for hydrophobic substances in addition: corresponding concentration in SPM)	• Based on Uniform Principles (CD 97/57/EC): $QS_{water,\ annual} = NOEC_{min}$ / TER-trigger $_{long\text{-}term}$ $QS_{water,\ transient\ peak}$ = L(E)C50min / TER-trigger $_{short\text{-}term}$	8.5
benthic community	PPP	freshwater sediment (SPM)	• QS for sediment derived as for "normal" organic chemicals, under consideration of the argumentation related to this compartment in the risk assessment monograph	8.5; 8.4.2.1
pelagic community	ME	freshwater (filtered sample) (corresponding concentration in SPM in addition)	• Added risk approach (QS = $C_{background}$ + MPA) • SSD method to derive the MPA for data rich metals • TGD assessment factor method (freshwater AFs) to derive MPA if application of SSD method not possible	8.6.1 8.6.2
pelagic community	ME	saltwater (filtered sample) (corresponding concentration in SPM in addition)	• Added risk approach (QS = $C_{background}$ + MPA) • SSD method to derive the MPA for data rich metals • TGD assessment factor method (saltwater AFs) to derive MPA if application of SSD method not possible	8.6.1 8.6.2 8.6.6
benthic community	ME	freshwater sediment (SPM) QS derived if log $Kp_{sediment\text{-}water} \geq 3$	• Added risk approach (QS = $C_{background}$ + MPA) • SSD method to derive the MPA for data rich metals • TGD assessment factor method (freshwater sediment AFs) to derive MPA if application of SSD method not possible • Equilibrium partitioning approach if no or only insufficient data for sediment organisms available	8.6.1 8.6.2 8.6.5

continued overleaf

Table 8.2: (continued) Overview on the methods proposed for the derivation of quality standards in relation to the different objectives of protection

Objective of protection	Type of substance	Compartment	Method proposed	Description in section
benthic community	ME	marine sediment (SPM) QS derived if log $Kp_{sediment\text{-}water} \geq 3$	• Added risk approach (QS = $C_{background}$ + MPA) • SSD method to derive the MPA for data rich metals • TGD assessment factor method (marine sediment AFs) to derive MPA if application of SSD method not possible • Equilibrium partitioning approach if no or only insufficient data for sediment organisms available	8.6.1 8.6.2 8.6.5 8.6.6
secondary poisoning of top predators	OC, PPP, ME	water (freshwater & saltwater) (for hydrophobic substances in addition: corresponding concentration in SPM) QS only derived if triggers are exceeded (see table 8.1a)	• Based on the lowest relevant threshold level (e.g. NO(A)EL divided by appropriate AF) and the standard figures given in the TGD for food consumption and body weights of the predators (birds, mammals), concentrations in fish (and/or mussels) are calculated ruling out adverse effects by seafood ingestion. Based on these "safe" levels calculated for fish or mussels, water concentrations are derived using the BCF (preferred) or the octanol water partition coefficient (the latter not for metals) of the substance concerned. The resulting water concentrations are the quality standards for secondary poisoning.	8.4.3 (OC) 8.5 (PPP) 8.6.7 (ME)
human health (drinking water consumption)	OC, PPP, ME	freshwater Derivation of QS only if no standard is fixed in CD 75/440/EEC	Derivation of DW abstraction QS only if the following cases apply: A “A1 value” is fixed in Directive 75/440/EEC and this value is lower than the QS for other objectives of protection: ⇒ QS = "A1 value" of CD 75/440/EEC No "A1 value" is fixed in CD 75/440/EEC but a DW Standard is available in CD 98/83/EC and the DWS is lower than the QS for other protection objectives: ⇒ Assessment (Experts): Identification of the substance specific removal efficiency in DW processing. QS = DWS / Fraction not removable No A1 value or DW Standard exists for the substance concerned: ⇒ a) Calculation of a provisional DWS b) Assessment based on expert knowledge with regard to: 1. Removal efficiency of substance in DW processing; 2. toxicological appropriateness of DWS QS = appropriate DWS / Fract. not removable	8.4.4
human health (food consumption)	OC, PPP, ME	water (freshwater & saltwater) (for hydrophobic substances in addition: corresponding concentration in SPM) Derivation of QS only if triggers are exceeded (see table 8.1b)	• Based on the lowest relevant threshold level for human health (e.g. NO(A)EL divided by appropriate AF, ADI/TDI or unit risk value) and the standard figures given in the TGD for seafood consumption and body weights of humans, concentrations in fish (and/or mussels) are calculated ruling out adverse effects by seafood ingestion. Based on these "safe" levels calculated for fish or mussels, water concentrations are derived using the BCF (preferred) or the octanol water partition coefficient (the latter not for metals) of the substance concerned. The resulting water concentrations are the quality standards for human health effects due to food uptake.	8.4.3 (OC) 8.5 (PPP) 8.6.7 (ME)

8.4 Derivation of Quality Standards for Organic Chemicals (other than Plant Protection Products)

8.4.1 Quality Standards Referring to Substance Levels in the Water Phase

For hydrophobic organic substances (exceeding the triggers given in table 8.1) the quality standards referring to water will be given as concentration in the unfiltered water sample (i.e. water plus SPM) and in addition as corresponding concentration in suspended particulate matter (SPM) of the EU standard water as defined in section 2.3.4, Vol. II of the TGD [6, 38] (15 mg/l SPM dry weight). This approach offers the Member States the option to do compliance monitoring in the matrix (unfiltered water sample or SPM) that is deemed the most suitable for various reasons (e.g. existing monitoring tradition, available technical equipment, analytical reasons).

The algorithms to calculate the concentration in SPM from the total concentration in water and vice versa are as follows:

$$QS_{SPM.wat}\ [\mu g/kg] = \frac{QS_{wat.tot}\ [\mu g/l]}{C_{SPM}\ [mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [l/kg]}$$

$$QS_{wat.tot}\ [\mu g/l] = QS_{SPM.wat}\ [\mu g/kg] * (C_{SPM}\ [mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [l/kg])$$

with:

$QS_{SPM.wat}$	Quality standard for water referring to the substance concentration in SPM
$QS_{wat.tot}$	Quality standard for water referring to the total (unfiltered) water sample
C_{SPM}	Concentration of SPM in the water sample (standard water: 15 mg dry weight / l)
Kp	Substance specific partition coefficient SPM – water

In case compliance checking is based on quality standards referring to SPM, the SPM concentration in the water samples should be monitored in addition. The SPM concentration is required to allow for a correction of the $QS_{SPM.wat}$ with the real C_{SPM}.

8.4.1.1 Freshwater

It is proposed to apply the procedures for aquatic effects assessment and the calculation of the PNEC ($\approx QS_{freshwater}$) by the Assessment Factor method as laid down in section 3.3 of Part II of the draft revised TGD [38] as standard approach (required also by Annex V WFD), i.e. assessment factors are used to derive the $QS_{freshwater}$ depending on the quality and the quantity of the data available (see table 5.1 and section 5.1.3.1 of this report).

In all Member States or Accession Countries for which information on the procedures used for QS derivation is available, approaches based on the application of assessment factors are followed as the only method of choice or as one of the methods that can be used to derive the standards, although the factors may be applied in slightly different manners and may differ in size. The assessment factor approach is generally considered as indispensable for substances for which no extensive toxicity data base is available and it is broadly accepted

as an in scientifically terms acceptable method to deal with uncertainties arising from limited data availability and knowledge in extrapolating "safe" environmental levels of substances. Since the procedures recommended in the TGD are agreed between Member States and used for the risk assessment for existing substances, these procedures should therefore be adopted for QS setting wherever useful.

However, in cases in which conditions are met to use a statistical extrapolation method for the derivation of quality standards, this approach shall also be applied (see section 8.4.1.3 for details).

8.4.1.2 Transitional, Coastal and Territorial Marine Waters

It is proposed to apply the procedures for the marine effects assessment as described in section 4.3 of the draft revised Part II of the TGD [38] as standard method, i.e. assessment factors are used to derive the $QS_{saltwater}$ depending on the quality and the quantity of the data available (see table 5.5 and section 5.1.6.1 of this report) and statistical extrapolation methods for the calculation of the PNEC for marine organisms may be used when sufficient data are available.

In order to derive quality standards for transitional, coastal and territorial marine waters it is proposed to generally use combined toxicity data sets of marine and freshwater species as data reviewed and current marine risk assessment practice suggest a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota [38] (i.e. the same data sets can be used interchangeably for freshwater and saltwater effects assessment and QS setting). Where this appears not justified based on the available evidence QS for freshwater and marine water must be derived on the basis of distinct data sets for freshwater and marine organisms.

For the derivation of QS for saltwater the assessment factors as proposed for marine risk assessment in the draft revised TGD [38] will be used (see table 5.5 of this report). Thus, for several substances the assessment factors that need to be applied might be more stringent than the standard TGD assessment factors used to derive the QS for the freshwater environment. However, the application of more stringent assessment factors for the marine environment is justified by the requirement to account for additional uncertainty due to peculiarities of the marine ecosystem such as, e.g., greater species diversity or limited data availability for marine species and use of freshwater toxicity data as surrogate. The greater species diversity in the marine environment, including the presence of a number of taxa that occur only in that environment, may mean that the distribution of sensitivities of species is broader. Thus, where only data for freshwater or saltwater algae, crustaceans and fish is available a higher assessment factor than that used for the derivation of the $PNEC_{freshwater}$ should be applied, to reflect the greater uncertainty in the extrapolation. Where data is available for additional taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a data set can be lowered [38] (see table 5.5).

Thus, an additional assessment factor is not automatically applied in the marine effects assessment but only if the data do not appropriately represent the community that dwells in the marine ecosystem. If marine life forms are sufficiently represented in the data set available, the assessment factors to be applied are not different from those used in the freshwater effects assessment.

In case of coastal and territorial marine waters additional consideration should be given to the prevention of pollution of the entire maritime area, including the open sea. Therefore,

quality standards for the coastal and territorial marine environment should prevent any significant input of hazardous substances into the open sea. According to Article 1 of the Water Framework Directive [1], this may be achieved by “continuously reducing discharges, emissions and losses, with the ultimate aim of achieving concentrations in the marine environment near background values for naturally occurring substances and close to zero for man-made synthetic substances” (this is consistent with the OSPAR strategy for the North-East Atlantic with regard to hazardous substances and a similar strategy of HELCOM for the Baltic Sea).

For Priority Hazardous Substances effect based quality standards are inappropriate to control the risks exerted by these substances in the open sea. Instead, the focus for this group of chemicals should primarily be on identifying sources, major emissions and pathways to the marine environment in order to establish the most appropriate and effective measures to reduce the releases which lead to contamination of the marine environment [38]. For Priority Hazardous Substances it should therefore be considered to define the **detection limit as Borderline Quality Standard** for territorial marine waters in the case of man made synthetic substances. For naturally occurring substances such as, for instance, cadmium and mercury the upper limit of the natural background level range in these marine waters should apply in order to achieve the objectives of the WFD.

Background levels of naturally occurring substances in marine waters have yet not been defined and agreed by Member States. Endeavours to define such agreed levels are therefore required, but beyond the scope of this study.[19]

8.4.1.3 Application of Statistical Extrapolation Methods to Derive Quality Standards

According to the draft revised TGD [38] the effects assessment performed with the assessment factor method can be supported by a statistical extrapolation method if the data basis is sufficient for its application.

Therefore, it is suggested to use statistical extrapolation methods supplementary to the QS derivation with the standard TGD assessment factor method in case the data base of the substance concerned is sufficient. To this end the recommendations given in section 5.1.3.2 of this report may be followed and, in principle, the same approach can be used as described in section 8.6.2. The decision which of the two quality standards derived by application of the extrapolation method or by the assessment factor method may be finally adopted as QS should be based on expert judgement.

8.4.2 Quality Standards Referring to Substance Levels in Sediment

8.4.2.1 Freshwater Sediment

The quality standard for sediment dwelling organisms is, in principle, calculated as outlined in section 5.1.3.3 for the calculation of the $PNEC_{sediment}$. If results of toxicity tests with sedi-

[19] OSPAR has developed and adopted "Background/Reference Concentrations" (BRCs) as assessment criteria for naturally occurring substances. BRCs for trace metals in sea water, sediments and biota (mussel tissue) and for some persistent organic contaminants in sediments and sea water are given in the OSPAR Status Report 2000 for the North-East Atlantic (Chapter 4: Chemistry). The report can be downloaded from the OSPAR web-site (http://www.ospar.org/eng/html/welcome.html).

ment organisms are available, the quality standard is calculated using the assessment factors given in table 5.2.

However, as toxicity data for benthic organisms are normally lacking for many substances, in such cases the $QS_{sediment}$ is calculated using the equilibrium partitioning method as described in section 3.5.3 of Part II of the draft revised TGD [38]:

$$QS_{sed.wet\_weight}\ [mg.kg^{-1}] = \frac{Kp_{SPM\text{-}water}\ [m^3.m^{-3}]}{bulk\ density_{SPM.wet}\ [kg.m^{-3}]} * QS_{water}\ [mg.l^{-1}] * 1000$$

with:

$Kp_{SPM\text{-}water}$	partition coefficient suspended particulate matter – water
$bulk\ density_{SPM.wet}$	1150 $kg.m^{-3}$

As the formula only considers uptake via the water phase, a correction is made for substances with log Kow >5 as significant uptake by food ingestion may take place. To this end, the PNEC sediment is divided by 10.

In case there is only a marginal effects data base for benthic organisms available the QS should be derived on the basis of both the effects data and the equilibrium partitioning approach. A recommendation for the final QS will be given based on expert judgement taking all available information into account.

8.4.2.2 Marine Sediment in Transitional, Coastal and Territorial Waters

With respect to the quality standards setting for marine sediments it is proposed to follow the strategy recommended in section 4 of the draft revised TGD [38] for effects assessment with marine benthic organisms (this is basically the same approach as proposed in section 8.4.2.1 of this report for freshwater sediment. However, more stringent assessment factors may apply depending on the quality and quantity of toxicity data available; see section 5.1.6.2 and tables 5.6 and 5.7 for details).

