

**Manual on the Methodological Framework
to Derive Environmental Quality Standards for
Priority Substances in accordance with Article 16
of the Water Framework Directive (2000/60/EC)**

Peter Lepper

Fraunhofer-Institute Molecular Biology and Applied Ecology
Schmallenberg, Germany

15 September 2005

Contents

1	Background	1
2	Concept Development.....	1
3	Objectives of the Approach for the Derivation of Environmental Quality Standards	3
4	Methodological Framework to Derive Environmental Quality Standards for Water, Sediment and Biota.....	5
4.1	Evaluation and Selection of Data Required for Quality Standard Derivation	5
4.2	General Approach to set Environmental Quality Standards.....	8
4.3	Derivation of Annual Average Environmental Quality Standards (AA-EQS) for Organic Substances.....	14
4.3.1	Adaptive Transformation of Quality Standards to Water or Suspended Particulate Matter as Reference Matrix to Allow for the Use of Economic and More Reliable Analytical Methods	15
4.3.2	Use of the Assessment Factor Method for EQS derivation.....	16
4.3.2.1	Water – Protection of the Pelagic Community of Inland Surface Waters.....	16
4.3.2.2	Water – Protection of the Pelagic Community of Transitional, Coastal and Territorial Waters.....	18
4.3.2.3	Sediment – Protection of the Benthic Community of Inland Surface Waters	22
4.3.2.4	Sediment – Protection of the Pelagic Community of Transitional, Coastal and Territorial Waters.....	22
4.3.2.5	Secondary Poisoning of Predators – Substance Levels in Biota	23
4.3.2.6	Adverse Health Effects upon Ingestion of Fishery Products – Substance Levels in Biota.....	25
4.3.3	Quality Standards Referring to Levels in Water Intended for the Abstraction of Drinking Water	26
4.3.4	Use of Species Sensitivity Distributions to Derive EQS referring to Substance Concentrations in Water or Sediment	27
4.3.4.1	Quality and Quantity of Data required.....	29
4.3.4.2	Aggregation of Multiple Data for One Species	29
4.3.4.3	Testing Distributions for Goodness of Fit.....	30
4.3.4.4	Specific Considerations Regarding the Use of the SSD Method for the Derivation of EQS Referring to Transitional, Coastal and Territorial Marine Waters	30
4.3.5	Specific Considerations Regarding the Use and Interpretation of Simulated Ecosystem Studies (Micro/Mesocosms) for EQS Derivation	31
4.3.5.1	Differences in the Objectives of the Risk Assessment under CD 91/414/EEC and the Quality Standard in the Context of the WFD	32
4.3.5.2	Conclusions	36
4.3.6	Derivation of EQS Accounting for Acute Effects of Transient Exposure Peaks (MAC-EQS).....	36
4.3.6.1	Derivation of a MAC-EQS by the Assessment Factor Method for Intermittent Releases	37
4.3.6.2	Derivation of a MAC-EQS by the SSD Method	37

4.3.6.3	Derivation of a MAC-EQS based on Simulated Ecosystem Studies	37
4.4	Derivation of Quality Standards for Metals – Use of the Added Risk Approach.....	38
4.4.1	Consideration of Water Quality Parameters in QS Setting for Metals	39
4.4.2	Calculation of Quality Standards for Metals	40
4.4.2.1	Calculation of the Maximum Permissible Addition (MPA) and the Environmental Quality Standard for Inland Waters (Freshwater).....	40
4.4.2.2	Calculation of the Maximum Permissible Addition and the Environmental Quality Standard for Sediments of Inland Waters (Freshwater).....	41
4.4.3	Specific Considerations with Respect to the derivation of MPAs and EQS referring to the protection of Water and Sediment of Transitional, Coastal and Territorial Marine Waters.....	42
4.4.4	Secondary Poisoning of Predators – Metal Levels in Biota.....	42
4.4.5	Adverse Health Effects upon Ingestion of Fishery Products – Metal Levels in Biota	43
4.4.6	Metal Quality Standards Referring to Levels in Water Intended for the Abstraction of Drinking Water.....	43
4.4.7	Derivation of MPAs and Environmental Quality Standards Accounting for Acute Effects of Transient Exposure Peaks (MAC-MPA and MAC-EQS).....	43
5	Conclusions and Future Steps	44
6	References	46

Glossary

5P-COV	5 th Percentile Cut-Off Value; the 5 th percentile of a species sensitivity distribution.
AA-EQS	Annual Average Environmental Quality Standard
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
DT50	Disappearance Time in which the concentration of a substance drops to 50% of its level at T ₀
EAC	Ecologically Acceptable Concentration
EC	European Community
EC50	Effect concentration for 50% of the individuals in a toxicity test
EEC	European Economic Community
EQS	Environmental Quality Standard
EU	European Union
HC₅	Hazardous concentration for 5% of the species (based on the SSD)
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-EQS	Maximum Acceptable Concentration Environmental Quality Standard
MPA	Maximum Permissible Addition
NO(A)EL	No Observed (Adverse) Effect Level
NOEAC	No Observed Ecologically Adverse Effect Concentration
NOEC	No Observed Effect Concentration in a toxicity test
PEC	Predicted Environmental Concentration
PNEC	Predicted No-Effect Concentration
PPP	Plant Protection Product
PPP-RA	Risk Assessment for Plant Protection Products
QSAR	Quantitative Structure Activity Relationship
RA	Risk Assessment
RAR	Risk Assessment Report
SPM	Suspended Particulate Matter
SSD	Species Sensitivity Distribution
TDI	Tolerable Daily Intake
TER	Toxicity Exposure Ratio
TGD	Technical Guidance Document
WFD	Water Framework Directive
WHO	World Health Organisation

1 Background

Article 16 of the Water Framework Directive (WFD, Directive 2000/60/EC^[1]) lays down the Community Strategy for the establishment of harmonised quality standards and emission controls for the priority substances posing a significant risk to, or via, the aquatic environment. The setting of quality standards applicable to the concentrations of the priority substances in surface water, sediment or biota is one element of the strategy to achieve the protection objectives of the WFD.

This Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC) is an updated summary of the concept originally laid down in the Final Report of the Study Contract No. B4-3040/2000/30637/MAR/E1: Identification of quality standards for priority substances in the field of water policy. Towards the Derivation of Quality Standards for Priority Substances in the Context of the Water Framework Directive. By P. Lepper, Fraunhofer-Institute Molecular Biology and Applied Ecology, September 2002 (Carried out for the European Commission, Directorate General for Environment). The Manual was presented to the Scientific Committee on Toxicity, Ecotoxicity and the Environment (SCTEE) which agreed an opinion on the methodology and the derivation of EQS on 28 May 2004^[19]. The comments of the SCTEE were taken into account when revising and finalising this document.

2 Concept Development

The concept for the derivation of environmental quality standards (EQS) proposed in this report was presented to the Expert Advisory Forum on Priority Substances (EAF) at different stages of its development. Furthermore, an Expert Group on Quality Standards discussed specific elements of the proposed methodology. Comments received upon the different discussion rounds have been taken into account, where appropriate. In principle, the proposed approach was endorsed by the EAF at its meeting in March 2002. However, discussions were continuing in 2003 and 2004 and a list of open issues was identified by the EAF. As mentioned above, some further revisions of the methodological framework were made as result of the opinion of the Scientific Committee on Toxicology, Ecotoxicology and the Environment (SCTEE) on the setting of environmental quality standards for the priority substances of the Water Framework Directive in accordance with Article 16 thereof^[19].

In order to develop a scientifically sound and practicable concept and to derive most appropriate quality standards ensuring a good chemical status¹ 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 EQS 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^[1]. However, while the provisions of Annex V may suffice as general scheme to derive environmental quality standards

¹ 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.

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 additional aspects for effects assessment and quality standard setting into account.

To this end, the EU (i.e. CSTÉ) and Member States methods for the purpose of deriving water quality standards^[5] 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^[3]) or for plant protection products (Directives 91/414/EEC and 97/57/EC^[4, 8, 9]) 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 the report "Towards the Derivation of Quality Standards for Priority Substances in the Context of the Water Framework Directive"^[2].

All approaches for quality standard setting or risk assessment are very similar in so far as the application of assessment (i.e., safety) factors depending on the quality and quantity of available toxicity data is a common core element. As an alternative to this assessment factor approach, the use of statistical extrapolation methods (i.e., species sensitivity distributions) is recommended, respectively preferred, e.g. in the context of the EU risk assessments^[3, 4], if the data requirements for the application of this approach are met. Simulated ecosystem studies (e.g. meso or microcosm studies) are also accepted tools to assess impacts of chemicals under more realistic conditions than laboratory single species tests do allow for.

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 build the methodological framework for EQS-setting as far as possible on the state-of-the-art, internationally acknowledged, effects assessment procedures used in the EU-risk assessment frameworks for new and existing substances and biocides^[3] or plant protection products^[4, 9, 10, 11]. In addition, the methodology was supplemented with elements of Member State approaches for quality standard setting or latest findings in research, if deemed pertinent (e.g. in the EQS-setting procedure for metals). The reasons for this approach are as follows:

- 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 environmental quality standard derivation methodological framework that are already accepted and agreed by Member States and introduced on Member State level.

The general approach chosen for the derivation of environmental 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^[5], as possible impacts on aquatic ecology, 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 was deemed necessary to use today's state of the art methods for the derivation of quality standards in the context of the Water Framework Directive.

3 Objectives of the Approach for the Derivation of Environmental Quality Standards

The methodological framework elaborated for the derivation of environmental 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, all valid information and data available shall be used to derive the environmental quality standards. For the entire set of objectives of protection, i.e. the pelagic and benthic communities (\approx water and sediment) in freshwater, brackwater or saltwater ecosystems, the top predators of these ecosystems and human health, it is assessed by means of pre-defined trigger criteria (see table 1 a and b for triggers) whether a substance may pose a risk to a certain objective. For those objectives for which a possible risk (\approx 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 environmental quality standard.

Thus, an environmental 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 exposure via drinking water uptake are accounted for. Further, all relevant modes of toxicity are considered, e.g. for ecosystems direct and indirect toxicity (\approx 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.²

In order to cover both long-term and short-term effects resulting from exposure to a chemical, it is deemed pertinent to derive two kinds of EQS referring to (i) the annual average concentration and (ii) to short-term concentration peaks. To this end, a long-term environmental quality standard is calculated which is referring to the annual arithmetic mean concentration (AA-EQS) and, in addition, the so-called maximum acceptable concentration EQS (MAC-EQS) that is referring to protection against acute toxic effects exerted by exposure to short-term peak concentrations. The MAC-EQS is a figure not to be exceeded any time. In conjunction, the AA-EQS and the MAC-EQS are intended to protect the structure and function of the addressed aquatic ecosystems from significant alterations by the impact of chemical substances.