Regarding the sediment quality standards for synthetic, man made Priority Hazardous Substances, it is proposed to define the detection limit of these substances in suspended marine sediment of territorial marine waters as borderline quality standard for the same reasons as outlined in section 8.4.1.2 for seawater.

8.4.3 Quality Standards referring to Substance Levels in Biota

Quality standards referring to substance levels in biota need to be derived in order to prevent secondary poisoning of top predators as well as adverse effects on human health through ingestion of contaminated food.

It is proposed to calculate the respective quality standards for substance levels in biota if the triggers given in table 8.1 concerning secondary poisoning or human health effects are met. The standard figures and procedures as given in section 3.8.3 of the draft revised TGD [38] will be used (see also sections 5.1.4 and 5.1.6.3 of this report).

Based on the lowest relevant threshold level for top predators or human health (e.g. NOEC, NO(A)EL or ADI/TDI in case of humans) and the standard figures given in the TGD for (sea)food consumption, body weights of top predators (birds, mammals) and humans, food conversion factors and other assessment factors, concentrations in fish and/or mussels are calculated ruling out adverse effects due to ingestion of these aquatic organisms. The calculated "safe" levels for fish or mussels are the biota quality standards.

However, as – for various reasons - it is not desirable to perform routine monitoring of biota for compliance checking, a corresponding concentration in water will be calculated as surrogate standard, using the safe level in biota and the BCF (or octanol water partition coefficient) of the substance concerned[20].

Quality standards referring to levels in biota will thus be given for two different objectives of protection: top predators and human health.

In accordance with the respective TGD [38] scenarios on secondary poisoning, it is assumed that top predators prey to 100% on the aquatic organisms (i.e. the $NOEC_{food}$ for the predators may be exhausted for 100 %).

With regard to "seafood" uptake by humans no standard approach or convention exists. The use of a consumer intake model considering all uptake routes was deemed too complex and, moreover, often not possible as not all exposure routes and the contamination levels of the relevant food commodities might be known. Therefore, proposals for dealing with that issue in a rather simple but practicable manner have been made and the Expert Advisory Forum was invited to express its opinion on this issue.

The majority of comments received after EAF(2) were in favour of the proposal that by convention the uptake of a substance with fishery products should not contribute to more than 10% of the relevant threshold level for humans (i.e. the ADI/ TDI /$NO(A)EL_{oral}$ must not be exhausted for more than 10% by uptake of food originating from aquatic environments)[21]. Therefore, this approach has been adopted for the derivation of the quality standard referring to the protection of human health from adverse effects due to the ingestion of food originating from aquatic environments.

8.4.4 Quality Standards Referring to Levels in Water Intended for the Abstraction of Drinking Water

In accordance with Articles 7(2,3) and 16(1) of the WFD it is required to protect the possibility of drinking water abstraction from surface waters. As according to the opinion of the majority of the Expert Advisory Forum drinking water limit values should not be used to set quality standards for drinking water, the procedure described in the following was devised:

1. In case a "A1 value" referring to simple surface water treatment (e.g. rapid filtration and disinfection) is fixed in the "drinking water abstraction" Directive 75/440/EEC [17] and this "A1 value" is lower than the quality standard required to safeguard the other objectives of protection (freshwater community, sediment quality, and quality of biota in order to protect humans or top predators from secondary poisoning by food ingestion), it is proposed to adopt the "A1 value" as quality standard for surface freshwater.

   If no "A1 value" has been set in CD 75/440/EEC but a drinking water standard is available according to Council Directive 98/83/EC [20] (concerning the quality of water intended for human consumption) and this drinking water standard is lower than the quality standard

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[20] For hydrophobic organic substances (exceeding the triggers given in table 8.1) the biota quality standards may be also given as concentration in suspended particulate matter of the EU standard water. For details see section 8.4.1.

[21] Another proposal was to base the maximum acceptable percentage up to which substance uptake by seafood ingestion may contribute to the threshold level for human health on the energy content of seafood and the energy requirement of a human being. However, this proposal was given preference in only one comment received after EAF(2). In another comment, it was suggested that the approach should be as far as possible in line with the methods for determining the maximum residue levels for plant protection products.

required to safeguard the other objectives of protection, the subsequent procedure is suggested:

2. An assessment is performed with the objective to derive a quality standard ensuring the possibility of drinking water abstraction by simple treatment (category A1 in CD 75/440/EEC). In this context, the substance specific removal efficiencies of the simple surface water treatment methods in use must be considered. As there is no sufficiently accurate method for the prediction of removal efficiencies for surface water treatment available [6], experts in drinking water processing technology should be involved in the assessment. The final quality standard for drinking water abstraction from surface water should be no higher than the drinking water standard according to CD 98/83/EC divided by the fraction not removable by simple treatment.

3. For those substances on the working list for which "A1 values" or quality standards have not been fixed in the context of Council Directives 75/440/EEC or 98/83/EC, provisional drinking water quality standards are calculated by the TGD-procedure described further below in this section. If this provisional drinking water quality standard is lower than the quality standard required to safeguard the other objectives of protection, in principle the same assessment procedure as described under (2.) is proposed:

   An assessment is performed with the objective to derive a quality standard ensuring the possibility of drinking water abstraction by simple treatment. Experts in drinking water processing technology should be involved for the reasons given under (2.). In addition, the participation of experts in human toxicology might also be required in order to assess the appropriateness of the provisional standards calculated by the rather simple TGD-procedure, not taking account of possible substance specific toxicological peculiarities. The final quality standard for drinking water abstraction from surface water should be no higher than the concentration in drinking water considered as acceptable in terms of toxicological aspects divided by the fraction not removable by simple treatment.

Calculation of provisional drinking water quality standards according to the TGD

Based on the recommendations given in Part I of the TGD [6] (section 2.4.3 and Appendix VII) it is proposed to calculate the quality standards for water intended for human consumption using assumptions as follows:

Water uptake 2l/d, body weight 70 kg. Threshold level for human health: either ADI/TDI, lowest relevant NOEL*100^{-1} or the 10^{-6} unit risk value for cancer risk. The provisional quality standard for drinking water is calculated with the consideration that uptake by drinking water should in any case not exceed 10% of the threshold level for human health.

$$QS_{DW} = \frac{0.1 * TL_{HH} * BW}{Uptake_{DW}}$$

with:

QS_{DW}	quality standard for drinking water (mg/l)
TL_{HH}	threshold level for human health (ADI/TDI etc. in mg/kg body weight per day)
BW	body weight (70 kg)
$Uptake_{DW}$	uptake drinking water (2 l per day)

8.5 Derivation of Quality Standards for Plant Protection Products

Where available, the quality standard setting for plant protection products (PPP) is exclusively based on the effects data identified as relevant in the monograph produced in the course of the risk assessment according to Council Directive 91/414/EEC for the respective substance.

As the aquatic effects assessment according to Directive 91/414/EEC is – in principle - equivalent to the aquatic effects assessment for new and existing substances as laid down in the TGD (cf. section 5.4), it is proposed to divide the lowest relevant long-term toxicity datum (e.g. a single species NOEC) by the long-term TER-trigger (10; TER ≈ Toxicity Exposure Ratio) in order to derive a PNEC-equivalent and the QS_{water} not to be exceeded.

$$QS_{water,\ PPP} = NOEC_{min} / TER\text{-}trigger_{\ long\text{-}term}$$

However, as risk assessment for plant protection products in the context of CD 91/414/EC is focused on the acceptability of effects that may occur in small water courses (e.g. ditches) in the vicinity of the treated area, specific weight is given to the recovery potential of these systems after transient exposure. This might be the reason why effects on algae are not considered exactly the same way as any other effects on invertebrates or fish. Many alga species have a high recovery potential and recover fast once the toxicant concentration falls below the effect level.

Thus, the objective of the PPP risk assessment differs to some extent from the objective that is followed by the quality standard. The long-term quality standards refer to "annual average" concentrations and it is, therefore, required to give the algae toxicity data another weight for the purpose of quality standard setting. Hence, it is proposed to apply an assessment factor of 10 (equivalent to the long-term TER trigger for aquatic invertebrates or fish) to the lowest valid $NOEC_{algae}$ in the data set, if algae are the organisms most sensitive to the PPP concerned.

If in a higher tier risk assessment a multi-species study (e.g. a mesocosm study) is identified as most relevant, this study is considered and the NOEC of that higher tier study is used in the derivation of the QS_{water}, if proposed in the monograph as appropriate.

In addition to the quality standard referring to a annual reference concentration, it is suggested to calculate a second MAC-QS accounting for transient concentration peaks as proposed in sections 7.2 and 8.2 of this report.

In order to derive the MAC-QS, the lowest relevant acute $L(E)C_{50}$ in the data set may be divided by the relevant short-term TER-trigger (in analogy to the calculation of short-term TER in the PPPRA):

$$MAC\text{-}QS_{water,\ PPP} = L(E)C50_{min} / TER\text{-}trigger_{\ short\text{-}term}$$

This short-term TER trigger is 100 for fish and invertebrates or 10 for algae. If algae are the organisms most sensitive to acute effects, it should be carefully assessed whether the application of a TER-trigger of 10 for algae is justified, given the differences in the objectives of the PPP risk assessment and a quality standard[22]. Generally, the guidance given in the TGD with respect to the variation of assessment factors when assessing possible effects due to intermittent release of a substance should be taken into account (see section 7.2). In addi-

[22] In this context it should also be considered that compliance monitoring is usually not carried out in small water bodies adjacent to fields. Therefore, taking possible dilution into account, it is most likely that headwaters feeding the water bodies in which compliance monitoring is conducted are even more polluted.

tion, the MAC-QS should in no case be higher than the long-term QS referring to the annual reference concentration.

With regard to sediment, secondary poisoning and human health effects it is proposed to conduct the quality standard derivation as for the "normal" organic chemicals, under consideration of the argumentation related to these issues in the risk assessment monograph (if available).

Historic plant protection products (in this study: DDT and its isomers as well as the "Drins" aldrin, dieldrin, endrin, isodrin) should be considered as "normal" organic chemicals and the quality standards for these substances are derived according to the procedures proposed in section 8.4.

8.6 Derivation of Quality Standards for Metals

For metals, it could be required to differentiate between freshwater and marine water in quality standard setting. Reasons are of both biological (ecological and physiological) and geochemical (metal phase distribution and speciation) nature. For several metals differences in sensitivity larger than a factor of 10 were found between saltwater and freshwater species of the same taxonomic groups [38]. Therefore, where appropriate, toxicity data sets (as well as BCF data) for marine and freshwater organisms may not be combined and it may be necessary to set specific quality standards referring to freshwater or marine ecosystems.

8.6.1 Use of the "Added Risk" Approach

Since metals are naturally occurring substances it is proposed to adopt the "added risk" approach as used in the Netherlands for the derivation of EU quality standards for metals (see section 4.1.3.1 of this report). This approach facilitates to account for natural background concentrations in an appealingly simple manner: A maximum permissible addition (MPA) to the background level of a certain metal is calculated. The MPA is the amount of metal that maximally may be added to the background concentration of this metal without adversely affecting the assessed ecosystem.

$$QS_{add} = C_{backg} + MPA$$

Two assumptions are the basis of this approach:

1. It is not relevant to which extent the background concentration of a metal has an impact on ecosystem structure and function since any potential adverse or positive effect of the background concentration can be considered as effect contributing to the natural biodiversity of ecosystems.
2. As species in an ecosystem are adapted to the prevailing background level, it is assumed that the same amount of a metal added by human activities causes in principle the same effect, provided all environmental parameters determining metal toxicity are equal except the background level of the metal concerned (i.e. not the "absolute" level of a metal is decisive for the occurrence/extent of adverse effects but only the added amount).

The background concentration and the MPA are independently derived values. Real world background concentrations can be derived on the basis of monitoring data of relatively pristine areas or be based on calculations using geological and hydrological data (estimation of

real world background levels for metals is beyond the scope of this study). For the purpose of quality standard setting, background levels may be defined and set by the competent bodies for any spatial level/resolution (e.g. EU, Member States, regions in MS) that is considered reasonable[23].

With regard to effects assessment, the added risk approach implies that the MPA is derived from toxicity data that are based on the added metal concentration in toxicity tests (i.e. the added metal concentration is considered 100% bioavailable). Thus, the maximum permissible addition and hence the quality standard derived by the added risk approach refer to the "bioavailable" fraction in "real world" samples.

The use of the added risk approach implies further that there is no risk for deficiency of essential metals at the level of the calculated quality standard, as the QS derived in this approach is defined as the maximum permissible addition to the background concentration. By definition, the background concentration in a given ecosystem provides the organisms in that ecosystem with the required essential metals.

8.6.2 Use of Statistical Extrapolation Technique and TGD Assessment Factor Method for Quality Standard Derivation

For metals with large databases (including many long-term toxicity data of a range of aquatic species) it is proposed to use a statistical extrapolation method as standard method for the calculation of the maximum permissible addition. The method of Aldenberg and Jaworska (2000) [31] seems most suitable for this purpose as it is possible with this method to calculate a confidence interval (normally the 90% interval) for the 5-percentile cut-off value of the species sensitivity distribution (SSD). The input data used to estimate the SSD should be NOEC data selected according to the criteria recommended in the draft revised TGD [38] (cf. section 5.1.3.2 of this report).

The 5-percentile cut-off value according to Aldenberg and Jaworska is calculated as follows:

$$\log P5 = X_m - k * s$$

with:

P5 =	5^{th}-percentile cut-off value
X_m=	mean of log-transformed NOEC data
k =	extrapolation constant depending on protection level and sample size (according to Aldenberg and Jaworska [31], see Annex 2 of this report)
s =	standard deviation of log-transformed data

The extrapolation constant *k* is taken from Aldenberg and Jaworska [31] (cf. Annex 2 of this report). Three values are given for *k*. The 5-percentile cut-off-value (5P-COV) is calculated with the median estimate for *k* whereas the confidence limits are calculated using the upper and lower estimates of *k*.