Therefore, an environmental 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.

² 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.

Table 1a: Environmental protection objectives and triggers to derive environmental quality standards

Water (protection of the pelagic community)	Sediments (suspended particulate matter) (protection of the benthic community)	Substance concentration in biota (prey; protection of predators against secondary poisoning)
<p>No trigger value applies. EQS are derived for <u>all</u> priority substances.</p> <p>For hydrophobic / adsorbing substances the EQS referring to the concentration in water are additionally reported as concentration in suspended particulate matter (SPM) if this is meaningful.</p> <p>Trigger value: $\log K_{pSPM-water} \geq 3$</p>	<p>EQS are derived for all substances with a $\log K_{pSPM-water} \geq 3$</p> <p>The EQS_{sediment} refers to suspended particulate matter in order to protect the new sediment.</p>	<p>EQS are derived for organic substances and metals with experimental $BCF \geq 100$ or $BMF > 1$.</p> <p>If a reliable BCF is not available, the trigger is $\log Pow \geq 3$ (applies only to organic substances)</p> <p>In order to avoid routine monitoring of biota the concentrations in animal tissue are normally transformed to concentrations in water or suspended particulate matter, using appropriate model estimates / partition coefficients. However, if the partition coefficients are highly variable or uncertain, the setting of biota standards may be considered.</p>

Table 1b: Human health related protection objectives and triggers to derive environmental quality standards

Substance concentration in biota (fishery products; protection of humans against adverse effects upon consumption of fishery products)	Possibility to abstract drinking water from surface water
<p>An EQS is derived for substances:</p> <ol style="list-style-type: none"> 1. being a known or suspected carcinogen (cat. I-III, R-phrases R45 or R40) 2. being a known or suspected mutagen (cat. I-III, R-phrases R46 or R40) 3. being a substance known or suspected to affect reproduction (cat. I-III, R-phrases R60, R61, R62, R63 or R64) 4. having the potential to bioaccumulate (experimental $BCF \geq 100$ or $BMF > 1$ (or $\log Pow \geq 3$, for organic substances only)) <p><i>plus</i></p> <ul style="list-style-type: none"> - classification as harmful or (very) toxic if swallowed or in contact with skin (R-phrases R21, R22, R24, R25, R27 or R28); <u>or</u> - danger of serious damage to health by prolonged exposure (R48) <p>The proposed EQS for Cd, Hg and Pb will be checked for compliance with the maximum permissible levels in fishery products fixed by existing EU-legislation (e.g. Council Regulation (EC) No 466/2001).</p>	<p>Derivation of an EQS referring to DW* abstraction only if the following cases apply (see section 4.3.3 for details):</p> <ol style="list-style-type: none"> 1. A "A1 value" is fixed in Directive 75/440/EEC and this value is lower than the EQS for other objectives of protection: $\Rightarrow EQS = \text{"A1 value" of CD 75/440/EEC}$ 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 EQS for other protection objectives: \Rightarrow Assessment (Experts): Identification of the substance specific removal efficiency in DW processing. $EQS = DWS / \text{Fraction not removable}$ 3. No A1 value or DW Standard exists for the substance concerned: \Rightarrow a) Calculation of a provisional DWS b) Assessment based on expert knowledge with regard to: <ol style="list-style-type: none"> 1. Removal efficiency of substance in DW processing; 2. toxicological appropriateness of the provisional DWS $EQS = \text{provisional DWS} / \text{Fract. not removable}$

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

4 Methodological Framework to Derive Environmental Quality Standards for Water, Sediment and Biota

4.1 Evaluation and Selection of Data Required for Quality Standard Derivation

The data base for each substance for which an environmental quality standard is to be derived in the context of the WFD should be as comprehensive as possible (i.e. with reasonable effort achievable). The data themselves should be **reliable** and **relevant**. The two terms are defined in the Technical Guidance Document (TGD) ^[3] as follows: **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 on a particular question addressed, for instance, in the effects assessment. **Only reliable, relevant data should be considered valid for use in quality standard setting.** This is in line with the opinion of the SCTEE ^[19], who argued that it is of utmost importance to base a standard on a comprehensive and valid data base given the possible consequences of a legally binding quality standard in terms of health, environmental and economical aspects.

In order to ensure that only valid data are used for quality standard setting, data quality control needs to be carried out. Guidance on the principles of data validation and the aspects to be considered is given in section 3.2 of chapter 3 of the TGD ^[3]. These principles of data validation are fully applicable for the purpose of quality standard setting.

A further validation of data generated or assessed under Community legislation such as Regulations (EC) 793/93 & 1488/94 (existing chemicals) or Directives 91/414/EC (plant protection products) or 98/8/EC (biocides) is normally not required because data published in the risk assessment reports under these legal frameworks already were subjected to data quality assurance controls and peer-review. The same may, in principle, apply for peer-reviewed data or guidance values (e.g. Tolerable Daily Intakes or Drinking Water values) published by (inter)national organizations such as, e.g., the World Health Organization (WHO), the United Nations Food and Agriculture Organization (FAO), the Organization for Economic Development (OECD) or the OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic. However, if data published by (inter)national organisations are used for quality standard derivation it should be considered case by case if the data source is reliable enough to warrant use of the data without further quality control.

For the selection of data to be used for quality standard setting the following principles apply:

1. Only data that can be considered as valid may be used, irrespective of the source of the data.
2. The relevant data are selected from the different sources available. This means that not all data mentioned in the different sources must be transferred to the data base for the respective substance but only those that could be relevant for quality standard setting.
3. Data for 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 principles laid down in sections 3 & 4 of chapter

3 of the TGD on effects assessment. That is, usually the lowest acute and long term toxicity data available for the different species³ are used, or in case of other data such as partition coefficients or bioconcentration factors, the figures resulting in realistic worst-case assumptions are selected.

4. If a risk assessment conducted under EU-legislation (e.g. Regulation (EC) No. 793/93 or Directives 98/8/EC or 91/414/EEC) is available for a substance for which EQS need to be derived, then the data validated in this risk assessment should be used for EQS-setting with the highest priority in order to ensure coherence with other EU-legislation. However, if new information relevant for the derivation of an EQS became available since the finalisation of a risk assessment report, this information should be given due consideration.
5. If a standard for a specific objective of protection cannot be derived since the required data are lacking, this is flagged.

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, and fish. However, for the purpose of quality standard setting it is important to consider available data of any other taxonomic groups or species as well, provided these data are relevant and reliable.

Both acute and chronic effect data may 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 includes effects on behaviour if it is conceivable that the effect described may impair the competitive fitness of the population. Avoidance reactions are also relevant, as the organisms concerned may be forced to abandon the habitat where they would normally be present.

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, by the time a QS must be set, adequate tests addressing this effect parameter are not available for a substance suspected to exert an endocrine disrupting potential, this substance is flagged for further consideration of this particular property in the future.

For the derivation of the long-term "annual average" environmental quality standards (AA-EQS, see section 4.2.1), chronic data (e.g. NOECs) are preferred. However, acute toxicity data (L(E)C₅₀) may be used to check the plausibility of the long-term data and of the quality standard derived on the basis of these long-term data⁴. In addition, acute toxicity data are required to derive the maximum acceptable concentration quality standard (MAC-EQS, see section 4.2.1) that is referring to the protection against acute effects of transient exposure peaks. Acute data may further be used to set long-term QS if no sufficient chronic toxicity data are available and cannot be acquired with reasonable effort. However, long-term annual average EQS shall not be derived exclusively on the basis of acute toxicity data.

³ In case more than one test result for the same species and end-point is available, the geometric mean (GM) may be calculated. Prior to calculating the GM an analysis of test conditions must be carried out with the objective to find possible reasons for the observed differences in response.

⁴ An annual average standard derived on the basis of long-term toxicity data should normally not be higher than a standard that would be obtained on the basis of acute toxicity data under consideration of the appropriate assessment factors. Derogations from this principle must be explained and justified.

Tests conducted with freshwater organisms may be used to derive EQS for transitional, coastal and territorial waters (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 organisms used in the tests are 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 “indicative” EQS for sediment, as long as no tests for sediment dwelling organisms are available. Legally binding sediment EQS should however preferably be based on results of toxicity tests with sediment organisms.

Results from test systems other than single species test (e.g. multi species / ecosystem simulation studies in micro- or mesocosms) should also be accounted for if the test system and the results meet the quality criteria (see section 4.3.5).

As in the quality standard setting framework protection of predators against secondary poisoning is addressed as one objective, mammalian or avian NOECs or NO(A)ELs of feeding studies are required for substances with a potential for bioaccumulation. Data obtained in long-term tests shall normally be given preference over acute data. The effects observed in the mammalian or avian toxicity tests must be of relevance for the population of the species concerned (e.g. reproductive developmental and behavioural performance, mortality).

Quantitative structure activity relationship (QSAR) estimates for toxicity may be referred to as supporting information in the derivation of QS, but such QSAR estimates cannot exclusively be used to derive a standard (i.e., experimental toxicity data supporting the QSAR estimates are required).

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. Oral Reference Doses (RfD), ADI or TDI values adopted by national or 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 may be used.

Data related to bioaccumulation and persistence

Data on bioaccumulation (bioconcentration, biomagnification and/or the octanol-water partition coefficient (K_{ow})) are required if a substance has a known or suspected potential to bioaccumulate (identified by the trigger-values given in table 1). Preference should be given to the most reliable data, i.e. field observations on bioaccumulation and biomagnification factors (BAFs, BMFs) or experimentally derived 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 but may be used as supplementary information, e.g. for risk management.⁵

Data referring to physical and chemical properties

Partition coefficients may be required in order to conduct transformation calculations (e.g. from mass/volume [mg/L] to mass/mass [mg/kg]) as explained in section 4.3.1 of this manual. Those coefficients (K) are, for instance: K octanol-water (K_{ow}), K suspended particulate matter – water (K_{susp-water}), K sediment – water (K_{sed-water}), K organic carbon (K_{oc}).

Other properties for which data should be available as supplementary information (e.g. for plausibility checks) are water solubility, vapour pressure and 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. Further information regarding the determination of natural background concentrations of metals has been elaborated by the Expert Group on Analysis and Monitoring of Priority Substances (AMPS).

4.2 General Approach to set Environmental Quality Standards

According to Article 16(7) WFD, quality standards shall be applicable to concentrations in water, sediments or biota. This implies that the setting of quality standards for the mentioned compartments is optional. An environmental quality standard (EQS) may not be required for the water, sediment or biota compartment if – based on the current scientific knowledge - there is no indication that a given substance poses this particular 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 referring to the concentration of a substance in biota may not be required if there is no indication for bioaccumulation (\approx secondary poisoning of top predators), or risk to human health due to consumption of fishery products.

In terms of working economy it is therefore foreseen to derive an EQS for each priority substance only for **water** by default. This quality standard is given in a mass per volume unit (e.g. $\mu\text{g/l}$) and intended to protect the pelagic community from adverse effects. However, for hydrophobic or strongly adsorbing substances this standard is additionally expressed as concentration in suspended particulate matter ($\mu\text{g substance / kg SPM}$) if this appears meaningful, e.g. for analytical reasons⁶.

⁵ 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 not to 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.

⁶ Thus, for hydrophobic organic substances, the quality standard referring to water will be given for unfiltered water samples ($\mu\text{g/l}$; i.e the "total" concentration in "whole" water) and for the corresponding concentration in suspended particulate matter ($\mu\text{g/kg SPM}$). See section 4.3.1 for transformation algorithms.

In line with the provisions of the TGD on marine effects assessment^[3], distinct QS are derived for **freshwater and saltwater** environments, respectively, if the effects data available are not sufficient to conclude that both environments can be considered as equally vulnerable. The setting of quality standards for the further objectives of protection, i.e. the possibility of drinking water abstraction from surface water, substance concentrations in biota that will prevent secondary poisoning of predators or adverse health effects in humans upon ingestion of fishery products, and concentrations in sediment that will not impair benthic life, is triggered by the criteria presented in tables 1a and b.

The lowest specific standard calculated for the different objectives of protection is adopted as **overall quality standard**. However, if different quality standards for the freshwater and the marine environment need to be derived, the lowest standards relevant for either the marine or the freshwater environment are adopted as specific overall QS_{saltwater} or overall QS_{freshwater}.

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 reported as those) in order to avoid routine monitoring (and thus sampling) of biota for compliance checking with quality standards⁷. The respective algorithms for transformation are given in the following sub-sections of chapter 4.3.

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 substances, the so-called equilibrium partitioning method may be used in order to extrapolate an indicative quality standard applicable to the concentration in sediment (for the protection of benthic life) from the quality standard derived for the protection of the pelagic community in water (see sections 4.3.2.3 & 4.3.2.4 for details).

For the purpose of compliance checking, the sediment quality standard may be compared with the substance concentration 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 substrate 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 the current task.

With respect to **drinking water quality**, existing standards will be accounted for, e.g. those laid down in Council Directive 75/440/EEC concerning the quality required of surface water intended for the abstraction of drinking water^[6] or in Council Directive 98/83/EC concerning the quality of water intended for human consumption^[7]. 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

⁷ In order to conduct the respective transformations supplementary information like partition coefficients or bioaccumulation data are required. If there is much uncertainty associated with these data it may be better to refrain from transforming quality standards, because in this case the transformation might compromise the reliability of the result obtained. In such a case it might be more appropriate to set additional biota or sediment standards beside the standard for water.

increase in the pollution of waters used for the production of drinking water⁸. In this sense, the "A1 values" of Council Directive 75/440/EEC^[6] referring to "simple treatment" (i.e. filtration and disinfection) to produce drinking water from surface water are considered as minimum quality standards. 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 4.3.3.

In order to derive the human health related quality standards for **biota** (consumption of fishery products), it is suggested to follow the guidance and models given in the TGD^[3] and in the context of Council Directives 91/414/EEC and 97/57/EC^[8, 9] as far as possible (see section 4.3.2.6). Existing maximum permitted levels such as, e.g., those fixed for cadmium, lead and mercury in Council Regulation (EC) No 466/2001^[17] for fishery products are generally to be considered in the derivation of the quality standards for the respective substances.

Table 2 gives an overview of the methods used for the derivation of quality standards referring to the different objectives of protection. The methods are outlined in sections 4.3 & 4.4 (including sub-sections).

In order to cover both long-term and short-term effects resulting from exposure to a chemical, it is deemed pertinent to derive two different kinds of environmental quality standards referring to:

- (i) **the annual average concentration (AA-EQS)** accounting for the protection against the occurrence of chronic effects, and
- (ii) **short term concentration peaks** (the maximum acceptable concentration, **MAC-EQS**) accounting for protection against the occurrence of acute toxicity.

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

The **annual average environmental quality standard** refers by definition to the **annual arithmetic mean** of the samples taken for operational monitoring at a sampling station. As Annex V.1.3.4 of the WFD specifies a sampling frequency of 1 sample per month the annual average concentration at a sampling station will normally be calculated as an arithmetic mean of 12 samples taken in monthly intervals⁹. This implies that for a certain percentage of time the concentration in the compartment concerned (water, sediment, biota) may considerably exceed the annual average concentration due to concentration peaks resulting, e.g., from intermittent releases of the chemical in question, varying concentrations due to seasonal differences in the use of a substance (e.g. plant protection products) or in the flow regime of the water body concerned, etc. In case of substances showing a very high acute toxicity (or a narrow acute to chronic toxicity ratio) it can thus not be excluded that an EQS only referring to the annual average concentration is insufficient to protect the aquatic ecosystem against acute effects by transient concentration peaks.

⁸ See Article 7 of Council Directive 75/440/EEC, Article 4 of 98/83/EC and Articles 7(2,3) and 16(1) of the Water Framework Directive.

⁹ For seasonally variable substances (in practice predominantly plant protection products) Annex V.1.3.4 specifies 12 monthly samples per year, with increased frequency during periods where use might lead to seasonal differences. It could for instance be envisaged that in addition to the 12 monthly samples per year, increased frequency is required during periods where use might lead to seasonal differences. The number of additional samples could be at least one per month (i.e. raising the frequency to 2-weekly) for at least three months. The relevant use period may be identified by the Member States.

In order to account for potential **acute toxic effects** exerted by transient exposure to peak concentrations of highly toxic chemicals, it is therefore required to establish in addition to the annual average quality standard a second quality standard setting a **maximum acceptable concentration** (MAC) which must not be exceeded at any time in order to protect aquatic life. As emissions to the aquatic environment normally occur in water first and because subsequent partition between water, settled sediment and biota is normally rather slow, it is deemed appropriate to derive this MAC-EQS for water only. Exposure concentrations in water might change to a significant extent much quicker than in sediment or biota.

During the consultation process, there was a discussion whether the MAC should take the form of a statutory or guidance value. The proposed methodology for deriving the MAC is independent of the outcome of this political/legal question. Similarly, the setting of a MAC may consider other aspects than the ecotoxicological considerations presented in this manual. For example, the frequency of monitoring (see footnote 9) may lead to a situation where an AA-EQS is not complied with if at least one value exceeds 12 times the AA-EQS value. In consequence, any MAC-EQS which is higher than 12 times the AA-EQS may be meaningless in the regulatory practice of compliance checking. It is up to the legal and political discussion to take account of such issues. No further recommendations are made in the context of this document.

Table 2: Overview of the methods used 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 including plant protection products; EQS: environmental quality standard; SPM: suspended particulate matter; SSD: species sensitivity distribution; TGD: technical guidance document)

Objective of protection	Sub-stance	Compartment	Method used	Description in section
pelagic community	OC	freshwater (unfiltered sample) (for hydrophobic substances in addition: corresponding concentration in SPM)	<ul style="list-style-type: none"> TGD Assessment Factor method (freshwater AFs) SSD method (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.3.2(.1), 4.3.1 4.3.4 4.3.5 4.3.6 (MAC-EQS)
pelagic community	OC	marine water (unfiltered sample) (for hydrophobic substances in addition: corresponding concentration in SPM)	<ul style="list-style-type: none"> TGD Assessment Factor method (saltwater AFs) SSD method (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.3.2(.2), 4.3.1 4.3.4 4.3.5 4.3.6 (MAC-EQS)
benthic community	OC	freshwater sediment (SPM) EQS are derived if $\log K_{pSPM-water} \geq 3$	<ul style="list-style-type: none"> TGD Assessment Factor method (AFs for freshwater sediment) Equilibrium partitioning approach (if no or only insufficient toxicity data of sediment organisms are available) SSD method (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.3.2(.3) 4.3.2.3 4.3.4 4.3.5
bentic community	OC	marine sediment (SPM) EQS are derived if $\log K_{pSPM-water} \geq 3$	<ul style="list-style-type: none"> TGD Assessment Factor method (AFs for marine sediment) Equilibrium partitioning approach (if no or only insufficient data for sediment organisms are available) SSD method (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.3.2(.4) 4.3.2.4 4.3.4 4.3.5
pelagic community	ME	freshwater (filtered sample, "dissolved concentration") (corresponding concentration in SPM in addition)	<ul style="list-style-type: none"> Added risk approach ($EQS = C_{background} + MPA_{freshwater}$) TGD assessment factor method to derive MPA (freshwater AFs) SSD method to derive the MPA (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.4, 4.4.2.1 4.4.7 (MAC-EQS)
pelagic community	ME	marine water (filtered sample, "dissolved concentration") (for hydrophobic substances in addition: corresponding concentration in SPM)	<ul style="list-style-type: none"> Added risk approach ($EQS = C_{background} + MPA_{saltwater}$) TGD assessment factor method to derive MPA (saltwater AFs) SSD method to derive the MPA (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.4, 4.4.2.1, 4.4.3 4.4.7 (MAC-EQS)
benthic community	ME	freshwater sediment (SPM) EQS are derived if $\log K_{pSPM-water} \geq 3$	<ul style="list-style-type: none"> Added risk approach ($EQS = C_{background} + MPA_{sediment.fw}$) TGD assessment factor method to derive MPA (freshwater sediment AFs) SSD method to derive the MPA (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.4, 4.4.2.2
benthic community	ME	marine sediment (SPM) EQS are derived if $\log K_{pSPM-water} \geq 3$	<ul style="list-style-type: none"> Added risk approach ($EQS = C_{background} + MPA_{sediment.sw}$) TGD assessment factor method to derive MPA (marine sediment AFs) SSD method to derive the MPA (if sufficient data are available to use this approach) Interpretation of Simulated Ecosystem Studies (if valid studies are available) 	4.4, 4.4.2.2, 4.4.3

continued overleaf

Table 2: (continued) Overview of the methods proposed for the derivation of quality standards in relation to the different objectives of protection