According to the recommendations given in the draft TGD [38] the 5P-COV of the SSD should be derived as an intermediate value in the determination of the MPA. The final MPA is calculated as 5-percentile cut-off value divided by an assessment factor reflecting further uncertainties identified.

MPA = P5-COV / AF (AF: max. 5 – min. 1; default: 5)

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[23] In Germany, Finland, the Netherlands and Sweden metal background levels for inland waters and, in the case of Finland and Sweden, for marine waters have been defined. In Austria the definition of such levels for inland waters is in progress.

In determining the size of the additional assessment factor to be applied in order to derive a MPA based on the 5th percentile, the following points can be used as a guide [38, 39]:

- The overall quality of the database and the end-points covered, e.g., if all the data are generated from ”true” chronic studies (e.g., covering all sensitive life stages);
- The diversity and representativeness of the taxonomic groups covered by the database, including also the variation represented relating to differences in the life forms, feeding strategies and trophic levels of the organisms;
- The mode of action of the chemical;
- Statistical uncertainties around the 5th percentile estimate, e.g., reflected in the goodness of fit or the size of confidence interval around the 5th percentile;
- Comparisons between field and mesocosm studies and the 5th percentile and mesocosm/field studies to evaluate the laboratory to field extrapolation.

Besides the derivation of the MPA by statistical extrapolation of the SSD, the MPA should be derived using the standard TGD assessment factor approach for PNEC derivation on the same database. If mesocosm studies are available, they should also be evaluated and a MPA derived following the TGD. A comparison of the two, possibly three points above should be carried out and a final MPA determined with full justification. In case the database is not sufficient to apply statistical extrapolation, it is suggested to follow the standard TGD approaches as recommended.

8.6.2.1 Quality and Quantity of Data required

Where possible and appropriate, a pre-selection of the data should be performed in relation to realistic environmental parameters for Europe. Confidence can be given to the MPA derivation based on statistical extrapolation if the database contains preferably more than 15, but at least 10 NOECs, for different species covering at least 8 taxonomic groups (see table 8.3). Deviations from these recommendations can be made, on a case-by-case basis, through consideration of sensitive endpoints, sensitive species, mode of toxic action and/or knowledge from structure-activity considerations.

Table 8.3: Species required to apply statistical extrapolation for freshwater [38] [24]

• Fish (species frequently tested include salmonids, minnows, bluegill sunfish channel catfish, etc.)
• A second family in the phylum Chordata (fish, amphibian, etc.)
• A crustacean (e.g. cladoceran, copepod, ostracod, isopod, amphipod, crayfish etc.)
• An insect (e.g. mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge, etc.)
• A family in a phylum other than Arthropoda or Chordata (e.g. Rotifera, Annelida, Mollusca, etc.)
• A family in any order of insect or any phylum not already represented
• Algae
• Higher plants

[24] For saltwater and sediment no specific species requirements (or better: taxonomic groups and foraging strategies) have been defined so far. However, it is evident from the concept of the SSD extrapolation methodology that different taxonomic groups and foraging strategies should be adequately represented in the input data set.

It is important to include any available knowledge on the mode of action of the chemical, in order to evaluate the need to include possible other (sensitive) taxonomic groups or exclude possible over-representation of certain taxonomic groups, realising that the mode of action may differ between short-term effects and long-term effects and between taxonomic groups. The acute toxicity database of the substance can be used to assist in evaluating the representativeness and the sensitivity of particular species in the SSD. It can also identify acutely sensitive species, which may be missing from the NOEC database. [39]

8.6.2.2 Aggregation of Multiple Data for One Species

It is proposed to follow the recommendations given in the draft report of the "London Workshop" [39], which also have been adopted in the draft revised TGD [38]:

1. The full database should be carefully evaluated to extract information (e.g., on sensitive species and/or end-points), which may be lost when ”averaging” the data to a single value (to be used for either the SSD or the ”standard” PNEC).
2. The data of the most sensitive end-point should be used as the representative for the species. In this context, demographic parameters and bio-markers can be used as endpoints, if they are relevant in terms of population dynamics.
3. Multiple values for the same endpoint with the same species should be investigated on a case-by-case basis, looking for reasons for differences between the results.
4. For comparable data on the same end-point and species the geometric mean should be used as the input value for the calculation of the SSD. If this is not possible, e.g. because results which are considered valid are too variable, then consider grouping and combining the values, e.g. by pH ranges, and using reduced numbers of values. The full data set could also be used if necessary.
5. Where it is considered that the results are limited to certain conditions (e.g. not appropriate for low pH) then these limitations should be explained.

8.6.2.3 Testing Distributions for Goodness of Fit

Different distributions like e.g. log logistic, log normal or others may be used. The log-normal distribution is a pragmatic choice from the possible families of distributions because of the available description of its mathematical properties (methods exist that allow for most in depth analyses of various uncertainties). The Anderson–Darling goodness of fit test can be used in addition to the Kolmogorov-Smirnov-test, as a criterion for the choice of a parametric distribution for comprehensive data sets, because it gives more weight to the tails of the distribution. [38]

Further guidance is given in the draft of the revised TGD [38]:

- Whatever the fit to a distribution, results should be discussed with regards to the graphical representation of the species distribution and the different p values that were obtained with each test.
- Finally, any choice of a specific distribution function should be clearly explained.
- If the data do not fit any distribution, the left tail of the distribution (the lowest effect concentrations) should be analysed more carefully. If a subgroup of species can be identified as particularly sensitive and if the number of data on this subgroup is sufficient, the distribution can be fit to this subgroup.

- The SSD method should not be used in cases where the data do not fit a distribution.

8.6.3 Consideration of Water Quality Parameters in QS Setting for Metals

For metals, it is important to define the bioavailable concentration, since this is the fraction of the total concentration which is important for toxicity, both in the laboratory tests and in the "real" environment. Due to several physico-chemical processes, metals exist in different chemical forms which might differ in bioavailability. Thus, the bioavailability of metals in both laboratory tests and in the environment may be affected by several physico-chemical parameters [44] such as the pH, hardness of water and the content of dissolved organic matter (DOM).

Although metal bioavailability to different aquatic life forms as well as the modifying influence of water quality parameters are subject of extensive ongoing research programs, there is – for most metals - not yet enough scientific knowledge available to describe quantitatively the influence of water quality parameters on bioavailability and long-term toxicity for the different aquatic life forms representing freshwater or marine communities [59] and, hence, to take these parameters into consideration in setting quality standards.

This is in the following illustrated for the water quality parameters hardness, pH and dissolved organic matter:

- ***Hardness:*** Hardness is usually considered as one of the main factors or as the main factor influencing metal bioavailability[25]. However, the generally assumed inverse relationship between hardness and metal toxicity is based mainly on the results from acute toxicity tests conducted with relatively high metal concentrations. These acute tests were mostly conducted with fish, it is not clear whether such a relationship between hardness and toxicity exists for other species which may have different uptake mechanisms. Furthermore, the relationship between hardness and chronic toxicity of metals appears to be much less consistent, especially in the range of hardness between 50 and 200 mg/l (as $CaCO_3$): The available chronic toxicity studies with zinc, cadmium, copper and chromium usually showed a 2- to 3-fold decrease in toxicity with increasing hardness, with a maximum of around 5-fold. Besides this also examples of tests exist in which no effect or even an increase of toxicity with increasing hardness was found [40, 44]. Recently it has been shown for copper that there is no correlation between hardness and long-term toxicity to algae and daphnids [47]. As for acute toxicity, the effects of hardness on chronic toxicity can be species dependent, because of differences in uptake mechanisms [44]. In both the cadmium and zinc risk assessment draft reports the generic PNEC is not corrected for water hardness [40, 41]. However, for cadmium an increasing trend of chronic values with increasing water hardness was established for *Daphnia magna*, *Pimephales promelas* and *Salmo trutta* in a recent EPA-study (reference not given in [41]). Therefore it is proposed in the draft risk assessment report for cadmium [41] to consider a water hardness correction of the $PNEC_{water}$ for risk characterisation at a local or regional scale.
- ***pH:*** With regard to the relationship between pH and metal toxicity the body of evidence seems also poor. For instance, no significant correlation was found between pH and the

[25] In some MS the national QS of some metals are hardness related (**Cd**: F; **Pb**: F, IRL, UK; **Cu**, **Ni**: F, IRL, SP, UK). However, only Spain provided some information with regard to the underlying methodological approaches and assumptions (section 4.6.2).

Industry proposes to consider relationships between hardness (as well as other water quality parameters such as pH and DOM) and metal toxicity by, e.g., using the US-EPA methods [50]. However, the relationships described in the EPA document are only based on short term toxicity data.

log-transformed acute or long-term cadmium toxicity data in an analysis conducted in the context of the ongoing cadmium risk assessment [42]. The relation between pH and zinc toxicity was also investigated in the ongoing zinc risk assessment [40]. In the respective draft report it is concluded that the few contradicting studies with only two species cannot be used as a basis for a pH-normalisation of aquatic toxicity. Also, Crommentuijn et al. [44] concluded in their study on maximum permissible concentrations for metals that pH related EQS cannot be derived on the basis of the current knowledge. However, recent research results indicate that for daphnids and algae a correlation between long-term copper toxicity and pH exists. The effect of pH on long-term toxicity was inverse for the investigated species. Whereas for daphnia a drop in toxicity with rising pH was observed copper toxicity to algae increased with rising pH. The reasons for the observed differences are not yet known [47].

- ***Dissolved organic matter (DOM):*** In the draft zinc and cadmium risk assessment reports [40, 42] the possibilities to consider the influence of DOM on metal toxicity are discussed. Conclusions regarding Cd are that complexation of cadmium by dissolved organic ligands cannot be calculated unequivocally and that the free metal ion is very rarely an order of magnitude smaller than the total concentration [42]. For zinc the available data and the model parameters proposed by industry are deemed not sufficient to correct for binding of Zn to DOM [40]. In the voluntary draft risk assessment for mercury in the marine environment conducted by Euro Chlor [49] it is mentioned that positive relationships between dissolved mercury and DOM or between mercury adsorbed to particles and their organic carbon content exist. However, no quantitative relationships are given. Thus, in none of the risk assessments bioavailability is corrected for metal sorption to DOM. However, for copper an inverse correlation between DOC and long-term toxicity to daphnids and algae could be shown recently [47].

Proposal:

For the time being, it is recommended to take no account of the influence of the above mentioned physico-chemical parameters on metal bioavailability and, hence, long-term toxicity to different aquatic life forms because of the uncertainties in the data and/or the possible methodological approaches. This recommendation applies for the metals, lead, mercury and nickel.

For cadmium the situation is different, as for this metal an (approximate) assessment of bioavailable concentrations might be possible. A regression function based on increasing chronic toxicity values of *Daphnia magna*, *Pimephales promelas* and *Salmo trutta* with increasing water hardness could be established recently and it is suggested in the ongoing cadmium risk assessment [41] to consider this water hardness correction of the $PNEC_{water}$ for risk characterisation at a local or regional scale.

The development of biotic ligand models (BLMs) for Cd, Ni, Pb and other metals (such as Cu and Zn) is in progress [52, 54, 55, 56, 57, 58, 59]. Industry expects that BLM models applicable for the prediction of long-term effects will be available within 2 years for some of the mentioned metals. If in the future these models and comprehensive data for validation become available, it is recommended to carefully evaluate their utility in the assessment of bioavailability and the calculation of appropriate local quality standards.

However, for metals that are classified as priority hazardous substances (i.e. cadmium and mercury), this exercise may not be justified as the controls proposed for the priority hazardous substances shall aim at the cessation or phasing out of discharges, emissions and

losses no longer than 20 years after the adoption of these proposals by the European Parliament and the Council.

8.6.4 Calculation of Quality Standards for Metals

Bioavailability of Metals in Toxicity Tests

It is proposed to consider metals that are added to the test medium as dissolved and 100% bioavailable under the conditions used in laboratory tests (usually very low content of dissolved organic matter and suspended particulate matter, use of flow through test systems with a rapid turnover rate for test media, use of soluble metal salts etc.). Thus, the maximum permissible addition refer to the "bioavailable" fraction in "real world" samples. This proposal is in line with the approach followed by the Netherlands [28] and in the draft risk assessments for Cd [41] and Zn [40].

"Bioavailable" Metal Fraction in "Real World" Water Samples

As for most metals adequate methods / data are lacking to quantitatively determine the fraction of a metal that is bioavailable to the aquatic life forms (i.e. species from various phyla differing in physiology and feeding types) representing the aquatic community, there may mainly two options be available to address bioavailability of "real world" samples:

1. Only the "dissolved" fraction is considered bioavailable. This is the approach followed in the ongoing risk assessment for Cd and Zn and in the Netherlands.

   ⇒ Total amount of a metal in a water sample is corrected for metal sorption to SPM.

   By convention, the metal fraction present in a water sample after filtration through a 0.45µm filter is considered as "bioavailable". However, it should be noted that not the entire amount in this "dissolved" fraction may be bioavailable as a certain amount of metal may be bound to colloids or be sequestered.

2. The "total" content of a metal in a water sample is considered as bioavailable. This approach is followed by Germany, Norway and Sweden.

   ⇒ Reasons to follow this approach are:
   - Sequestered or otherwise bound / sorbed metals may become bioavailable as physico-chemical water parameters change
   - Organisms like filter feeders may also take up metals from SPM during gastro-intestinal passage

Although the comments received after the session of the Expert Advisory Forum in October 2001 indicate that a majority of delegations support the consideration of bioavailability in the setting of quality standards for metals, opinions differ how this could be best achieved. Approximately one half of the comments received were in support of option 1 whereas the other half was in favour of option 2.