Objective of protection	Substance	Compartment	Method used	Description in section
secondary poisoning of top predators	OC, ME	water (freshwater & saltwater) (for hydrophobic substances in addition: corresponding concentration in SPM) EQS only derived if triggers are exceeded (see table 1a)	<ul style="list-style-type: none"> Tolerable body concentrations in prey (fish and/or mussels) are calculated that prevent adverse effects on predators based on the lowest relevant mammalian or avian oral NOAEL or NOEC_{food}, the food web scenario and the figures given in the TGD for food consumption (\Rightarrow EQS_{secpois.biota}). Based on these "safe" levels in prey organisms water concentrations are derived using the BCF (preferred) or the octanol water partition coefficient (the latter not for metals) of the substance concerned (\Rightarrow EQS_{secpois.water}). Taking account of the potential uncertainty associated with the transformation of the biota body burden based standard to the corresponding water concentration it may be decided substance by substance to which matrix this standard should refer to (i.e. biota or water). 	4.3.2.5 4.4.4
human health (drinking water consumption)	OC, ME	freshwater derivation of EQS only if no standard is fixed in CD 75/440/EEC	<p>Derivation of DW abstraction EQS only if the following cases apply:</p> <p>An "A1 value" is fixed in Directive 75/440/EEC and this value is lower than the EQS for other objectives of protection: \Rightarrow EQS = "A1 value" of CD 75/440/EEC</p> <p>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 EQS for other protection objectives: \Rightarrow Assessment (Experts): Identification of the substance specific removal efficiency in DW processing. EQS = DWS / Fraction not removable</p> <p>No A1 value or DW Standard exists for the substance concerned: \Rightarrow 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 EQS = appropriate DWS / Fract. not removable</p>	4.3.3, 4.4.6
human health (food consumption)	OC, ME	water (freshwater & saltwater) (for hydrophobic substances in addition: corresponding concentration in SPM) Derivation of EQS only if triggers are exceeded (see table 1b)	<ul style="list-style-type: none"> 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 TGD standard figures for consumption of fishery products and body weights of humans, concentrations in fish (and/or mussels) are calculated that prevent adverse effects by ingestion of fishery products. Based on these biota standards (EQS_{hh.biota}) referring to concentrations in fish or mussels the corresponding water concentrations are derived using the BCF (preferred) or the octanol water partition coefficient (the latter not used for metals) of the substance concerned (\Rightarrow EQS_{hh.water}). Taking account of the potential uncertainty associated with the transformation of the biota body burden based standard to the corresponding water concentration it may be decided case substance by substance to which matrix this standard should refer to (i.e. biota or water). 	4.3.2.6 4.4.5

4.3 Derivation of Annual Average Environmental Quality Standards (AA-EQS) for Organic Substances

In the European Union the risks of most industrial chemicals (i.e. existing as well as new substances and biocides) are assessed according to the provisions laid down in the TGD^[3], the risks exerted by plant protection products (PPP) are assessed according to the principles laid down in Council Directives 91/414/EEC^[8] and 97/57/EC^[9]. However, although PPP are assessed and authorized under another legal framework than the other chemicals, the principles and procedures applied for aquatic effects and risk assessment are compatible with respect to their results (i.e. indication as to whether the assessed chemical exerts an environmental risk at the conditions of its uses). For this reason it is possible to derive the environmental quality standards required by the WFD for both PPP and other substances with the same methodological approach as presented in the sub-sections to section 4.3 of this manual. This is explained further in the following.

The most obvious difference in the aquatic risk assessment protocols laid down in the TGD (TGD-RA) or used for plant protection products (PPP-RA) is the fact that in the TGD-RA a predicted no effect concentration (PNEC) is calculated, normally based on toxicity data of the most sensitive organism and an assessment factor accounting for the quality and quantity of available data, which is set in relation to the predicted environmental concentration (PEC). A PEC/PNEC ratio >1 is used as indicator for risk. For plant protection products a PEC is calculated as well and related to a set of acute and chronic toxicity tests with algae, invertebrates and fish, thereby establishing toxicity exposure ratios (TER, i.e. result of the acute or chronic toxicity test of each species divided by the relevant PEC). The resulting TER-ratios are compared with predetermined TER trigger values of 10 or 100, depending on the taxonomic group and the type of effects (chronic or acute) to be assessed. The calculated TER values must normally not be lower than the triggers in order to permit the authorisation of the PPP. Thus, only the application of safety factors accounting for uncertainties is different although the factors are in most instances the same for a comparable data set (i.e. 10 or 100, see table 11).

Therefore, despite the apparent formal differences, both approaches are in principle equivalent and will, in most instances, for the same data set give the same result with regard to the acceptability of risk, because in essence the TER ratio 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" (TGD-RA) or "higher tier" (PPP-RA) risk assessment may be conducted utilising more sophisticated means for exposure and effects assessment such as, e.g., species sensitivity distributions or multi-species studies (micro/mesocosms).

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 PPP-RA, only acute toxicity to algae (EC50) is considered whereas in the TGD-RA also the no-effect level (NOEC or 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 TGD-RA, assessment factors of 10 for NOEC/EC10 values and 100 for EC50 data are normally used (cf. Table 3) whereas the respective PPP-RA TER-ratio for the EC50_{algae} must not fall below 10 (equivalent to an assessment factor of 10 in TGD-RA, cf. Table 11).

These differences in the consideration of toxicity to algae may be a result of the philosophy behind the risk assessment for plant protection products. For PPP beneficial effects of its (intentional) use are taken into account and, therefore, the risk characterisation in the PPP-RA is focused on the acceptability of in practice inevitable side effects occurring in the vicinity of the treated area. To this end, specific consideration is given to the recovery potential of affected ecosystems (e.g. small water courses in the immediate vicinity of the area of application after transient exposure to a PPP). This might be the reason why effects on algae are not considered in 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).

The “ditch at the edge of a field” exposure pattern normally assessed in the PPP-RA is different from the exposure situation in larger water bodies for which EQS in the context of the WFD are to be set. Peak concentrations will normally be lower in the water courses draining an agricultural area than the initial concentration in a ditch adjacent to the application area but exposure may not cease as quick as in the ditch. Therefore, the recovery potential of aquatic ecosystems cannot be taken into account for the purpose of setting an annual average quality standard because exposure in draining water bodies is not transient but will prevail for at least the use period of the active substance in the river basin. Consequently, for the purpose of environmental quality standard setting, algal toxicity of plant protection products needs to be assessed and considered the same way as for any other pollutant (in other words, the assessment factors referred to in table 3 should apply; further implications for the use and interpretation of Higher-Tier studies conducted in the context of the PPP-RA for quality standard derivation are addressed and discussed in section 4.3.5.1 of this Manual).

4.3.1 Adaptive Transformation of Quality Standards to Water or Suspended Particulate Matter as Reference Matrix to Allow for the Use of Economic and More Reliable Analytical Methods

For organic substances the EQS are normally expressed as concentration in whole water (i.e. the unfiltered water sample \approx water plus suspended particulate matter). For hydrophobic organic substances (i.e. those exceeding the partition coefficient triggers given in table 1) a corresponding concentration in suspended particulate matter (SPM) of the EU standard water as defined in the TGD^[3] (15 mg/l SPM dry weight) may be calculated and used as a surrogate standard. This approach offers the option to conduct compliance monitoring in the matrix (i.e. the unfiltered water sample or SPM) that is deemed the most suitable for analysis of the substance in question.

In case compliance checking is based on quality standards referring to SPM as matrix, the SPM concentrations in the water samples must be monitored in addition. Knowledge of the SPM concentrations is required to allow for a correction of the $EQS_{SPM,water}$ (calculated for an EU-standard SPM concentration of 15 mg/l) with the real SPM content (C_{SPM}) of the samples.

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

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

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

with:

$QS_{SPM,water}$	Quality standard for water referring to the substance concentration in SPM
QS_{water}	Quality standard for water referring to the total (unfiltered) water sample
C_{SPM}	Concentration of SPM in the water sample (EU standard freshwater: 15 mg/l; saltwater: 3 mg/l)
Kp	Substance specific partition coefficient SPM – water

4.3.2 Use of the Assessment Factor Method for EQS derivation

The assessment factor method (AF-method) as laid down in the TGD is the standard approach to derive environmental quality standards in the context of the Water Framework Directive (cf. Annex V, 1.2.6). It is generally considered indispensable for substances for which no extensive toxicity data base is available and it is broadly accepted in scientific terms as an acceptable method to deal with uncertainties arising from limited data availability and knowledge in extrapolating "safe" environmental levels of substances. However, the minimum data requirements as described in section 4.1.1 and the following sections on EQS derivation by the assessment factor method in water, sediment or biota must be fulfilled in order to derive a standard.

If preconditions are met to use the species sensitivity distribution method or the results of simulated ecosystem studies for the derivation of quality standards (see sections 4.3.4 & 4.3.5 including the respective sub-sections) these more sophisticated approaches should preferably be used to calculate standards. However, it is required to derive the same EQS as well with the AF-method for comparative purposes. Potential discrepancies in the results obtained with the different procedures need to be discussed and the decision for the finally preferred EQS derivation method needs to be justified.

4.3.2.1 Water – Protection of the Pelagic Community of Inland Surface Waters

The procedures for aquatic effects assessment and the calculation of the PNEC ($\approx QS_{freshwater}$) with the Assessment Factor method as laid down in section 3.3 of Part II of the TGD^[3] are used as the standard approach (required also by Annex V, 1.2.6 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 3).

Table 3: Assessment factors to derive a Quality Standard for **freshwater** (adaptation from table 16 of chapter 3 of the TGD^[3])

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:	
<p>(a) The assessment factor 1000 is a conservative and protective factor. For a given substance there may be evidence that the factor 1000 is too high or too 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.</p> <p>(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.</p> <p>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)C₅₀ 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)C₅₀ of the short-term tests.</p> <p>(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.</p> <p>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)C₅₀ 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)C₅₀ of the short-term tests.</p> <p>(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.</p> <p>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.</p> <p>(e) Basic considerations and minimum requirements as outlined in section 3.3.1.2 of the TGD^[3], see also section 4.3.4 of this document.</p> <p>(f) The AF to be used on mesocosm studies or (semi) field data will need to be reviewed on a case by case basis.</p>	

4.3.2.2 Water – Protection of the Pelagic Community of Transitional, Coastal and Territorial Waters

The procedures for the marine effects assessment as described in section 4.3 of Part II of the TGD^[3] are used as the standard approach for transitional, coastal and territorial waters, i.e. the assessment factor method together with specific assessment factors for marine effects assessment (see table 4) is applied to derive the $QS_{\text{saltwater}}$.

The SCTEE has been critical about the distinction made between marine and freshwaters in the revised TGD^[19, 20]. In particular the Committee is unconvinced about the need for extra application factors to reflect uncertainties regarding the relative sensitivity of uniquely marine taxa and therefore criticised the general TGD approach to apply an additional assessment factor of 10 when no information on the sensitivity of additional marine groups is available. The SCTEE acknowledged and welcomed however that for the setting of quality standards referring to the protection of transitional, coastal and territorial waters specific assessments are foreseen that involve a critical evaluation of the information available. They considered this a derogation from the TGD rules which is however not the case. As further outlined in the following, the TGD provides scope for an in-depth evaluation of the information available and a case-by case decision on the appropriate assessment factor.

In order to derive environmental quality standards for transitional, coastal and territorial waters combined toxicity data sets of marine and freshwater species are normally used as toxicity data because current marine risk assessment practice suggests a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota^[3] (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, EQS for inland surface waters and transitional, coastal and territorial waters must be derived on the basis of distinct data sets for freshwater and marine organisms.

According to the TGD, freshwater effects data of plant protection products (PPP) shall normally not be used in place of saltwater data, because within trophic levels differences larger than a factor of 10 were found for several PPP^[3]. This means that for PPP the derivation of quality standards addressing the protection of water and sediment in transitional, coastal and territorial waters is not possible if there are no effects data for marine organisms available or if it is not possible to determine otherwise with high probability that marine organisms are not more sensitive than freshwater biota (consideration of the mode of action may be helpful in this assessment).

As for the derivation of quality standards referring to transitional, coastal and territorial waters the assessment factors for marine risk assessment of the TGD^[3] are to be used, the resulting quality standards might be more stringent than the standards derived 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 a 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 are available a higher assessment factor than that used for the derivation of the inland water (freshwater) quality standard should be applied to reflect the greater uncertainty in the

extrapolation. Where data is available for additional marine 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^[3] (see table 4).

Thus, an additional assessment factor is not automatically applied in the effects assessment and quality standard setting procedure referring to transitional, costal and territorial waters. This additional AF is only used if the available data do not appropriately represent the communities that dwell in the addressed marine ecosystems. If marine life forms are sufficiently represented in the data set available, the recommended assessment factors do not differ from those used in the freshwater effects assessment.

Table 4: Assessment factors to derive PNEC_{water} for **saltwater**^[3]

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 and/or crustaceans and/or fish) representing three trophic levels + 2 long-term NOECs from additional marine taxonomic groups (e.g., echinoderms, molluscs)	10
<p>NOTES</p> <p><i>General:</i> 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.</p> <p>(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.</p> <p>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.</p> <p>Evidence for varying the assessment factor could include one or more of the following:</p> <ul style="list-style-type: none"> • 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). <p>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)C₅₀ data for <i>Daphnia</i>. In these exceptional cases, the PNEC should be calculated with a factor of 10000.</p> <p style="text-align: right;">(continued overleaf)</p>	

Table 4: (continued) Assessment factors proposed for use to derive PNEC_{water} for saltwater

(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)C₅₀ 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)C₅₀ 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 1000. 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)C₅₀ of the short-term tests. This should not apply in cases 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)C₅₀ 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)C₅₀ 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, or 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)C₅₀ 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)C₅₀ 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.

4.3.2.3 Sediment – Protection of the Benthic Community of Inland Surface Waters

If results of long-term toxicity tests with sediment organisms are available, the quality standard (EQS_{sediment}) is calculated as laid down for the $PNEC_{\text{sediment}}$ in section 3.5.4 of Part II of the TGD^[3], using the assessment factors given in table 5.

$$EQS_{\text{sediment}} [\text{mg/kg}] = \text{lowest NOEC or EC10} [\text{mg/kg}] / \text{AF (range 100 – 10)}$$

Table 5: Assessment factors to derive a EQS_{sediment} (table 19 of^[3])

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

However, as toxicity data for benthic organisms are normally lacking for many substances an *indicative* EQS_{sediment} is calculated in such cases with the equilibrium partitioning method as described in section 3.5.3 of the TGD^[3]:

$$EQS_{\text{sed.wet.weight}} [\text{mg/kg}] = \frac{K_{p\text{SPM-water}} [\text{m}^3/\text{m}^3]}{\text{bulk density}_{\text{SPM.wet}} [\text{kg}/\text{m}^3]} * EQS_{\text{water}} [\text{mg}/\text{l}] * 1000$$

with:

$K_{p\text{SPM-water}}$ partition coefficient suspended particulate matter – water
 $\text{bulk density}_{\text{SPM.wet}}$ 1150 kg/m^3

As the formula only considers uptake via the water phase, a correction is made for substances with $\log K_{ow} > 5$ as significant uptake by food ingestion may take place. To this end, the EQS_{sediment} is divided by a factor of 10.

In case there is only a marginal short-term effects data base for benthic organisms available an *indicative* EQS_{sediment} may be derived on the basis of both the short-term effects data (applying an assessment factor of 1000 to the lowest) and the equilibrium partitioning approach. The final value is selected by expert judgement, taking all available information into account.

All sediment quality standards that are not derived on the basis of at least 3 long-term tests with sediment organisms representing different life and feeding conditions should only be considered as indicative. Due to the high level of uncertainty, firm EQS_{sediment} may only be derived for a statutory purpose if the mentioned minimum data set is available for the substance in question.

4.3.2.4 Sediment – Protection of the Pelagic Community of Transitional, Coastal and Territorial Waters

With respect to the quality standards setting for sediments in coastal and territorial waters the strategy recommended in section 4 of Part II of the TGD^[3] for effects assessment with marine benthic organisms is followed. This is in principle the same approach as outlined in section

4.3.2.3 with regard to sediment of inland surface waters. However, more stringent assessment factors may apply depending on the quality and quantity of toxicity data available; see table 6.

Table 6: Assessment factors for derivation of the PNEC_{marine sediment} based on the lowest available NOEC/EC₁₀ from long-term tests^[3]

Available test results	Assessment factor ^{a)}
One acute freshwater or marine test (LEC ₅₀)	10000 ^{b)}
Two acute test including a minimum of one marine test with an organism of a sensitive taxa (lowest LEC ₅₀)	1000 ^{b)}
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 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.

b) If an indicative EQS_{sediment.marine} is calculated with short-term toxicity data, an alternative EQS must be calculated using the equilibrium partitioning approach (see section 4.3.2.3). The final value is selected by expert judgement, taking all available information into account.

4.3.2.5 Secondary Poisoning of Predators – Substance Levels in Biota

The respective quality standards for substance levels in biota are calculated if the triggers given in table 1b concerning secondary poisoning or human health effects are met.

The standard figures and procedures as laid down in section 3.8.3 and 4.3.3 of Part II of the TGD^[3] are used.

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. As secondary poisoning effects on bird and mammal populations rarely become manifest in short-term studies, 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.

$$\text{NOEC}_{\text{oral}} = \text{NOAEL}_{\text{oral}} * \text{CONV}$$

with:

CONV: conversion factor from NOAEL to NOEC (table 7)

Table 7: Conversion factors from NOAEL to NOEC for several species^[3]

Species	Conversion factor (BW/DFI*)
<i>Canis domesticus</i>	40
<i>Macaca sp.</i>	20
<i>Microtus spp.</i>	8.3
<i>Mus musculus</i>	8.3
<i>Oryctolagus cuniculus</i>	33.3
<i>Rattus norvegicus</i> (> 6 weeks)	20
<i>Rattus norvegicus</i> (≤ 6 weeks)	10
<i>Gallus domesticus</i>	8

* BW = body weight (g); DFI: daily food intake (g/day)

The quality standard referring to the concentration in food of the predator ($QS_{\text{secpois.biota}} \approx PNEC_{\text{oral}}$) is then derived from the $NOEC_{\text{oral}}$ applying an assessment factor (table 8).

$$QS_{\text{secpois.biota}} = NOEC_{\text{oral}} / AF_{\text{oral}}$$

Table 8: Assessment factors for extrapolation of mammalian and bird toxicity data^[3]

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

If several $NOEC_{\text{oral}}$ for bird or mammal species are available, the lowest of the resulting $EQS_{\text{secpois.biota}}$ is used as quality standard.

As for several reasons it is currently not desirable or possible to perform routine monitoring of biota for compliance checking, a corresponding concentration in water may be calculated as a surrogate standard ($\approx EQS_{\text{secpois.water}}$), using the safe level in prey ($EQS_{\text{secpois.biota}}$) and bioaccumulation data (bioconcentration factor (BCF) and biomagnification factor (BMF)) of the substance concerned¹⁰. The calculation is done with a transformation of the formulae used in the TGD to calculate the PEC_{oral} (sections 3.8.3.4 and 4.3.3.2 of Part II of the TGD). Accounting for the longer food chains in the marine environment, not only biomagnification in the prey of predators (BMF₁, as for freshwater) but also in the prey of top predators (BMF₂) is considered.

Freshwater

$$EQS_{\text{secpois.water}} [\mu\text{g/l}] = \frac{QS_{\text{secpois.biota}} [\mu\text{g/kg}]}{BCF [l/kg] * BMF_1}$$

¹⁰ For hydrophobic organic substances (exceeding the triggers given in table 1) the biota quality standards may also be expressed as concentration in suspended particulate matter of the EU standard water; for transformation see section 4.3.1.

Marine water

$$EQS_{\text{secpois.water}} [\mu\text{g/l}] = \frac{QS_{\text{secpois.biota}} [\mu\text{g/kg}]}{BCF [l/kg] * BMF_1 * BMF_2}$$

The BMFs used should ideally be based on measured data but the availability of such data is at present very limited. Therefore it may be considered to use the TGD default BMF values as listed in table 9.

However, there may too much uncertainty being associated with the use of default data but variable experimental bioaccumulation data as well. It may therefore be considered to refrain from transforming the biota quality standard into a water quality standard because transformation might compromise the reliability of the result. Expert judgement is required to decide on a case-by case basis as to whether it might be more appropriate to maintain the $QS_{\text{secpois.biota}}$ or to transform it to the $QS_{\text{secpois.water}}$.

Table 9: Default BMF-values for organic substances^[3]

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

4.3.2.6 Adverse Health Effects upon Ingestion of Fishery Products – Substance Levels in Biota

The respective quality standards for substance levels in biota are calculated if the triggers given in table 1a concerning secondary poisoning or human health effects are met.

With regard to the uptake of fishery products 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, a rather simple but practicable approach for deriving a respective quality standard is used.

By convention, the uptake of a substance with fishery products shall not exceed more than 10% of the relevant threshold level for humans (e.g. the ADI / TDI / NO(A)EL_{oral}).

The quality standard referring to the substance concentration in fishery products ($EQS_{\text{hh.food}}$) is calculated as follows, using the standard figures of the TGD for human body weight (bw; 70 kg) and consumption of fishery products (115 g/day):

$$EQS_{\text{hh.food}} = \frac{0.1 * \text{threshold level} [\mu\text{g/kg bw}] * 70 \text{ kg (human bw)}}{0.115 \text{ kg seafood consumption}} = \mu\text{g/kg fishery product}$$

This $EQS_{hh.food}$ is transformed to the corresponding concentration in water, applying the same approach and considerations as described for the transformation of the $QS_{secpois.biota}$ in section 4.3.2.5 of this report.

$$EQS_{hh.food.water} [\mu\text{g/l}] = \frac{QS_{hh.food} [\mu\text{g/kg}]}{BCF [l/kg] * BMF_1}$$

The suggested approach does not specifically consider possible high risk groups such as, e.g., children or sub-populations that consume more fishery products than the European average. However, by limitation of the acceptable uptake of a substance with fishery products to 10% of its threshold value at the European average level of fishery product uptake the resulting margin of safety is considered sufficient to protect those high risk groups as well from adverse health effects.