Calculation of the Maximum Permissible Addition (MPA)

As, for the time being, it is not possible to decide whether one of the above described options for the consideration of metal bioavailability in “real world” water samples is generally superior in reflecting metal bioavailability under all possible environmental conditions and for all life forms, it is proposed to calculate two MPAs, one referring to metal levels in water and one referring to levels in suspended particulate matter of the EU "standard water" (15 mg/l SPM[26]) using reliable SPM – water partition coefficients.

- A MPA for water referring to the "bioavailable" (dissolved) metal [µg Metal / l] is calculated based on the underlying toxicity tests
- A MPA for SPM [µg Metal / kg SPM] is calculated based on the MPA_{water}

Quality standards for other SPM concentrations in water samples[27] may be calculated following the approach outlined in section 8.4.1.

Calculation of the final QS Referring to Metal Levels in Water Samples:

The background concentration is either added as concentration in water or as concentration in SPM in order to derive a QS_{water} or a QS_{SPM}.

- $QS_{water} = C_{background.water} + MPA_{water}$
- $QS_{SPM} = C_{background.SPM} + MPA_{SPM}$

8.6.5 Quality Standard Derivation for Sediment

The added risk approach as outlined for water in section 8.6.1 applies also to sediment.

If sufficient NOEC data for benthic organisms are available (≥ 10 NOEC data for different species representing different living and feeding conditions) it is recommended to use the same statistical extrapolation methodology as described in section 8.6.2 for the MPA_{water} to derive the $MPA_{sediment}$.

If not enough data for benthic organisms are available to use the species sensitivity distribution method, the standard TGD approach [38] as - in principle - described for organic substances in freshwater sediment (sections 8.4.2.1 and 5.1.6) should be followed (i.e. the assessment factor approach for toxicity data of benthic organisms and the equilibrium partitioning method for calculation of a $MPA_{sediment}$ on the basis of the MPA_{water}[28]). It should be decided by expert judgement whether the $MPA_{sediment}$ derived on the basis of toxicity data of benthic organisms or calculated from the MPA_{water} should be used.

Industry [52] proposes to integrate bioavailability into the evaluation of sediment toxicity data by the Acid-Volatile Sulphide (AVS) content in relation with the Simultaneously Extracted Metals (SEM). It is suggested to use the organic carbon normalised excess SEM concentration $(SEM-AVS)/f_{oc}$ as a basis for assessing the toxicity of metals in sediment, where f_{oc} is the organic carbon content of the sediment. A metal contaminated sediment is not expected

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[26] TGD Part II, section 2.3.8.4 – calculation of PEC_{local} for sediment [6]

[27] For instance, the Dutch "standard water" contains 30 mg/l suspended particulate matter and in Germany a SPM content of 25 mg/l is considered as a representative national average.

[28] In the case of metals, only empirically derived coefficients for the partition between water and sediment (i.e. $K_{water\text{ -suspended particulate matter}}$) should be used.

to cause adverse effects on the benthos if (SEM-AVS)/foc is less than 100 µmol/foc. At this concentration, the metals are unlikely to be bioavailable and therefore cannot cause toxicity. This approach has been accepted by the Technical Meeting (TM I, 2001) in the context of the ongoing zinc risk assessment for local risk assessments [52].

However, in the draft zinc risk assessment report some comments on limitations and uncertainties of the SEM/AVS concept are given [40].

1. In some cases there appeared to be a linear accumulation of metals with increasing sediment metal concentration irrespective of the SEM/AVS content. This questions the validity of the assumption that when the SEM/AVS < 1, the metals would not be bioavailable.
2. Both the qualities of the SEM-data and the AVS-data are under recent discussion. The experimentally determined SEM values may underestimate the actual concentration of metals, while the AVS values from pooled sediment samples may overestimate the actual AVS concentration in the top, aerobic sediment layer.
3. Further research is required to the proposed SEM/AVS concept to better implement its significance:
   - for benthic organisms that have a habitat at or slightly above the sediment surface where aerobic conditions prevail, and the AVS-content will be very low;
   - to protect aquatic systems from metal release associated with sediment suspension;
   - for the transport of metals into the food web either from sediment ingestion or the ingestion of contaminated benthos; and
   - for organisms that are capable of actively extracting (essential) metals to accelerate uptake.

Due to the above comments on the SEM/AVS concept, its use for a generic approach is not adopted in the ongoing Zn risk assessment.

With respect to the methodological approach for sediment quality standard setting of metals, the SEM/AVS concept seems also not applicable because the sediment quality standards shall refer to suspended particulate matter and not to sediment at the ground of water bodies (for reasons see section 8.3). As the suspended particulate matter is entirely aerobic, the SEM/AVS concept cannot be applied (negligible levels of metal sulphides under aerobic conditions).

8.6.6 Specific Considerations with Respect to Transitional, Coastal and Territorial Marine Waters

It is proposed to apply, in principle, the same approach as described for freshwater and freshwater sediment in sections 8.6.1 to 8.6.4 for the derivation of quality standards for transitional, coastal and territorial marine waters.

As for several metals differences larger than a factor 10 in sensitivity between saltwater and freshwater species of the same taxonomic groups were found, the recommendation in the marine risk assessment section of the draft revised TGD [38] should be followed and only toxicity data of marine organisms be used in the derivation of quality standards for coastal and territorial marine waters.

Quality standards for the territorial marine environment (water as well as sediment) should prevent any significant input of hazardous substances into the open sea. For Priority Hazardous Substances effect based quality standards are inappropriate to control the risks ex-

erted by these substances. In conclusion, for cadmium and mercury the upper limit of the natural background level range in sediment of territorial marine waters should apply as borderline quality standard.

Saltwater

In case the method to extrapolate the 5-percentile of the species sensitivity distribution as described in section 8.6.6 for metals in freshwater cannot be applied to derive the maximum permissible addition for saltwater ($MPA_{saltwater}$), the provisions set out for the marine effects assessment and PNEC derivation as described in the draft revised TGD [38] may be followed (see section 5.1.6.1), i.e. assessment factors are used to derive the $MPA_{saltwater}$ depending on the quality and the quantity of the data available (table 5.3).

Marine Sediment

If not enough data on benthic organisms are available to use the species sensitivity distribution method for the calculation of the $MPA_{sediment, marine}$ (see section 8.6.2), the provisions set out for the marine effects assessment and PNEC derivation as described in the draft revised TGD [38] may be followed (i.e. the assessment factor approach for toxicity data of benthic organisms and the equilibrium partitioning method for calculation of a $MPA_{sediment, marine}$ on the basis of the $MPA_{saltwater}$; see section 5.1.6.1). The decision whether the $MPA_{sediment, marine}$ derived on the basis of toxicity data of benthic organisms or calculated from the $MPA_{saltwater}$ should be used may be based on expert judgement taking into account all available information.

8.6.7 Metal Quality Standards Referring to Substance Levels in Biota

For metals, in principle the same TGD-based approach should be followed as outlined in section 8.4.3 for organic substances.

With regard to human health, quality standards for levels in biota are already set by Council Regulation (EC) No 466/2001 [43] for cadmium, lead and mercury in seafood. Corresponding metal concentrations in water may be derived using the relevant BCFs of the metals.

With respect to the use of BCF data it must be taken into account that inverse relationships have been observed for metals where the highest BCF values for metals were found in waters with the lowest metal concentrations (and vice-versa). Thus, BCF values of studies conducted in waters with extremely low (i.e. lower than in the upper range of background levels) or high metal concentrations will not be used for the calculation of quality standards. The required BCFs may be either obtained by calculating species specific geometric means from BCF studies conducted with environmentally relevant metal concentrations in the test media or by using BCFs observed in the field, this approach was followed in a study on secondary poisoning by Cd, Cu and Hg published by the Dutch RIVM [53].

9 Acquisition, Handling, Evaluation and Selection of the Data Used for Quality Standard Derivation

9.1 Data Required for Quality Standard Derivation

General

Similar to the elaboration of the method for quality standard setting, the data-related issues have been closely aligned with the guidance and requirements of the TGD [38]. Data used for the setting of quality standards should be **reliable** and **relevant**. **Reliability** means that the inherent quality of the method used to conduct the test is high and that all relevant details to judge on the performance and the results of the test are described. **Relevance** means the extent to which a test is appropriate to give insight in a particular question addressed, for instance, in the effects assessment. Only reliable, relevant data should be considered valid for use in quality standard setting.

Ecotoxicological Data

According to the provisions set out in Annex V of the WFD the "base set" of taxa that should be used in setting quality standards referring to the aquatic environment are:

- algae and/or macrophytes
- daphnia or representative organisms for saline waters
- fish

However, any other taxa are also considered if relevant and reliable data are available.

Both acute and chronic effect data will be used if the endpoint observed can be reasonably considered to reflect an adverse impact on the performance of the respective organism's population. This also includes effects on behaviour if it is conceivable that the effect described may impair the competitive fitness of the population. This includes avoidance reactions, as the organisms concerned may be forced to abandon the habitat where they would normally be present.

For the derivation of the long-term "annual" quality standards, chronic data (e.g. NOEC) are preferred. However, acute toxicity data ($L(E)C_{50}$) will be used to check the plausibility of the long-term data and of the quality standard derived on the basis of these long-term data. In addition, acute toxicity data are required to derive the MAC-QS (see section 7.2) and will further be used to set long-term QS if no sufficient chronic toxicity data are available. However, if possible, long-term QS will not be derived exclusively on the basis of acute toxicity data.

Tests conducted with freshwater organisms may be used to derive marine QS (and vice versa) as long as there is no evidence that this is not appropriate for the substance concerned or indications are available that the organism used in the test is not representative for the environment for which the effects assessment is conducted. Similarly, test results of organisms living in water may be used to derive QS for sediment, as long as no tests for sediment dwelling organisms are available.

Other ecotoxicological effects, such as endocrine disruption, are considered as a "normal" mode of toxic action of a chemical if appropriate tests accounting for the endpoint "endocrine disruption" are available. If adequate test results for substances suspected to exert an endocrine disrupting potential are not available, these substances are flagged for further consid-

eration of this particular property. Table 9.1 provides an indication whether a substance on the working list is a known or suspected endocrine disrupter.

As in the quality standard setting framework secondary poisoning of top predators is addressed, NOECs or NO(A)EL data of feeding studies with mammals and/or birds are required for several substances on the working list.

Results from test systems other than single species test (e.g. microcosm studies) are also considered if the test system and the results meet the quality criteria rendering a study valid (see section 9.2).

Qantitative structure activity relationship (QSAR) estimates for toxicity are not used in the derivation of quality standards.

Data related to bioaccumulation and persistence

Data on bioaccumulation (experimental data on bioconcentration or biomagnification or the octanol-water partition coefficient (Kow)) are required if a substance has a known or suspected potential to bioaccumulate (identified by the trigger-values given in table 8.1). Preference is given to experimental BCFs and BMFs, if available.

Data on persistence (biodegradation, hydrolysis or photodegradation) are not directly used in the derivation of the effect based quality standards (for reasons see section 8.2) but are given as supplementary information in the data sheet elaborated for each substance on the working list.

Toxicity data related to human health aspects

Data considered in setting quality standards referring to human health comprise information on oral toxicity, repeated dose toxicity, carcinogenicity, mutagenicity and effects on reproduction. Effect data used in deriving quality standards referring to human health are, for instance the relevant NOAEL, ADI, TDI values identified in the human health section of risk assessments according to Council Regulation (EEC) No. 793/93 or Council Directive 91/414/EEC. ADI or TDI values adopted by international bodies such as the World Health Organization may also be used. For effects for which a threshold level cannot be given, unit risk values corresponding to an additional risk of, e.g., cancer over the whole life of 10^{-6} (one additional cancer incident in 10^{6} persons taking up the substance concerned for 70 years) may be used, if available. Only data from reliable sources will be used.

Unfortunately, it is not possible to use the underlying toxicological data that were used to establish the R-phrases (according to Council Directive 67/548/EEC[16]) as this information could not be provided by the European Chemicals Bureau within the time frame of this study. The official R-phrases currently in force in the European Union are listed in table 9.1.

Data referring to physical and chemical properties

Partition coefficients may be required in order to conduct calculations as proposed in section 8 of this report. Those coefficients are, for instance:

- K octanol-water (Kow)
- K suspended particulate matter – water
- K sediment – water
- K organic carbon (Koc)

Other properties for which data should be available as supplementary information (e.g. for plausibility checks) are:

- water solubility
- vapour pressure
- molecular weight

Other Data

For naturally occurring substances data on natural background levels is pertinent supplementary information. For metals these data are required to calculate the quality standards for water and sediment [29].

Table 9.1: Classification and labelling of working list substances and indication of potential for endocrine effects

* Classification and Labelling in accordance with Council Directive 67/548/EEC [16] (28th Adaptation to Technical Progress of Annex I): submitted by ECB, August 2001

** Potential for effects on endocrine regulation according to COM(2001)262 final [63]
Table 2 of COM(2001)262: substances with evidence of ED or evidence of potential ED which are neither restricted nor currently being addressed under existing Community legislation
Table 3 of COM(2001)262: Substances with evidence of ED or evidence of potential ED, already regulated or being addressed under existing legislation
Table 4 of COM(2001)262: Substances with insufficient data in the BKH Report

#	CAS number	Name	Classification & Labelling *	ED potential **
1	15972-60-8	Alachlor	Xn, N; R: 22-40(Carc. Cat. 3)-43-50/53	table 3
2	120-12-7	Anthracene		
3	1912-24-9	Atrazine	Xn, N; R: 43-48/22-50/53	table 3
4	71-43-2	Benzene	F, T; R: 45(Cat. 1)-11-48/23/24/25	
5	n.a.	Brominated diphenylether	2,2',4,4'tetra BDE	table 2
	1163-19-5	(Bis(pentabromophenyl)ether)		table 3
	32536-52-0	(Diphenyl ether, octabromo deviate)		table 3
	32534-81-9	(Diphenyl ether, pentabromo derivative)	Xn, N; R: 48/21/22-50/53-64	table 3
6	7440-43-9	Cadmium and its compounds	Xn; N; R: 20/21/22-50/53 (cadmium compounds, with the exception of cadmium sulphoselenide (xCdS.yCdSe), mixture of cadmium sulphide with zinc sulphide (xCdS.yZnS), mixture of cadmium sulphide with mercury sulphide (xCdS.yHgS), and those specified elsewhere)	
7	85535-84-8	C_{10-13}-chloroalkanes	Xn, N; R: 40(Carc. Cat. 3)-50/53	table 4 (short chain chlorinated paraffins)
8	470-90-6	Chlorfenvinphos	T+, N; R: 24-28-50/53	table 4
9	2921-88-2	Chlorpyrifos	T, N; R: 24/25-50/53	table 4
10	107-06-2	1,2-Dichloroethane	Conc. < 20%: T; R: 45(Cat. 2)	

continued overleaf

[29] In the context of this study only background concentrations of the river Rhine have been used to illustrate the calculation of metal quality standards.