4.3.3 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. The procedure described in the following was devised to permit the derivation of a quality standard addressing this protection objective:

1. In case an "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^[6] 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), the "A1 value" is proposed as an overall quality standard for inland surface waters (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^[7] (concerning the quality of water intended for human consumption) and this drinking water standard is lower than the quality standard required to safeguard the other objectives of protection, the subsequent procedure is followed:

2. If possible, 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^[3], 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 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 applied.

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 described 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 for the purpose of EQS setting

Based on the recommendations given in Part I of the TGD^[3] (section 2.4.3 and Appendix III) the quality standards for water intended for human consumption are calculated 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)

4.3.4 Use of Species Sensitivity Distributions to Derive EQS referring to Substance Concentrations in Water or Sediment

Statistical extrapolation in line with the provisions of the TGD^[3], namely the species sensitivity distribution method (SSD), is preferably used for the derivation of EQS referring to substance concentrations in inland surface waters as well as in transitional, coastal and territorial waters¹¹ if the database of the substance concerned is sufficient to apply this methodology (see section 4.3.4.1 for details). Supplementary, the standard TGD assessment factor method is applied. If ecosystem simulation studies are available, these should also be evaluated and an EQS derived following the provisions laid down in sections 4.3.2 and 4.3.5 of this document. A comparison of the two, possibly three results should be carried out and a final EQS determined by expert judgement with full justification.

¹¹ In principle, it is conceivable that the SSD methodology may as well be used to derive quality standards for sediments or the QS referring to the concentration of food of predators (QS_{secpois.biota}, see sections 4.3.2.3 – 4.3.2.5). However, criteria with regard to the quantity and quality of data required to derive these standards with the SSD method are not yet defined because in practice there are normally not enough sediment toxicity data or mammalian and avian oral toxicity data available to use the SSD approach. (For sediment, long-term NOECs of 10 species representing different living and feeding conditions may be considered appropriate.)

The SSD method works as follows: Toxicity data are log-transformed and fitted to a distribution function and a percentile (normally the fifth percentile, the so called 5-percentile cut-off value) of that distribution is used as the criterion. 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 method of Aldenberg and Jaworska (2000)^[14] 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); its application is therefore described here as an example of the use of the SSD-approach. The input data used to estimate the SSD should be NOEC data selected according to the criteria recommended in section 4.3.4.1¹².

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

$$\log 5P\text{-COV} = X_m - k * s$$

with:

5P-COV = 5th-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^[14])

s = standard deviation of log-transformed data

The extrapolation constant k is taken from Aldenberg and Jaworska^[14]. 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 recommendation in section 3.3.1.2 of Part II of the TGD^[3] the 5P-COV of the SSD is considered as an intermediate value in the determination of the EQS. The final EQS is calculated as 5-percentile cut-off value divided by an assessment factor reflecting further uncertainties identified.

$$\text{EQS} = \text{P5-COV} / \text{AF} \quad (\text{AF: max. 5 – min. 1; default: 5})$$

In determining the size of the additional assessment factor to be applied in order to derive an EQS based on the 5th percentile, the following points should be used as a guide^[3]:

- 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.

¹² However, if the SSD approach is used to derive a MAC-EQS as described in section 4.3.6.2 E(L)C50 data referring to acute effects may be used.

4.3.4.1 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. With regard to the derivation of annual average quality standards input data may be all reliable NOECs from chronic/long-term studies, preferably on full life-cycle or multi-generation studies. SSDs for the derivation of MAC-EQS may be based on acute E(L)C50 data.

Confidence can be given to an SSD-based EQS if the database contains preferably more than 15, but at least 10 NOECs, for different species covering at least 8 taxonomic groups (see table 10). Deviations from these recommendations can be made, on a case-by-case basis, through consideration of sensitive endpoints, sensitive species, mode of toxic action¹³ and/or knowledge from structure-activity considerations. Deviations need however justification.

It is important to include any available information 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.

Table 10: Species required to apply statistical extrapolation for freshwater^{[3] 14}

-
- 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
-

4.3.4.2 Aggregation of Multiple Data for One Species

It is proposed to follow the recommendations given in the draft report of the "London Workshop", which also have been adopted in the TGD^[3]:

- 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).
- 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 end-points, if they are relevant in terms of population dynamics.

¹³ Especially if the substance in question exerts a specific mode of action, or is suspected to have such a specific mode, SSDs should not only be set up for the entire database but as well for the most sensitive taxonomic group(s). For substances with a specific mode of action it may in most instances be more appropriate to derive a quality standard on the basis of the SSD of the most sensitive group. However, any decision should be discussed and justified.

¹⁴ 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.

- 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.
- 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.
- 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.

4.3.4.3 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.^[3]

Further guidance is given in the TGD^[3]:

- Whatever the fit to a distribution, results should be discussed with regards to the graphical representation of the species distribution and the different p-values¹⁵ that were obtained with each test.
- 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.

4.3.4.4 Specific Considerations Regarding the Use of the SSD Method for the Derivation of EQS Referring to Transitional, Coastal and Territorial Marine Waters

For quality standards referring to transitional, coastal and territorial waters the same approach as described in the preceding sections 4.3.4 to 4.3.4.3 can in principle be used. Combined toxicity data sets of marine and freshwater species may be normally used if the evaluation of the toxicity data for the substance concerned suggest a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota^[3] (i.e. the combined data set can be used to establish a common SSD that is relevant for both freshwater and saltwater effects assessment and QS setting).

The same assessment factor on the result of the SSD (the 5% cut-off value) as considered appropriate for inland waters (see section 4.3.4) should however only be applied for transitional, coastal and territorial waters if the data set used to establish the SSD comprises long-term

¹⁵ p-value \approx probability value - expressing the probability of wrongly rejecting a statistical hypothesis if it is in fact true (e.g. $p < 0.05$, meaning a probability of $< 5\%$).

NOECs of at least 2 additional marine taxonomic groups other than fish, crustaceans and algae (e.g. echinoderms, molluscs, coelenterata), showing that these additional marine groups are not more sensitive than other taxa. Where this cannot be proven, or otherwise be established that marine organisms are not more sensitive, an additional assessment factor of 10 on the EQS referring to inland waters may be used to derive the corresponding EQS for transitional, coastal and territorial waters. This is in line with the provisions of the TGD for marine effects assessment where such an increased assessment factor is recommended to cover the increased uncertainty resulting from the larger diversity of marine ecosystems and the limited availability of effects data for marine life forms (see sections 4.3.2.2 & 4.3.2.4).

Where the hypothesis of a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota cannot be justified based on the available evidence, SSD based EQS for inland surface waters and transitional, coastal and territorial waters must be derived on the basis of distinct data sets for freshwater and marine organisms, respectively. For setting up the SSD with ecotoxicological data of marine organisms the same data requirements regarding the quantity and quality of input data as laid down in section 4.3.4.1 apply. However, with regard to the species requirements laid down in table 10, insects and higher plants may be replaced by more typical marine taxa such as, e.g., molluscs, echinoderms or coelenterata.

Freshwater effects data of **plant protection products** shall normally not be used instead of saltwater data according to the TGD, because within trophic levels differences larger than a factor of 10 were found for several PPP^[3]. This means that for PPP the derivation of quality standards addressing the protection of water and sediment in transitional, coastal and territorial waters is not possible with the SSD method if there are no effects data for marine organisms available or if it is not possible to determine otherwise with high probability that marine organisms are not more sensitive than freshwater biota (consideration of the mode of action may be helpful in this assessment).

4.3.5 Specific Considerations Regarding the Use and Interpretation of Simulated Ecosystem Studies (Micro/Mesocosms) for EQS Derivation

Simulated ecosystem studies like, e.g., microcosm or mesocosm¹⁶ studies can be a valuable tool to assess the impact of a chemical on populations or communities of aquatic ecosystems under environmentally more realistic conditions than achievable with standard single-species laboratory studies. Therefore, if such studies are available, they should be considered if they fulfil the criteria regarding reliability and relevance as defined in section 4.1 for the purpose of quality standard setting.

If simulated ecosystem studies are used for EQS derivation, other approaches like the assessment factor method or the species sensitivity distribution method should be considered as well. A comparison of the two, possibly three results should be carried out and a final EQS determined by expert judgement with full justification.

Although simulated ecosystem studies can in principle be used to assess the effects and fate of all kinds of chemicals, such studies may mainly be available for plant protection products and their active ingredients. This is due to the fact that such studies are frequently used in the

¹⁶ It is difficult to distinguish between microcosms and mesocosms based on size or volume as there is some overlap and differences of opinion. Cooper and Barmuta^[18] suggested the following distinctions: microcosms are 10^{-3} to 10^3 m³ in size, while mesocosms are 10 to 10^4 m³; larger mesocosms may be considered to be equivalent to natural systems (10^3 to 10^8 m³ in size). In Europe however, the term “microcosm” is normally used for indoor multispecies tests whereas “mesocosm” usually refers to outdoor multispecies tests^[4].

so-called Higher Tier risk assessment under Council Directive 91/414/EEC concerning the placing of plant protection products on the market. Since the objectives of risk assessment under CD 91/414/EEC and the quality standards of the Water Framework Directive are not 100% compatible, it is necessary to carefully re-assess the results and conclusions of those studies for the purpose of quality standard setting as outlined in the following (see as well section 4.3). However, the outlined basic principles for the evaluation and interpretation of micro/mesocosm studies for the purpose of quality standard setting apply for all kinds of simulated ecosystem studies.

4.3.5.1 Differences in the Objectives of the Risk Assessment under CD 91/414/EEC and the Quality Standard in the Context of the WFD

Plant protection products (PPPs) are intentionally released chemicals that are toxic for at least certain groups of species. It is therefore hardly possible to avoid any side effects on non-target species dwelling in the vicinity of treated areas. Given the beneficial effects of the use of PPPs in terms of agriculture and economy, the (Higher-Tier) risk characterisation in the plant protection product risk assessment (PPP-RA) is focused on the acceptability of side-effects occurring after exposure of non-target species and ecosystems, respectively. With respect to aquatic ecosystems, specific consideration is given to the unintended exposure of water bodies in the immediate vicinity of treated areas, effects observed upon exposure and recovery of affected communities and species after exposure.

Exposure of a water body in the immediate vicinity of the area of PPP application is considered as the worst-case situation in the PPP-RA. The maximum concentration that might occur in those water bodies upon exposure, taking account of the intended uses and the proposed application rates and frequency of the assessed PPP, is estimated and used for risk characterisation. In the **lower Tier** (or Tier 1) risk assessment the concentration in a ditch immediately adjacent to the treated field is set in relation to various short-term and longer-term/chronic single species studies in order to calculate toxicity-exposure ratios (TER). The types and sophistication level of studies which have to be presented are dependent on the mode of action, the fate and other physical-chemical properties of the product / active substance and on expert judgement. Usually, short-term TERs for fish and invertebrates should not fall below 100 and long-term TERs not below 10 (see table 11).

Table 11: Minimum Toxicity – Exposure Ratios (quotient: toxicity test result / PEC) to be achieved according to the Uniform Principles Directive (97/57/EC)

Species	short-term TER	long-term TER
Fish	100 (based on LC50)	10 (based on NOEC)
Daphnia	100 (based on EC50)	10 (based on NOEC)
Algae		10 (based on EC50)

The maximum predicted exposure concentration (PEC_{max}) is used for comparison to the acute toxicity data. For the long-term PEC a time-weighted average concentration (PEC_{TWA}) may be calculated, taking into account fate data¹⁷ 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 PEC_{TWA} values.

If the lower Tier risk assessment indicates potential for concern (e.g. one or more TER triggers not met) these potential concerns must be addressed by refining the exposure and/or effects assessment in the so-called **Higher-Tier assessment**.

Micro- and mesocosm studies may be conducted to investigate potential effects on populations and communities of organisms under conditions more relevant to the field^[4, 10, 11]. According to the Guidance Document on Aquatic Ecotoxicity^{[4] 18}, a number of endpoints are to be determined from the micro- or mesocosm data to further use them in the PPP risk assessment. A NOEC at the community level ($NOEC_{community}$) should be derived for the relevant taxonomic groups using appropriate statistical techniques. NOECs for populations of relevant organisms should be reported as well. If effects at the population level occurred, the time taken for recovery to occur should also be reported. The $NOEC_{community}$, the $NOEC_{population}$ and the time needed for recovery should then be used to determine a **No Observed Ecologically Adverse Effect Concentration (NOEAEC)**. The NOEAEC is defined as the concentration at or below which no long-lasting, adverse effects were observed in a particular Higher-Tier study. No long-lasting effects are defined as those effects on individuals that have no or only transient effects on populations and communities, and are considered of minor ecological relevance (e.g., effects that are shown not to have long-term effects on population growth, taking into account the life-history characteristics of the organisms concerned)^{[4] 19}.

The NOEAEC may be used directly in the PPP-RA (i.e. for comparison with the relevant PEC) if it is relevant for overall decision making and if there is clear knowledge of all relevant endpoints and long-term effects (i.e. no uncertainty left). Otherwise **an appropriate uncertainty factor (subject to expert judgement) must be applied in order to derive the ecologically acceptable concentration (EAC)**, defined by the HARAP-workshop^[10] as being the concentration at or below which no ecologically adverse effects would be expected.

In the Guidance Document on Aquatic Ecotoxicity the NOEAEC is defined as a study specific value whereas the EAC is defined as a value resulting from an overall evaluation of a compound. In the Guidance Document the EAC is therefore considered comparable in its concept to the PNEC derived in the context of the risk assessment for industrial chemicals. However, the latter assumption in the guidance document is questionable, as pointed out in the following.

Exposure of a water body in the immediate vicinity of the area of PPP application is considered as worst-case situation in the PPP-RA and therefore the exposure pattern (i.e. maximum concentration and dynamics of dissipation) that might occur in such a water body is estimated and used to decide on dosing in Higher-Tier studies and for the interpretation of the results of

¹⁷ The dissipation measured in laboratory water-sediment fate studies is normally used to calculate time-weighted averages.

¹⁸ This document is referring to aquatic risk assessment of PPP in the EU legal context (i.e. Council Directives 91/414/EEC^[8] and 97/57/EC^[9]).

¹⁹ In general (but depending on the study design and life-history of the organism concerned), recovery within a period of 8 weeks is considered acceptable for defining the NOEAEC (i.e., if initial effects are observed, but recovery is observed within 8 weeks, then the treatment concentration can be considered to have no ecologically adverse effects). The NOEAEC can therefore be higher than the $NOEC_{community}$ or $NOEC_{population}$ since recovery is incorporated^[5].

the study, including recovery of the affected populations. Normally, the expected PEC_{max} is bracketed by the selected concentrations in Higher-Tier studies. The initial concentration and dissipation of the active substance are normally monitored, however, effects observed as well as established NOEAECs or EACs are in the context of the PPP-RA usually only reported and interpreted with reference to the initially applied concentration ($\approx PEC_{max}$)²⁰ and not with regard to the prevailing average concentration (e.g. PEC_{TWA}).

For the purpose of quality standard setting in the context of the Water Framework Directive it is important to realise that the exposure conditions relevant at the edge of a field are not necessarily the conditions that might prevail in water bodies draining an agricultural area (e.g. tributary and main rivers in a river basin) or lakes that may receive pesticide loaded water via inflows. An active substance may be used in different plant protection products and, hence, in different crop types. Application patterns may vary depending on PPP and crop type, but depending on other factors as well (e.g. local weather conditions or growth stages of plants in individual fields, time schedule of farmers, etc.). In addition, flow regimes of draining water bodies will be different and therefore the transport velocity of pesticide loaded water. If an active substance is sufficiently mobile and persistent²¹, all these factors will result in an exposure pattern in receiving waters that is significantly different from the “edge of a field” scenario that is normally used in the PPP-RA. Peak concentrations will normally be lower in draining water bodies than the PEC_{max} calculated according to the PPP-RA scenario but exposure may be long lasting and not drop and cease as quick as calculated/monitored for a water body directly adjacent to the application area. Therefore, it is questionable in many instances whether the “edge of a field” exposure-scenario used in the PPP-RA can really be considered the worst-case scenario. **The exposure pattern in the water courses of a river basin might be best characterized as prolonged exposure over the entire period that an active substance is used and also for a certain time period thereafter, however at levels normally lower than the PEC estimates of the PPP-RA. The duration of the “post-use” exposure period will be dependent on the properties of the active substance and the prevailing hydrological and climatic conditions. As for any other priority substance, the long-term water quality standard for a PPP under the WFD must therefore refer to an average concentration over a prolonged time interval.**

This different exposure pattern in ditches adjacent to a field and larger draining water bodies has implications with respect to the interpretation of results of (Higher-Tier) simulated ecosystem studies. It is therefore necessary to carefully check any of these studies conducted for PPP-RA with respect to the relevance of the endpoints derived and the conclusions drawn for environmental quality standard setting in accordance with the objectives of the WFD. The following points are of particular importance:

1. It is essential that all relevant endpoints are addressed and the concentration of the active substance in the test system is monitored during the study in order to be able to calculate time-weighted average concentrations (C_{TWA}) for not fast dissipating active ingredients.
2. All effects observed (and all NOECs derived, respectively), must be related to the respective C_{TWA} in case a substance is not fast dissipating, in order to render the study results

²⁰ The nominal initial concentration is used as reference if the monitored initial concentration is in the range of 80 to 120 % of the nominal concentration. Otherwise it is recommended to make reference to the monitored concentration^[2].

²¹ All active substances that are priority substances under the WFD have been selected in the COMMPS process because they were frequently monitored in surface waters of several Member States^[7].

applicable for the derivation of a quality standard in the context of the WFD. It is not acceptable to use the initial concentration as reference.²²

3. Absence of the occurrence of effects upon exposure to the prevailing substance concentration (either C_{TWA} or $C_{initial}$, depending on the dissipation and mode of action of the substance) rather than the potential to recover to the *status quo ante* within a certain time interval, e.g. 8 weeks, upon exposure to a single peak is the decisive criterion. The long-term quality standard (AA-EQS) in the context of the WFD refers by definition to an average concentration over a prolonged time interval. Hence, not the potential to recover after transient exposure but long-term undisturbed function and lack of impact on community structure of aquatic ecosystems at a prevailing average concentration level set by the EQS is the protection objective under the WFD.
4. It may be possible to use the EAC, respectively NOEAEC, derived in Higher-Tier studies as MAC-EQS in certain cases. However, a thorough evaluation of the study results and the expected exposure pattern of the active substance in draining water bodies of a catchment area is required prior to the adoption of an EAC/NOEAC as MAQ-QS. Time needed to recover from impacts (if any) versus the probability that concentrations that caused the observed effects will recur is the decisive criterion. Ideally, a MAC-QS based on a Higher-Tier simulated ecosystem study should be the highest initial concentration that caused neither long-term nor ecologically relevant²³ short-term effects in that study.
5. The scope of protection of an environmental quality standard under the WFD is broader than that of the “acceptable concentration” in the PPP-RA. In deriving a surface water quality standard from a Higher-Tier simulated ecosystem study it is therefore indispensable to consider that the quality standard must be protective for all types of surface waters and communities that are addressed by the respective standard, as long as it is not possible to rule out that exposure to plant protection products may occur in particular types of water bodies. This means that in the interpretation of Higher-Tier studies an evaluation is necessary as to whether the test system and the tested community, respectively, can be considered as representative for all water bodies that potentially are subject to PPP exposure. Higher-Tier studies in the context of the PPP-RA are normally focused to eutrophic shallow water bodies usually occurring in the immediate vicinity of agriculturally used areas. An EQS under the WFD, however, must assure protection also for water bodies that significantly differ from this paradigm, such as those having different flow regimes or trophic status, for instance.

²² Exceptions may be applicable for fast dissipating substances with a knock-down effect (e.g. certain carbamates or phosphoric acid esters).

²³ It is suggested to consider slight transient effects on functional parameters such as pH or oxygen content not as relevant if no concomitant effects on the investigated species could be observed. Effects on community structure (i.e. the populations of investigated species) may be regarded as not ecologically relevant if complete recovery of affected species occurs within the time interval over which short-term toxicity tests for the affected taxa normally are conducted (e.g. 72 h for algae, 48 h for daphnia, etc.).