Table 9.1: (continued) Classification and labelling of working list substances and indication of potential for endocrine effects

#	CAS number	Name	Classification & Labelling	ED potential
11	75-09-2	Dichloromethane	Xn; R: 40(Carc. Cat. 3)	
12	117-81-7	Di(2-ethylhexyl)phthalate (DEHP)	T; R: 60-61(Repr. Cat. 2)	table 3
13	330-54-1	Diuron	Xn, N; R: 22-40(Carc. Cat. 3)-48/22-50/53	table 3
14	115-29-7	Endosulfan	T, N; R: 24/25-36-50/53	table 3
	959-98-8	(alpha-endosulfan)		table 3
15	206-44-0	Fluoroanthene		
16	118-74-1	Hexachlorobenzene	T, N; R: 45(Cat. 2)-48/25-50/53	table 3
17	87-68-3	Hexachlorobutadiene		
18	608-73-1	Hexachlorocyclohexane	T, N; R: 21-25-40(Carc. Cat. 3)-50/53	table 4
	58-89-9	(gamma-isomer, Lindane)	T, N; R: 23/24/25-36/38-50/53	table 3
19	34123-59-6	Isoproturon	Xn, N; R: 22-40(Carc. Cat. 3)-50/53	
20	7439-92-1	Lead and its compounds	T, N; R: 61(Repr. Cat.1)-20/22-33-50/53-62(Repr. Cat.3) (lead compounds with the exception of those specified elsewhere)	
21	7439-97-6	Mercury and its compounds	T+, N; R: 26/27/28-33-50/53 (inorganic compounds of Hg with the exception of HgS and those specified elswere)	
22	91-20-3	Naphthalene	Xn, N; R: 22-50/53	
23	7440-02-0	Nickel and its compounds	nickel monoxide, dioxide, trioxide: T; Carc. Cat. 1; R49 R43 R53 nickel sulphide: T; Carc. Cat. 1; R49 R43 N; R50-53 nickel dihydroxide: Carc. Cat. 3; R40 Xn; R20/22 R43 N; R50-53	
24	25154-52-3	Nonylphenols		
	104-40-5	(4-(para)-nonylphenol)		table 4
	84852-15-3	(4-nonylphenol, branched)	C, N; R: 22-34-50/53	
25	1806-26-4	Octylphenols		
	140-66-9	(para-tert-octylphenol)		table 2
26	608-93-5	Pentachlorobenzene	F, Xn, N; R: 11-22-50/53	table 4
27	87-86-5	Pentachlorophenol	T+, N; R: 24/25-26-36/37/38-40(Carc. Cat. 3)-50/53	table 4
28	n.a.	Polyaromatic hydrocarbons		table 4
	50-32-8	(Benzo(a)pyrene)	T, N; R: 45(Carc. Cat. 2)-46(Mut. Cat. 2)-60-61(Repr. Cat. 2) -50/53	table 4
	205-99-2	(Benzo(b)fluoroanthene)	T, N; R: 45(Carc. Cat. 2)-50/53	
	191-24-2	(Benzo(g,h,i)perylene)		
	207-08-9	(Benzo(k)fluoroanthene)	T, N; R: 45(Carc. Cat. 2)-50/53	
	193-39-5	(Indeno(1,2,3-cd)pyrene)		
29	122-34-9	Simazine	Xn, N; R: 40(Carc. Cat. 3)-50/53	table 3
30	688-73-3	Tributyltin compounds	T; R 25-48/23/25; Xn, R 21; Xi, R 36/38; N, R 50-53	table 3
	36643-28-4	(Tributyltin-cation)		
31	12002-48-1	Trichlorobenzenes		table 4
	87-61-6	(1,2,3-Trichlorobenzene)		
	120-82-1	(1,2,4-Trichlorobenzene)	Xn, N; R: 22-38-50/53	
	108-70-3	(1,3,5-Trichlorobenzene)		

continued overleaf

Table 9.1: (continued) Classification and labelling of working list substances and indication of potential for endocrine effects

#	CAS number	Name	Classification & Labelling	ED potential
32	67-66-3	Trichloromethane	Conc. < 5%: Xn; R 40(Carc. Cat. 3)	
33	1582-09-8	Trifluralin	Xi, N; R: 36-43-50/53	table 4
34		DDT		table 2
	50-29-3	DDT, 4,4'-isomer	T, N; R: 25-40(Carc. Cat. 3)-48/25-50/53	table 2
	789-02-6	DDT, 2,4'-isomer		
35	n.a.	Dioxins (PCDD)		table 4; table 3 (1,2,3,7,8-Pentachlorodibenzodioxin, 2.37.8-TCDD)
	n.a.	Furans (PCDF)		table 4; table 3
	n.a.	Drins		
36	309-00-2	Aldrin	T, N; R: 24/25-40(Carc. Cat. 3)-48/24/25-50/53	table 3
37	72-20-8	Endrin	T+, N; R: 24-28-50/53	table 3
38	465-73-6	Isodrin	T+, N; R: 26/27/28-50/53	
39	60-57-1	Dieldrin	T+, N; R: 25-27-40(Carc. Cat. 3)-48/25-50/53	table 3
40	1336-36-3	PCB	Xn, N; R: 33-50/53	table 3
	(7012-37-5)	(PCB 28)		table 4
	(35639-99-3)	(PCB 52)		table 4
	(37680-73-2)	(PCB 101)		
	(31508-00-6)	(PCB 118)		table 4
	(35065-28-2)	(PCB 138)		table 4
	(35065-27-1)	(PCB 153)		table 3
	(35065-29-3)	(PCB 180)		table 4
41	127-18-4	Tetrachloroethene	Xn, N; R: 40(Carc. Cat.3)-51/53	
42	56-23-5	Tetrachloromethane	T, N; R: 23/24/25-40(Carc. Cat. 3)-48/23-52/53-59	
43	79-01-6	Trichloroethene	T; R: 45(Carc. Cat. 2)-36/38-52/53-67(Muta. Cat. 3)	

9.2 Evaluation and Classification of Data

In the data inquiry, as set out in the working document for this study (EAF (1) 06/01/FHI, February 2001), it was asked to submit data to the consultant that can be considered as reliable according to the criteria given in table 9.2. All data should be rated by the senders accordingly and provided in a pre-defined format as Excel file. However, in hardly any case this provision was followed.

- First, in many cases data were provided as hardcopies on paper, or, if provided in electronic format, not as the proposed Excel data sheets but, for instance, as Excel files in other formats, as reports (text-files or pdf-files with tables from which the data had to be retrieved) etc.
- Second, if the data were rated at all, they were either rated according to the IUCLID system, according to the U.S. EPA's Klimisch criteria for quality data, according to the TGD reliability index (RI) system, or according to systems defined by the data provider.

Table 9.2: Proposed classification of tests with respect to data reliability

A	Test performed in full accordance with current internationally accepted guidelines (e.g.: OECD, EU, EPA, ISO). All relevant details are given. A clear dose-response relationship could be established for the observed effect(s). Results appear to be reliable.
B	Test performed according to internationally accepted guidelines. However not all relevant details are given. A clear dose-response relationship could be established for the observed effect(s). Results appear to be reliable.
C	Test was not performed in accordance with a current guideline. However, the results have been discussed and explained by the author(s). A clear dose-response relationship could be established for the observed effect(s). The author's interpretation of the results appears logic to the evaluating person. Results appear to be reliable.
D	Test was not performed in accordance with a current guideline and results have not been discussed and explained by the author(s). However, the evaluating person found the test design plausible and could explain and interpret the results. A clear dose-response relationship could be established for the observed effect(s). The results seem to be reliable
E	Due to various shortcomings in the test design and/or in the interpretation of the result(s) the test is not considered as reliable.

Fortunately, the different rating systems used by the US EPA or in the context of IUCLID and the TGD are very similar, and thus, their results are comparable (table 9.3). Only data of the reliability classes I and II are used for the derivation of quality standards. Data assigned to classes III and IV are not used. A further re-evaluation of the data provider's classification by the consultant was normally not possible as background information was usually not sufficient to do so (see first bullet point above).

The data that were not rated in terms of quality were in most cases provided by Member States. However, in most instances this data was already used by national authorities for regulatory purposes, such as the derivation of quality standards. Thus, it can be assumed that the respective data was reviewed and validated in terms of reliability and quality by national experts.

Finally, for many substances on the working list data collated and evaluated in the context of the risk assessment process for existing substances or for plant protection products are available for use in the derivation of quality standards. The data qualified as valid in the risk assessment reports (i.e. rated as TGD RI I or II) were subjected to an extensive peer review and evaluation process and are therefore used without any reservations.

Table 9.3: Comparison of different classification systems

Class	TGD Reliability index (RI)	US EPA	IUCLID
I	I (highly reliable)	high confidence	valid without restrictions
II	II (reliable)	moderate confidence	valid with restrictions
III	III (not reliable)	low confidence	invalid
IV	IV (unknown reliability)	unknown confidence	not assignable

9.3 Handling and Availability of Required Data

As already outlined in section 9.2, the data were mostly provided in a format that made it impossible to set up a uniform database for all substances, as originally intended and described in the working document (EAF (1) 06/01/FHI, February 2001). Given the time con-

straints, it was not possible to adapt all the different formats in which the data were sent to the consultant to the originally proposed format or to manually extract all data from the reports provided on paper. Thus, it was decided to set up substance data sheets containing all data and information used to derive the standards (cf. Annex 4).

The data and information sources listed in Annex 3 have been made available to the consultant until 20 February 2002.

9.4 Selection of Data for Derivation of Quality Standards

Data identified as valid in finalised risk assessment reports and in (consolidated) draft reports for existing substances (according to Council Regulation (EEC) No. 793/93) as well as for plant protection products (according to Council Directives 91/414/EEC & 97/57/EC) have been preferably used for the derivation of quality standards as they were already subjected to an extensive peer review and evaluation process. No differentiation with regard to the status of the risk assessment report (final or draft) was made in the context of this study. Therefore, quality standards that are proposed on the basis of information and data given in draft reports should be reviewed once the respective risk assessments are finalised (see Annex 3 for information regarding the status of the risk assessment reports).

If PNECs are already established in the risk assessment reports (which is the case for fourteen substances or substance groups on the working list), these PNECs (e.g. for water, sediment or secondary poisoning of top predators) were used for the derivation of the standards for the respective objectives of protection (see sections 8.2 & 8.3). Accordingly, the effects data identified as valid to establish the Toxicity Exposure Ratios (TER) in the RA-monographs for plant protection products (PPP) were used to derive the quality standards for plant protection products as described in section 8.5 (monographs are available for six PPP). In order to set quality standards referring to human health the relevant threshold levels identified in the risk assessment reports have been used (see section 9.1 for details).

For those 22 substances or substance groups on the working list for which the above mentioned risk assessment reports or monographs were not available, or in case data required to calculate the quality standards could not be retrieved from the RA reports, selection rules as follows were applied:

1. Only data that can be considered as reliable (see section 9.2) are used, irrespective of the source of the data.
2. The relevant data from the different sources available (see Annex 3) are collated in the substance data sheet. This means that not all valid data mentioned in the different sources are transferred to the data sheet but only those that may be required for quality standard setting.
3. Data to be used for the quality standard derivation are selected from the collated data making best use of supplementary information provided along with the data. In case no further ranking of data with regard to their utility and relevance for the derivation of quality standards is possible, final selection of data is made following the precautionary principle. I.e., usually the lowest acute and long-term toxicity data available for the different species and end points are used, or in case of other data, such as partition coefficients, the figures resulting in worst-case assumptions are selected. A justification for the selection of specific data is briefly given in the EQS data sheets of Annex 4.

4. Based on the selected data, the quality standards are derived as described in section 8. If a standard for a specific objective of protection cannot be derived since the required data are lacking, this is flagged.

10 Proposals for Quality Standards

An overview on the proposed overall quality standards for inland waters as well as transitional, coastal an territorial waters is given in table 10.1. Further, short remarks with regard to considerations undertaken in the derivation process or recommendations addressing possibilities to improve the reliability of the proposed standards are added.

All data and information sources used as well as the calculations performed and the considerations undertaken to derive the quality standards are comprehensively documented in the EQS data sheets that have been prepared for each substance or substance group of the working list (see Annex 4).

In these EQS data sheets additional information can be found regarding the quality standards derived for individual objectives of protection (water, sediment, secondary poisoning of predators, impact on human health due to ingestion of fishery products, drinking water abstraction from surface water) as far as it was required to derive these specific standards (i.e. trigger values for derivation were met, see table 8.1). Further, for those hydrophobic organic substances with a partition coefficient ($Kp_{susp.sediment-water}$) $\geq$ 1,000 the water based concentration values are additionally given as corresponding concentration in suspended particulate matter (SPM) of the EU standard freshwater and seawater (15 and 3 mg/l SPM, respectively).

All proposed quality standards should be considered as preliminary and it is recommended to subject them to a validation or peer review step.

Table 10.1: Proposed overall quality standards for the substances on the working list

@: WFD – Water Framework Directive; PS - Priority Substance; PHS –WFD Priority Hazardous Substance; PSR – WFD Priority Substance under Review; OSC – other substance of concern

#	CAS No	Name	WFD category @	Overall Quality Standards	Comments / Recommendations
1	15972-60-8	Alachlor	PS	Inland and transitional waters: **0.035 µg/l** Coastal and territorial waters: Derivation not possible due to lack of toxicity data for marine biota. MAC-QS: 1.15 µg/l	Alachlor is classified as a **category 3 carcinogen**. However, in the risk assessment monograph it is concluded that the mechanism leading to tumours in rats is not relevant for humans. The overall QS refers to the protection of the pelagic community. However, the decisive algae toxicity data are not conclusive. Therefore the proposed QS should only be considered as provisional standard. Moreover, alachlor is suspected to affect endocrine regulation but potential adverse effects of alachlor on the endocrine system in aquatic organisms and wildlife are not addressed in the monograph, which served as data source for the derivation of the proposed QS.
2	120-12-7	Anthracene	PSR	Inland and transitional waters: **0.063 µg/l** Coastal and territorial waters: **0.0063 µg/l** MAC-QS: 0.01 µg/l	The overall QS refers to the prevention of adverse effects on the pelagic communities in both freshwater and saltwater. The differences in the QS for saltwater and freshwater are due to the application of different assessment factors according to the TGD provisions (only insufficient effect data for marine organisms were available in the anthracene RAR). However, as data on additional marine taxonomic groups are available from other sources showing that marine species are not more sensitive than freshwater organisms, it should be considered to use the QS derived for freshwater as overall quality standard for both freshwater and saltwater.
3	1912-24-9	Atrazine	PSR	Inland waters as well as transitional, coastal and territorial waters: **0.34 µg/l** MAC-QS: 2 µg/l	The overall QS refers to the protection of the pelagic communities in both freshwater and saltwater. Atrazine is suspected to affect endocrine regulation. Potential adverse effects of atrazine on endocrine regulation in aquatic organisms are not addressed in the monograph, which served as data source for the derivation of the proposed QS.
4	71-43-2	Benzene	PS	No proposal for an overall QS can be made based on the available data. MAC-QS: 49 µg/l Specific QS: The QS derived for the protection of aquatic life (incl. top predators) are: Inland and transitional waters: 16 µg/l Coastal and territorial waters: 1.6 µg/l	Benzene is a **carcinogen of category I** (proven human carcinogen). In the benzene risk assessment report it is concluded that no safe level of exposure can be recommended. Therefore, the protection of human health from adverse effects due to drinking water uptake or the ingestion of seafood is the most relevant objective of protection. However, based on the available information, a sound proposal for a quality standard addressing the health concerns cannot be made. It is suggested to establish an expert group to address the open questions. The differences in the quality standards for saltwater and freshwater are due to the application of different assessment factors as required by the TGD for the case that only insufficient effect data for marine organisms are available.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
5	n.a.	Brominated diphenylethers		Derivation of an overall QS for the substance group not recommended.	The individual substances are very different with regard to their physico-chemical properties and their toxic potential. Therefore, it cannot be recommended to implement a quality standard common for the group.
	(1163-19-5)	(Bis(pentabromophenyl)ether)	PS	It is not possible to derive effect based quality standards for the pelagic communities in freshwater or saltwater based on the tentative PNECs derived in the risk assessment report. These tentative PNECs are based on unbounded toxicity test results (i.e. the highest concentration tested) and thus invalid according to the provisions given in the TGD. MAC-QS: Is not required because apparently no acute effects occur up to the water solubility limit.	Apparently, deca-BDE does not exert acute or longer-term effects in pelagic organisms up to its water solubility limit. For sediment dwelling organisms the toxicity of the substance seems also to be rather low. However, it should be kept in mind that these findings stated in the risk assessment report of the substance are only based on a small number of toxicity tests and that, therefore, there is considerable uncertainty about the "tentative" PNECs derived in the risk assessment. The derivation of quality standards referring secondary poisoning of predators, to drinking water abstraction or the protection of human health from adverse effects due to ingestion of food originating from aquatic environments is not necessary as the respective trigger criteria are not met. Deca-BDE is suspected to affect endocrine regulation. This issue is addressed and accounted for in the risk assessment report, which served as basis for the derivation of the proposed QS.
	(32536-52-0)	(Diphenyl ether, octabromo deviate)	PS	Inland waters as well as transitional, coastal and territorial waters: **1217 µg/kg** fishery products (wet wt) MAC-QS: Is not required because apparently no acute effects occur up to the water solubility limit.	The overall QS refers to the prevention of adverse effects on human health by ingestion of fishery products. The substance is not classified according to Directive 67/548/EEC. However, in the draft risk assessment report a classification as **harmful to reproduction** (Xn, R63) is suggested. Octa-BDE is suspected to affect endocrine regulation. This issue is addressed and accounted for in the draft RAR. Commercially available octabromodiphenyl ether preparations appear to contain significant amounts of by-products that are considerably more liable to bioaccumulation and more toxic than octa-BDE, in particular hexabromodiphenyl ether. A discussion is therefore required as to whether it is necessary to impose a quality standard for this latter compound. Example calculations are given in the EQS data sheet of octa-BDE.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
	(32534-81-9)	(Diphenyl ether, pentabromo derivative)	PHS	Inland and transitional waters: **0.0005 µg/l** Coastal and territorial waters: **0.00018 µg/l**. MAC-QS: 1.4 µg/l	Penta-BDE is classified as **harmful to reproduction** (Xn, R64). Protection of human health from adverse effects due to ingestion of fishery products is the objective that requires the lowest levels of penta-BDE in inland waters. With regard to marine (coastal and territorial) environments, the lowest quality standard is required to protect top predators from secondary poisoning. The differences in the overall quality standards for saltwater and freshwater environments are due to the application of different food web models for the assessment of the potential for secondary poisoning in freshwater and marine water, as recommended in the revised TGD. Penta-BDE is suspected to affect endocrine regulation. This issue is addressed in the risk assessment report, which served as data basis for the derivation of the proposed QS. In the report it is concluded that there are insufficient data currently available to assess the significance of the effects in terms of the commercial penta-BDE. Penta-BDE is categorised as PHS. Therefore, the detection limit may apply as borderline quality standard in territorial waters. The derived QS may, however, be lower than the detection limit of the substance.
6	7440-43-9	Cadmium and its compounds	PHS	QS = $C_{background}$ + MPA MPA for inland and transitional waters: Hardness $CaCO_3$ [mg/l] — MPA [µg/l, dissolved Cd] 40 - <100 — **0.08** 100 - <200 — 0.15 >200 — 0.25 Coastal and territorial waters: derivation of a MPA not possible (no marine toxicity data were available in the risk assessment report)	The suggested overall MPA refers to the protection of the pelagic community. In case it is decided to correct for influence of hardness on Cd toxicity, the 3 classes as defined may be used. Alternatively, only the MPA derived for the lowest hardness class could be used to derive the QS (Cd is a PHS and anthropogenic emissions are principally unwanted – minimisation of emissions is thus required). Under consideration of the water quality required to prevent secondary poisoning of top predators, the QS (i.e. $C_{background}$ + MPA) should in no case be higher than 0.26 µg/l (dissolved Cd). Sections on critical effects of Cd on kidney and bone were not included in the human health part of the risk assessment report available to the consultant. It might therefore be required to reconsider human health aspects and to update the MPA derivation upon finalisation of the respective sections of the human health risk assessment. Cadmium is categorised as priority hazardous substance. Therefore its natural background concentration in territorial waters may apply as quality standard at the border to the open sea.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
7	85535-84-8	C_{10-13}-chloroalkanes	PHS	Inland and transitional waters: **0.41 µg/l** (the corresponding level in food of top predators is 16.6 mg/kg food (wet weight)) Coastal and territorial waters: **0.1 µg/l** MAC-QS: 1.4 µg/l	Protection of top predators from secondary poisoning requires the lowest levels of C_{10-13}-chloroalkanes in inland and transitional waters. With regard to coastal & territorial waters, the lowest quality standard was derived for the protection of the pelagic community. C_{10-13} chloroalkanes are known to accumulate in the sediment, but, due to lack of effects data for sediment dwelling organisms, the standards derived for the sediment compartment are only a transformation of the freshwater or saltwater standards by the equilibrium partitioning method. Therefore, it cannot be ruled out that protection of the sediment compartment requires more stringent overall QS. The QS should be reviewed as soon as valid toxicity data for sediment dwelling organisms become available. C_{10-13} chloroalkanes are classified as a **category 3 carcinogen**. However in the risk assessment report it is concluded that the identified NOAEL for chronic toxicity is also protective with regard to cancer risk. The chronic NOAEL has been considered in the derivation of the quality standard.. The differences in the quality standards for saltwater and freshwater are due to the application of different assessment factors as required by the TGD for the case that only insufficient effect data for marine organisms are available. C_{10-13} chloroalkanes are categorised as PHS. Therefore, the detection limit may apply as borderline quality standard in territorial waters in order to prevent pollution of the open sea.
8	470-90-6	Chlorfenvinphos	PS	Inland waters as well as transitional, coastal and territorial waters: **0.01 µg/l** MAC-QS: 0.01 µg/l	The suggested overall QS refers to the protection of the pelagic communities in both freshwater and saltwater. It is protective for drinking water abstraction and sediments as well. However, chlorfenvinphos appears to be moderately bioaccumulating (worst case BCF >100) and is classified as very toxic if swallowed. Therefore, it is required to assess whether the standard derived for the pelagic community is also sufficient to protect predators from secondary poisoning or humans from adverse effects due to ingestion of fishery products. This was not possible in the context of this study as appropriate mammalian and avian toxicity data were lacking. The available tests indicate that acute and chronic toxicity is in the same range for the most sensitive taxonomic group (crustaceans). Therefore, overall QS and MAC-QS are identical.
9	2921-88-2	Chlorpyrifos	PSR	Inland waters as well as transitional, coastal and territorial waters: **0.00046 µg/l** MAC-QS: 0.001 µg/l	The overall QS is referring to the protection of pelagic communities in both freshwater and saltwater. As chlorpyrifos is partitioning to the sediment in significant amounts, the risk for sediment dwelling organisms should be assessed on the basis of experimental data for benthic organisms as soon as such data become available.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
10	107-06-2	1,2-Dichloroethane	PS	No proposal for an overall QS can be made based on the available data. Human health is the most critical objective of protection. **In view of the carcinogenic potential of 1,2-dichloroethane emissions and losses of the substance should be minimised as far as possible.** MAC-QS: 1080 µg/l	As 1,2-dichloroethane is a **carcinogen (class 2)**, the decisive issue for quality standard setting is human health. A limit value of 3 µg/l has been set for drinking water in CD98/83/EC. A standard referring to uptake of fishery products could not be calculated since appropriate mammalian toxicity data were not available. An evaluation is required as to whether the water quality standard currently in force (10 µg/l, CD 86/280/EEC) is sufficient to guarantee that the drinking water limit value of 3 µg/l can be achieved by application of simple means as defined in CD 75/440/EEC on drinking water abstraction. There are considerable inconsistencies in the data available for ecological effects assessment. Therefore, the validity of the critical effects data should be checked and the standards referring to the environmental protection objectives be amended, if required.
11	75-09-2	Dichloromethane	PS	Inland waters as well as transitional, coastal and territorial waters: **8.2 µg/l** MAC-QS: 162 µg/l	The overall QS is referring to the protection of pelagic communities in both freshwater and saltwater and should be considered as provisional because the protection of human health may require a lower standard. Dichloromethane is classified as a **class 3 carcinogen** but it was not possible to calculate the QS referring to human health concerns (uptake of fishery products, drinking water abstraction) since adequate mammalian toxicity data were not available.
12	117-81-7	Di (2-ethylhexyl)-phthalate (DEHP)	PSR	Inland and transitional waters: 1 µg/l (or according to the guidance given in the revised TGD: **0.33 µg/l**) Coastal and territorial waters: 0.5 µg/l (or according to the guidance given in the revised TGD: **0.17 µg/l**) MAC-QS: not required (no toxic effects up to water solubility limit)	The proposed standards are referring to secondary poisoning. According to the reasoning in the risk assessment report on which the QS proposal is based on, they should also cover possible effects of DEHP on endocrine regulation as the $PNEC_{food}$ used for the calculation covers effects on development, reproduction (DEHP is classified as **toxic to reproduction, class 2**) and sexual differentiation in mammals and fish. However, as the calculation of the PNECs by the amended method proposed in the revised TGD would result in a threefold lower QS for secondary poisoning as derived on the basis of the respective PNEC in the DEHP risk assessment report, it should be considered to lower the $QS_{secpois}$ accordingly. Protection of human health form adverse effects due to the ingestion of fishery products contaminated by DEHP might require an even lower quality standard than the protection of predators from secondary poisoning. However, in order to calculate this QS, advice from experts in human toxicology is required. Due to its very low water solubility DEHP apparently does not exert direct toxic effects on the pelagic communities of freshwater or saltwater environments.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
13	330-54-1	Diuron	PSR	Inland waters as well as transitional, coastal and territorial waters: **0.046 µg/l** MAC-QS: 1.1 µg/l	The suggested overall QS refers to the protection of the pelagic communities in both freshwater and saltwater. It should be considered as provisional, as it was not possible to derive the QS referring to uptake of fishery products by man (lack of appropriate mammalian toxicity data). Diuron is classified as a **carcinogen of class 3** and the derivation of the respective QS is therefore required. In addition, no information on the (eco)toxicological relevance of the potential impact of diuron on endocrine regulation was available and data on the environmental relevance of diuron metabolites were lacking too.
14	115-29-7 (959-98-8)	Endosulfan (alpha-endosulfan)	PSR	Inland waters as well as transitional, coastal and territorial waters: **0.004 µg/l** MAC-QS: 0.004 µg/l	The acute toxicity of endosulfan to many fish and invertebrate species is in the range of the lowest NOECs observed. Therefore, the overall QS refers to the protection of the pelagic communities in both freshwater and saltwater from acute effects of endosulfan. Endosulfan is suspected to affect endocrine regulation. However, in the risk assessment monograph it is concluded that there is weight of evidence that endosulfan is not an endocrine disruptor.
15	206-44-0	Fluoranthene	PS	Inland waters as well as transitional, coastal and territorial waters: **0.12 µg/l** MAC-QS: 0.9 µg/l	The proposed overall QS is only referring to the protection of the pelagic communities in both freshwater and saltwater and should therefore be considered as provisional. Standards referring to the benthic communities and to secondary poisoning of predators could not be derived due to lack of data.
16	118-74-1	Hexachlorobenzene	PHS	No overall QS could be derived based on the data available. In view of the carcinogenic properties of HCB and its ecological hazard potential **emissions and losses of the substance should be minimised as far as possible**. MAC-QS: 0.05 µg/l Specific QS: Environment (protection of predators from secondary poisoning and aquatic life in inland as well as transitional, coastal and territorial waters): 0.008 µg/l in the best case.	As hexachlorobenzene is a **carcinogen (class 2)**, the decisive issue for quality standard setting may be human health. However, as no appropriate toxicity data have been provided, a quality standard that covers cancer risk of humans could not be calculated. Regarding the environment, protection of predators from secondary poisoning is the most critical objective. There are considerable inconsistencies in the data available for ecological effects assessment (toxicity and bioaccumulation). Moreover, no data with regard to potential adverse effects of HCB on endocrine regulation were available. Therefore, the validity of the critical effects data should be checked and the standards referring to the environmental protection objectives be amended, if required. Hexachlorobenzene is categorised as PHS. Therefore, the detection limit may apply as borderline quality standard in territorial waters.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
17	87-68-3	Hexachloro-butadiene	PHS	Inland waters as well as transitional, coastal and territorial waters: **at most 0.003 µg/l** MAC-QS: 0.59 µg/l	Protection of predators from secondary poisoning and of humans from adverse effects due to seafood ingestion are the most critical objectives that require water concentrations of at most 0.003 µg/l. Hexachlorobutadiene is categorised as PHS. The detection limit may therefore apply as borderline quality standard in territorial waters.
18	608-73-1	Hexachlorocyclo-hexane	PHS	Inland and transitional waters: **0.042 µg/l** Coastal and territorial waters: **0.01 µg/l** MAC-QS: 0.9 µg/l	It is suggested that the quality standards of hexachlorocyclohexane may apply for the sum of all HCH-isomers. However, the levels of γ-HCH (Lindane) must not exceed the quality standards specifically derived for this isomer. Hexachlorocyclohexane is classified as a **class 3 carcinogen** (however, not so the gamma-isomer). Appropriate data referring to this aspect or to human health in general were not available. Therefore, the proposed overall QS should be considered as provisional. The suggested overall QS for freshwater and transitional waters refers to the protection of predators from secondary poisoning. The proposed overall QS for coastal and territorial waters refers to the protection of the saltwater pelagic community. The differences in the QS for saltwater and freshwater are due to the insufficient availability of toxicity data for marine organisms and, resulting, the application of different assessment factors according to the TGD provisions. Hexachlorocyclohexane is categorised as PHS. Therefore, the detection limits of the individual isomers may apply as borderline quality standards in territorial waters.
	(58-89-9)	(gamma-isomer, Lindane)		Inland and transitional waters: **0.02 µg/l** Coastal and territorial waters: **0.002 µg/l** MAC-QS: 0.03 µg/l	The suggested overall QS refer to the protection of the pelagic communities in freshwater and saltwater, respectively. The differences in the QS for saltwater and freshwater are due to apparent differences in the sensitivity of freshwater and marine invertebrates. Lindane is suspected to affect endocrine regulation. Potential adverse on mammals have been addressed and accounted for in ADI derivation in the risk assessment monograph, which served as data basis for the proposed QS.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
19	34123-59-6	Isoproturon	PSR	Inland and transitional waters: **0.32 µg/l** QS for coastal and territorial waters: derivation was not possible due to lack of effects data for marine biota. MAC-QS: 1.3 µg/l	Isoproturon is classified as a **carcinogen of class 3**. However, in the risk assessment monograph an acceptable daily intake for humans was calculated. This ADI was considered in the QS derivation and the proposal for the overall QS, respectively. The proposed overall QS for inland waters is referring to the protection of the pelagic community. It is not clear whether the QS for inland waters is protective for drinking water abstraction in all cases. An assessment by experts in drinking water technology with regard to the question which percentage of the amount of isoproturon present in raw water can be removed by usual simple treatment procedures might be helpful. If the respective percentage was known, this figure could be used together with the drinking water standard to estimate the maximum level in surface water that can be removed during drinking water production by simple treatment.
20	7439-92-1	Lead and its compounds	PSR	QS = $C_{background}$ + MPA Overall MPA for inland waters as well as transitional, coastal and territorial waters: **1 µg/l** (dissolved Pb, corresponding to MPAs of 58.8 mg/kg in freshwater SPM and 200 mg/kg in saltwater SPM, respectively) MAC-MPA: 2 µg/l	Lead and its compounds are classified as having **adverse effects on reproduction (class 1).** The MPAs derived for the protection of the pelagic communities in both freshwater and saltwater environments may not be low enough to guarantee that lead body burdens of bivalve molluscs remain below the maximum level set by Commission Regulation (EC) No 466/2001 in order to protect humans from adverse effects due to ingestion of these organisms as food. Therefore, the MPAs should be considered as provisional. An in depth assessment of lead levels in mussels and the bioaccumulation potential of lead in filtrating molluscs is deemed necessary in order to be able to set a reliable QS for lead. The proposed overall MPAs should further be considered as provisional since it was not possible to derive specific standards addressing secondary poisoning or the protection of sediment organisms due to lack of appropriate experimental data.
21	7439-97-6	Mercury and its compounds	PHS	QS = $C_{background}$ + MPA No overall MPA can be suggested. MAC-MPA: 0.07 µg/l (dissolved Hg) Specific MPA: Pelagic communities in inland waters as well as transitional, coastal and territorial waters: 0.036 µg/l dissolved Hg)	The MPA calculated for the pelagic communities is presumably not low enough for the protection of predators from secondary poisoning or the protection of humans from adverse health effects. Due to considerable uncertainties associated with the available data on bioaccumulation and toxicity of (organic) Hg no reliable QS for the latter objectives of protection could be derived. Hg is categorised as priority hazardous substance. Therefore its natural background concentration in territorial waters may apply as quality standard at the border to the open sea.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
22	91-20-3	Naphthalene	PSR	Inland and transitional waters: **2.4 µg/l** Coastal and territorial waters: **1.2 µg/l** MAC-QS: 80 µg/l	Protection of the pelagic communities in freshwater and saltwater is the objective of protection that requires the lowest levels of naphthalene in aquatic ecosystems. The differences in the quality standards for saltwater and freshwater are due to insufficient availability of marine effects data and, resulting, the application of different assessment factors according to the TGD provisions.
23	7440-02-0	Nickel and its compounds	PS	QS = $C_{background}$ + MPA MPA for inland waters as well as transitional, coastal and territorial waters: **0.6 µg/l** (dissolved Ni); corresponding concentration in freshwater suspended particulate matter 24 mg/kg and in saltwater SPM 46 mg/kg (dry wt). MAC-QS: MAC-MPA 1.3 µg/l (dissolved Ni)	The proposed MPA should be considered as provisional as it is only referring to the protection of pelagic communities in both freshwater and saltwater. It was only possible to derive this MPA for the protection of the pelagic communities. MPAs or quality standards for the other objectives of protection such as sediments, top predators or human health could not be derived as the toxicity data required for this purpose were lacking. However, according to some provided documents on nickel, accumulation through the food web and thus secondary poisoning of predators and humans due to the uptake of food from aquatic environments is not a relevant problem. Therefore, it is suggested to adopt the sum of the MPA and the relevant Ni background level as provisional overall quality standard. It should however be verified that the potential of Ni for secondary poisoning of predators or for adverse effects on human health after oral ingestion of fishery products is really negligible.
24	25154-52-3 (104-40-5) (84852-15-3)	Nonylphenols (4-(para)-nonylphenol) (4-nonylphenol, branched)	PHS	Inland and transitional waters: **0.33 µg/l** Coastal and territorial waters: **0.033 µg/l** MAC-QS: 2.1 µg/l	The proposed overall QS refer to the protection of the pelagic communities. Nonylphenols and nonylphenol ethoxylates are known to affect endocrine regulation by exerting estrogenic activity, e.g. in fish. However, according to the risk assessment report on used as data source for the suggested QS, these effects start to occur at 10-20 µg/l. Hence, they are covered by the proposed QS. Nonylphenols are categorised as Priority Hazardous Substances. Therefore, the detection limit may apply as borderline quality standard in territorial waters in order to prevent pollution of the open sea.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
25	1806-26-4 (140-66-9)	Octylphenols (para-tert-octylphenol)	PSR	Inland and transitional waters: **0.1 µg/l** Coastal and territorial waters: **0.01 µg/l** MAC-QS: 0.133 µg/l	The suggested overall QS refer to the protection of the pelagic communities in both freshwater and saltwater. The differences in the QS for saltwater and freshwater are due to the insufficient availability of toxicity data for marine organisms and, resulting, the application of different assessment factors according to the TGD provisions. Compared to the risk that octylphenols may pose to aquatic live the health risks due to ingestion of fishery products or uptake of drinking water appear to be low. Also, the risk for mammals to suffer from secondary poisoning seems not to be significant. However, no conclusion is possible regarding the risk for birds, as no respective toxicity data were available. The secondary poisoning risk of birds should therefore be assessed as soon as the required data become available. Accordingly, it is recommended to refine the provisional sediment quality standards as soon as the required toxicity data for sediment organisms are available. Para-tert-octylphenol is suspected to affect endocrine regulation. However, as no toxicity data addressing this aspect were available, this issue could not be considered in the derivation of the proposed QS.
26	608-93-5	Pentachloro-benzene	PHS	Inland waters as well as transitional, coastal and territorial waters: **presumably < 0.05 µg/l** MAC-QS: 1 µg/l	No definitive overall quality standard can be suggested. Protection of predators from secondary poisoning is the objective that requires the lowest quality standard. However, the available bioaccumulation data cover a very wide BCF range and do, therefore, not allow for the derivation of a reliable standard. An in depth assessment of the bioaccumulation potential is required in order to get a reliable figure. Pentachlorobenzene is categorised as PHS. Therefore, the detection limit may serve as borderline quality standard in territorial waters in order to prevent pollution of the open sea.
27	87-86-5	Pentachlorophenol	PSR	QS for inland waters as well as transitional, coastal and territorial waters: **0.1 µg/l** MAC-QS: 1 µg/l	The suggested overall QS refers to the protection of the pelagic communities in both freshwater and saltwater and should only be considered as provisional. It covers the protection objectives drinking water abstraction and protection of predators from secondary poisoning, but as no data with relevance to sediment organisms and protection of human health from adverse effects due to ingestion of fishery products were available, it is not possible to conclude whether these latter objectives are also covered by the proposed overall QS of 0.1 µg/l. Pentachlorophenol is classified as a **category 3 carcinogen**.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
28	n.a.	Polyaromatic hydrocarbons	PHS		Due to lack of data for benzo(b)fluoranthene, benzo(g,h,i)perylene and indeno(1,2,3-cd)pyrene it was not possible to derive overall quality standards for the group PAH. As the group polyaromatic hydrocarbons is categorised as PHS, the detection limits of the individual substances assigned to this group (or their natural background levels in territorial waters) may serve as borderline quality standards for the respective compounds in territorial waters.
	(50-32-8)	(Benzo(a)pyrene)		No overall QS could be derived since relevant toxicity data for birds and mammals required to address secondary poisoning of predators or human health (ingestion of fishery products) as objectives of protection are lacking. MAC-QS: 0.05 µg/l Specific QS: Pelagic communities in freshwater & transitional waters: 0.05 µg/l; coastal & territorial waters: 0.005 µg/l	B(a)P is classified as **carcinogenic, mutagenic and as having adverse effects on reproduction (class 2 for each of the CMR properties)**. Further, it is a bioaccumulating substance. Hence, human health and protection of predators from secondary poisoning may be the most critical objectives of protection. However, no relevant mammalian and avian oral toxicity data required for the derivation of the respective QS were available. The differences in the specific QS for saltwater and freshwater are due to the insufficient availability of toxicity data for marine organisms and, resulting, the application of different assessment factors according to the TGD provisions.
	(205-99-2)	(Benzo(b)fluoranthene)			Derivation of QS not possible due to lack of data. B(b)F is classified as a **carcinogen of class 2.**
	(191-24-2)	(Benzo(g,h,i)perylene)			Derivation of QS not possible due to lack of data.
	(207-08-9)	(Benzo(k)fluoranthene)		No overall QS could be derived since relevant toxicity data for birds and mammals required to address secondary poisoning of predators or ingestion of fishery products by humans as objectives of protection are lacking. MAC-QS: derivation not possible due to insufficient availability of acute toxicity data Specific QS: Pelagic communities in freshwater & transitional waters: 0.0054 µg/l; coastal & transitional waters: 0.00054 µg/l	B(k)F is classified as a **class 2 carcinogen** and it is a bioaccumulating substance. Hence, human health and protection of predators from secondary poisoning may be the most critical objectives of protection. However, no relevant mammalian and avian oral toxicity data required for the derivation of the respective QS were available. The differences in the specific QS for saltwater and freshwater are due to the insufficient availability of toxicity data for marine organisms and, resulting, the application of different assessment factors according to the TGD provisions.
	(193-39-5)	(Indeno(1,2,3-cd)-pyrene)			Derivation of QS not possible due to lack of data.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
29	122-34-9	Simazine	PSR	Inland waters: **< 1 µg/l** Transitional, coastal and territorial waters: **1.1 µg/l** MAC-QS: 4.2 µg/l	Simazine is classified as a **category 3 carcinogen**. However, in the risk assessment monograph it is concluded that the mechanism leading to tumours in rats is not relevant for humans. The inland water overall QS is referring to the possibility of drinking water abstraction from surface water. The respective A1-value of the drinking water abstraction directive 75/440/EEC is 1 µg/l for Σpesticides (the specific QS derived for the protection of aquatic life in freshwater is 1.1 µg/l, as for transitional, coastal and territorial waters). The MAC-QS and the overall QS referring to the protection of aquatic life in transitional, coastal and territorial waters have been derived on the basis of the data compiled in the simazine risk assessment monograph. However, significantly lower short-term and long-term toxicity test results than used for risk assessment in this monograph have been reported elsewhere. Further, simazine is suspected to affect endocrine regulation. This issue is not addressed in the monograph. It is therefore deemed necessary to critically assess whether the toxicity data of the simazine monograph do represent all relevant information with regard to the aquatic toxicity of simazine. Therefore, the proposed QS should be considered as provisional.
30	688-73-3 (36643-28-4)	Tributyltin compounds (Tributyltin-cation)	PHS	Inland waters as well as transitional, coastal and territorial waters: **0.0001 µg/l** MAC-QS: 0.0015 µg/l	The overall QS refers to the protection of the pelagic communities in freshwater and saltwater environments. This standard may be considered as provisional as due to lack of appropriate mammalian and avian oral toxicity data no quality standard for the protection of top predators from secondary poisoning could be derived. However, secondary poisoning may be no relevant issue, as biomagnification through the food chain apparently does not occur. In addition, vertebrates can metabolise TBT compounds to by far less toxic compounds. TBT compounds are known to affect endocrine regulation. Respective toxicity data of molluscs (the most sensitive group known) are considered for the derivation of the proposed QS. Tributyltin compounds are categorised as Priority Hazardous Substance. Therefore, the detection limit may serve as borderline quality standard in territorial waters in order to prevent pollution of the open sea.

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
31	12002-48-1 (87-61-6) (120-82-1) (108-70-3)	Trichlorobenzenes (1,2,3-Trichloro-benzene) (1,2,4-Trichloro-benzene) (1,3,5-Trichloro-benzene)	PSR	Inland and transitional waters: **1.8 µg/l** Coastal and territorial waters: **0.4 µg/l** MAC-QS: 50 µg/l	As commercial trichlorobenzene consists predominantly of 1,2,4-TCB and the individual uses of the 1,2,3- and 1,3,5- isomers appear to be very limited, it is proposed to derive the required QS not for the individual isomers but for Σtrichlorobenzenes on the basis of the toxicity data available for 1,2,4-TCB (for the other isomers many of the required data for QS derivation are not available). The suggested overall QS for inland waters refers to the protection of humans from adverse effects on health due to ingestion of fishery products. For coastal and territorial waters the standard derived for the marine pelagic community may apply. This saltwater QS is lower than the QS for the freshwater pelagic community due to insufficient availability of marine toxicity data and, resulting, the application of a more stringent assessment factor according to TGD provisions.
32	67-66-3	Trichloromethane	PS	Inland waters as well as transitional, coastal and territorial waters: **3.85 µg/l** MAC-QS: 38.5 µg/l	The suggested overall QS refers to the protection of the pelagic communities in both freshwater and saltwater. It should be considered as provisional since trichloromethane is classified as a **class 3 carcinogen**. The protection of human health from adverse effects may therefore require lower levels in the aquatic environment than the suggested overall QS. The part of the risk assessment report dealing with human health was not yet available. However, since the substance is deemed sufficiently regulated for human exposure by the Competent Authorities, it cannot be expected that much additional measures will be initiated based on this document.
33	1582-09-8	Trifluralin	PSR	Inland waters as well as transitional, coastal and territorial waters: **0.03 µg/l** MAC-QS: 0.42 µg/l	The suggested overall QS is referring to the protection of the pelagic communities in both freshwater and saltwater. It should be considered as provisional because the potential of trifluralin to adversely affect the benthic community as well as its potential for secondary poisoning could not be evaluated. The required data were not available. In view of the high BCF of trifluralin and the high Koc values, the respective assessments and QS calculations should be carried out as soon as appropriate data are available
34	n.a.	DDT	OSC	Proposal will be provided at a later date	
	50-29-3	(DDT, 4,4'-isomer)			
	789-02-6	(DDT, 2,4'-isomer)			
35	n.a.	Dioxins (PCDD) / Furans (PCDF)	OSC	Proposal will be provided at a later date	
	n.a.	Drins	OSC	Proposal will be provided at a later date	
36	(309-00-2)	(Aldrin)			
37	(72-20-8)	(Endrin)			

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
38	(465-73-6)	(Isodrin)			
39	(60-57-1)	(Dieldrin)			
40	1336-36-3	PCB	OSC	Proposal will be provided at a later date	
	(7012-37-5)	(PCB 28)			
	(35639-99-3)	(PCB 52)			
	(37680-73-2)	(PCB 101)			
	(31508-00-6)	(PCB 118)			
	(35065-28-2)	(PCB 138)			
	(35065-27-1)	(PCB 153)			
	(35065-29-3)	(PCB 180)			
41	127-18-4	Tetrachloroethene	OSC	Inland and transitional waters: **10 µg/l** Coastal and territorial waters: **5.1 µg/l** MAC-QS: 36 µg/l	Tetrachloroethene is classified as a **carcinogen of class 3**. Hence, protection of human health from adverse effects is the objective that may require the lowest levels in the aquatic environment. However, toxicity data referring to health effects were not available and therefore the respective quality standards could not be calculated. Given the potential risk of tetrachloroethene exposure for human health, the quality standard derived for the protection of the freshwater community (36 µg/l) should not be exhausted. Instead, the quality standard set in Council Directive 86/280/EEC should be adopted as provisional overall QS, as long as it is not possible to derive a standard that reliably addresses the human health concerns. However, for coastal and territorial waters a lower overall QS may apply, referring to the protection of the pelagic community in these waters (the saltwater QS for the pelagic community is lower than the corresponding freshwater QS due to insufficient availability of toxicity data for marine biota and the resulting application of more stringent assessment factors according to TGD provisions).

Table 10.1: (continued) Proposed overall quality standards for the substances on the working list

#	CAS No	Name	WFD category	Overall Quality Standards	Comments / Recommendations
42	56-23-5	Tetrachloromethane	OSC	Inland waters as well as transitional, coastal and territorial waters: **7.2 µg/l** MAC-QS: 24.6 µg/l	Tetrachloromethane is classified as a **carcinogen of class 3**. Hence, the protection of human health from adverse effects due to the potential carcinogenic properties of tetrachloromethane is the objective that may require the lowest levels in the aquatic environment. But without toxicity data addressing these effects no respective effect based quality standard can be calculated. Respective QS referring to the health risk of tetrachloromethane upon oral uptake (drinking water / food from aquatic environments) should be calculated as soon as appropriate data become available. The proposed overall QS is referring to the protection of the pelagic communities both in freshwater and saltwater. For the reasons given above It should be considered as provisional.
43	79-01-6	Trichloroethene	OSC	Inland waters as well as transitional, coastal and territorial waters: **10 µg/l** MAC-QS: 210 µg/l	Trichloroethene is classified as a **class 2 carcinogen and a mutagen of class 3**. Protection of human health from adverse effects due to the carcinogenic and probable mutagenic properties of trichloroethene is therefore the objective that may require the lowest levels in the aquatic environment. However, in the final draft risk assessment report (part environment) it is stated that a threshold exposure level for adverse health effects cannot be identified. Hence, no respective effect based quality standards could be calculated. Assuming that cancer risk was considered in the derivation of the legal standard set by Council Directive 86/280/EEC, it is proposed to adopt this value (10 µg/l) as provisional overall QS. However, this QS should be reviewed based on the results of the human health part of the trichloroethene risk assessment as soon as this part is finalised.

11 Conclusions and Recommendations

The two main objectives of this study are the development of (i) a practicable methodological framework that enables the Commission to submit proposals for quality standards applicable to the concentrations of the priority substances of the Water Framework Directive (2000/60/EC) and other substances of concern, and (ii) to elaborate for a working list of substances quality standards with the approach developed.

The elaboration of quality standards for the substances on the working list with the developed methodological framework clearly showed that the proposed approach is applicable for the derivation of specific quality standards addressing the particular objectives of protection (i.e. pelagic and benthic communities, secondary poisoning of predators, human health, and drinking water abstraction) as well as for the identification of the overall quality standard that finally may be imposed to safeguard the entire set of objectives of protection.

Also, with regard to the effort required to work with the concept, it can be considered as economic. This is attributable to the fact that despite the comprehensive consideration of all relevant routes of exposure and objectives of protection the different quality standards for the specific objectives are normally only derived if certain pre-defined trigger values are exceeded. This avoids the assessment of irrelevant exposure routes and the calculation of unnecessary standards.

Problems encountered during the elaboration of the standards were in general not attributable to the proposed methodological framework but mostly to the limited availability of data or to the limitations of the available data.

For 21 substances on the working list risk assessment reports according to Council Regulation (EEC) No. 793/93 (6 final reports and 9 consolidated drafts or parts thereof) or Council Directive 91/414/EEC (7 monographs in final or consolidated form or data summaries thereof) were available and have been used as data basis for QS derivation. As all draft reports were already in a consolidated stage, it is not expected that substantial amendments of data or conclusions drawn will be made during further discussions until finalisation of the reports. However, amendments in some cases can, of course, not be excluded. For some of the substances on the working list for which a risk assessment according Regulation 793/93 is still ongoing it can be expected to get toxicity data and evaluations regarding risks for human health that will help to fill the respective data gaps identified in this study (see table 10.1). Four more risk assessment reports according to the existing substances regulation (nickel and compounds) and the plant protection products directive (chlorfenvinphos, diuron, trifluralin) are pending. Once they are available the proposed QS for these substances should be reviewed.

For most substances or substance groups for which quality standards have been derived so far (36) there were sufficient toxicity data available to calculate a quality standard referring to the protection of the pelagic community. Only for the PAHs benzo(b)fluoranthene, benzo(g,h,i)perylene and indeno(1,2,3-cd)pyrene this was not possible due to lacking data. For the brominated diphenylethers octa-BDE and deca-BDE as well as di (2 ethylhexyl)-phthalate the respective standards could also not be derived. However, in these cases this is due to the fact that the substances are apparently not directly toxic to aquatic organisms up to the limits of their water solubility.

For freshwater organisms by far more toxicity data have been provided as for saltwater species. However, for those substances for which toxicity data were available for freshwater and

saltwater organisms, in only one case (gamma-HCH) evidence could be found that freshwater and saltwater organisms differ in their sensitivity to the substance concerned[30]. Therefore, in all these cases, with the exception of gamma-HCH, it was suggested to derive the quality standard for water on the basis of the pooled freshwater and saltwater toxicity data and to use this standard for both freshwater and saltwater (20 substances). For 15 substances different quality standards for freshwater and saltwater have been suggested. With the exception of gamma-HCH, this is however not attributable to observed differences in sensitivities of freshwater and marine organisms but is the consequence of the fact that either no toxicity data for saltwater organisms were provided or that the marine data basis available was to small to assess whether freshwater and saltwater organisms are comparable in their sensitivity. In these cases the provisions of the marine effects assessment in the draft revised TGD [38] have been followed which foresee the use of higher assessment factors for saltwater than for freshwater, leading to lower quality standards for marine ecosystems.

The specific quality standards addressing secondary poisoning of top predators or adverse effects on human health due to consumption of fishery products could in many cases not be calculated since the required oral toxicity data for mammals or birds were lacking. This was especially the case for substances for which EU risk assessments were not available. If for a substance classified as having CMR-properties effect data referring to these properties were lacking, an overall QS for this substance has not been proposed in case these CMR-properties fall within classes 1 or 2. Because of the potentially high risk for humans it is deemed indispensable to conduct in depth assessments of health risks for the respective substances before overall QS can be proposed. For substances for which only weak evidence is available that their CMR properties may be relevant for man (class 3) overall QS have been proposed as far as possible, even if data addressing human health concerns were lacking. However, if done so, this has been indicated in table 10.1 and the respective EQS data sheets in Annex 4.

Data availability was worst for sediment dwelling organisms. In no case a reliable standard for sediment could be calculated on the basis of experimental results obtained with sediment organisms. Almost any standards derived for sediment have been calculated with the equilibrium partitioning approach as suggested in the TGD and are therefore no “real” sediment standards but merely a transformation of the standard derived for the protection of the pelagic community. It is recommended to use these figures only as "tentative values".

An occasionally occurring problem was inconsistency of the data. In some few cases a part of the provided toxicity data appear not plausible when compared to the other available results obtained for the same species or taxonomic group (i.e. the non plausible results are more than, e.g., a factor > 50 lower than the usual range obtained for the species concerned). Data that are deemed not plausible have not been used for the derivation of standards and this was flagged in the respective EQS data sheet. It is recommended to assess the validity of the rejected data and to amend the proposed quality standards accordingly, if the exclusion of the rejected data is not justified.

Further inconsistencies (respectively high data variability) have been observed with data on bioaccumulation and with partition coefficients (reported coefficients or BCF and BMF values cover a very wide range). This was, for instance, the case with the metals lead and mercury and with hexachlorobutadiene and pentachlorobenzene. For these substances it was there-

[30] Comparable sensitivity of freshwater and saltwater biota of the same groups was not only observed for organic substances with a narcotic mode of action but also for most plant protection products with specific modes of action or for metals for which bioavailability and toxicity may depend on geochemical parameters (e.g. salinity).

fore not possible to derive meaningful overall quality standards as for some of the protection objective specific standards no reliable calculations could be performed. Where these problems occurred this has been indicated in the EQS data sheet of the respective substances.

All proposed quality standards should be considered as preliminary and it is recommended to subject them to a validation or peer review step. In this review step attempts should be made to fill data gaps and to assess uncertainties identified and described in the EQS data sheets and to derive with the proposed methodological framework the protection objective specific or overall quality standards that could not be established in this study because information was lacking or was not reliable.

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