4.3.5.2 Conclusions

- All simulated ecosystem studies must be checked with regard to their validity (i.e. relevance and reliability, see section 4.1) for the purpose of environmental quality standard setting in the context of the WFD.
- While an EAC/NOEAEC derived in a Higher-Tier simulated ecosystem study might adequately characterize acceptable impacts from PPP use in the immediate vicinity of the target area, these endpoints normally cannot be imposed as “general” surface water environmental quality standard in the context of the WFD. Hence, the terms “Ecologically Acceptable Concentration” and “No Observed Ecologically Adverse Effect Concentration” are misleading if they are used without the reservation that these observations are only valid under specific exposure conditions considered in the PPP-RA, which is normally the case. The terms should therefore not be used without explaining the conditions under which they apply or, better, be replaced by more matching terms.
- Nonetheless, a simulated ecosystem study might well be suitable as a data basis for the derivation of an aquatic quality standard. However, a careful re-evaluation of the observed effects and NOECs, respectively, and the calculation of the corresponding time-weighted average concentrations for not fast dissipating substances will be required in order to derive a long-term EQS meeting the protection objectives of the WFD. For the derivation of the MAC-QS the highest initial concentration in a simulated ecosystem study that caused no ecologically relevant effects may be used.
- Uncertainties with respect to the representativeness of the study for all water bodies within the scope of the WFD must be addressed also, e.g. by application of a supplementary assessment factor on the relevant NOEC used to derive the EQS. Determination of the appropriate size of the AF is subject to expert judgment.

4.3.6 Derivation of EQS Accounting for Acute Effects of Transient Exposure Peaks (MAC-EQS)

In order to cover both long-term and short-term effects resulting from exposure to a chemical, a second kind of quality standard referring to possible acute effects of transient exposure peaks, the maximum accceptable concentration EQS (MAC-EQS) is derived. The MAC-EQS must not be exceeded any time in order to protect aquatic life. As emissions to the aquatic environment normally occur in water first and because subsequent partitioning between water, settled sediment and biota is normally rather slow, it is deemed appropriate to derive this MAC-EQS for water only. In water exposure concentrations might change much quicker to a significant extent than in sediment or biota.

The MAC-EQS may be derived by three different approaches, depending on the quality and quantity of the data available. As standard method the TGD provisions for effects assessment for substances with intermittent release may be used. If enough short-term EC50/LC50 data are available to fulfil the conditions for the use of the SSD method this approach should be used as well. In certain cases, it may as well be possible to base a MAC-EQS on results obtained in simulated ecosystem studies (e.g. micro or mesocosm studies). Potential discrepancies in the results obtained with the different approaches need to be discussed and the decision for the finally preferred MAC-EQS derivation method be justified.

As mentioned earlier, the use of the MAC within a regulatory framework may also take into account other considerations which go beyond the derivation of an MAC on the basis of (eco-) toxicological data as presented subsequently (see section 4.2).

4.3.6.1 Derivation of a MAC-EQS by the Assessment Factor Method for Intermittent Releases

As standard method for the derivation of MAC-EQS the TGD provisions on effects assessment for substances with intermittent release may be used (section 3.3.2 of Part II of the TGD^[3]).

For exposure of short duration only short term effects may need to be considered. An assessment factor of 100 applied to the lowest L(E)C50 of at least 3 short term tests of three trophic levels is normally considered appropriate to derive the MAC-QS for such situations. However, for substances with a potential to bioaccumulate the lowered 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. Expert judgement and justification of the decision regarding the assessment factor chosen is therefore required. In no case should a factor lower than 10 be applied to a short-term L(E)C50 value.

4.3.6.2 Derivation of a MAC-EQS by the SSD Method

For the derivation of the MAC-EQS the same approach as described in sections 4.3.4 – 4.3.4.3 can in principle be applied. However, instead of long-term NOECs, acute E(L)C50 data will serve as input data. Combined acute toxicity data sets of marine and freshwater species may be used as well if the evaluation of the toxicity data for the substance concerned suggest a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota.

The result of a SSD with short-term E(L)C50 data is the 5-percentile cut-off value for the occurrence of acute effects. Therefore, an assessment factor accounting for extrapolation from the short-term acute 50%-effects level to the short-term no-effect level must be applied on the 5-percentile cut-off value in order to derive the MAC-EQS. This assessment factor should normally be 10, unless it can be justified that a higher assessment factor will be required or a lower one be sufficient. The acute to chronic toxicity ratios and the criteria presented in section 4.3.4 may be helpful to decide on the appropriate assessment factor.

4.3.6.3 Derivation of a MAC-EQS based on Simulated Ecosystem Studies

For the derivation of the MAC-QS the highest initial concentration in a simulated ecosystem study that caused no ecologically relevant effects may be used. Further guidance regarding the derivation of the MAC-EQS from micro/mesocosm studies is given in section 4.3.5.1.

4.4 Derivation of Quality Standards for Metals – Use of the Added Risk Approach

The methodologies for risk assessment of metals are constantly evolving. For several metals (cadmium, nickel and zinc), there are ongoing risk assessments in the context of the Existing Substances Regulation (793/93). In addition, voluntary risk assessment reports are being conducted for lead and copper by industry. At the time of finalisation of this document, none of these risk assessment reports had been finalised. It is expected that further methodological developments will emerge from this process in the future.

Metals are naturally occurring substances and hence it is useful to account for their natural background concentrations in the aquatic environment when setting quality standards. However, the Technical Guidance Document^[3] does not provide guidance on how to deal with elements that have a natural background concentration in the environment. In the context of the EU risk assessment (Regulation 793/93) both the “added risk” approach (Zn–RAR) and the “total risk” approach (Cd-RAR & Ni-RAR) have been applied and in the voluntary risk assessments for copper and lead the total risk approach is being pursued.

The total risk approach accounts for the total dissolved amount (cf. section 4.4.1) of a metal in a water body. This means that no distinction is made between the fraction of a metal that is present in a water body for natural reasons and the fraction added due to anthropogenic activities. If no correction for water quality parameter dependent toxicity for the metal in question can be made (which is yet the case for most metals, except Cd, Cu, Ni and Zn cf. 4.4.1) this will for metals with a significant natural background concentration in relation to the estimated effects threshold value (e.g. PNEC or quality standard) frequently result in the calculation of threshold values below local natural background concentrations.

The “added risk” approach is used in the Netherlands for the derivation of quality objectives for naturally occurring substances^[15, 16] and on the EU-level in the context of the risk assessment for zinc and its compounds^[20]. It has been proposed and discussed in detail for the purpose of setting EU-EQS in the context of the Water Framework Directive because this approach facilitates to account for natural background concentrations and to avoid setting regulatory standards below this background 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.

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

Two assumptions need to be made for 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. A concept for the estimation of background levels and the definition of the appropriate level of spatial resolution (e.g. river basin scale) is elaborated by the AMPS²⁴ working group. Therefore, no further considerations are attributed to this issue in this document.

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 EQS derived by 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.

However, although the added risk approach is the preferred approach in this manual because of its merits for setting regulatory standards, **it will finally be up to the Commission proposal to decide whether the "added risk" approach or the "total risk" approach or a case-by-case decision should be followed for a particular metal.**

4.4.1 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^[13] such as the pH, hardness of water and the content of dissolved organic matter (DOM).

In order to take account of the differences in bioavailability, the "dissolved fraction" and not the total concentration is used as an approximation to the, in toxicological terms, relevant concentration of a metal in water. For aquatic organisms, which are mainly exposed via water, especially the metal ions and other dissolved species are available and therefore relevant for toxicity. Thus, with respect to the aquatic toxicity data, the concentration of dissolved metal species in water is a better indicator of toxicity than the total concentration of the metal in question, which may include a significant non-bioavailable metal fraction (e.g. sequestered or adsorbed to particulate matter). The dissolved fraction however may also contain forms of the metal that are not or hardly bioavailable (e.g. metal associated with colloidal forms of organic matter). In practice, the dissolved fraction of a substance in water is defined as the fraction that passes a 0.45 µm filter.

Although metal bioavailability to different aquatic life forms as well as the modifying influence of water quality parameters are the 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

²⁴ AMPS = Analysis and Monitoring of Priority Substances

aquatic life forms representing freshwater or marine communities^[15] and, hence, to take these parameters into consideration in setting quality standards (for details refer to section 8.6.3 of^[2]).

Therefore, for the time being, 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 is taken because of the uncertainties in the data and/or the possible methodological approaches. This 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^[16] to consider this water hardness correction of the $PNEC_{\text{water}}$ 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. For some metals (copper and zinc) such models exist or are in an advanced stage of development. For some other metals, 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, their utility in the assessment of bioavailability and the calculation of appropriate local quality standards should be evaluated carefully. If for a particular metal such an evaluation results in the conclusion that BLM based local quality standard setting is reliable, practicable and meaningful²⁵ with regard to the protection objectives of the WFD, then for this metal it may be considered to replace standards derived with the approach described in this Manual by BLM based quality standards.

4.4.2 Calculation of Quality Standards for Metals

4.4.2.1 Calculation of the Maximum Permissible Addition (MPA) and the Environmental Quality Standard for Inland Waters (Freshwater)

In principle, the same methods as proposed for the derivation of quality standards for organic substances may be used to derive the MPA_{water} of metals (i.e. application of assessment factors, statistical extrapolation by means of species sensitivity distributions, or use of ecosystem simulation studies).

If enough data are available to derive the MPA_{water} with the SSD approach, this MPA should in addition be derived using the standard TGD assessment factor approach (see sections 4.3.2 & 4.3.4) on the same database. If ecosystem simulation studies such as micro/mesocosm tests are available, these should also be evaluated and a MPA derived following the provisions laid down in section 4.3.5. A comparison of the two, possibly three resulting MPA values should be carried out and a final MPA determined with full justification.

Calculation of the MPA_{water} and the QS_{water}

²⁵ The setting of biotic ligand model (BLM) based local quality standards may not be meaningful for priority hazardous metals such as cadmium and mercury because the objective of the WFD is the cessation of emissions and losses and the achievement of concentrations close to the background level for naturally occurring substances.

- The MPA_{water} referring to the "bioavailable" (using dissolved fraction as the best available approximation) metal [$\mu\text{g Metal} / \text{l}$] is calculated on the basis of long-term NOEC data (e.g. by the species sensitivity distribution method if enough data are available to apply this method or by the assessment factor method)
- The corresponding MPA_{SPM} for SPM [$\mu\text{g Metal} / \text{kg SPM}$] is calculated based on the MPA_{water} and the locally relevant²⁶ $K_{\text{p,water-SPM}}$ ($MPA_{\text{SPM}} = MPA_{\text{water}} * K_{\text{p,water-SPM}}$)

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} .

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

4.4.2.2 Calculation of the Maximum Permissible Addition and the Environmental Quality Standard for Sediments of Inland Waters (Freshwater)

The added risk approach as outlined in section 4.4 applies also for sediment.

If sufficient NOEC data for benthic organisms are available (≥ 10 NOEC data for different species representing different living and feeding conditions) the same statistical extrapolation methodology as described in section 4.4.2 for the MPA_{water} is used to derive the MPA_{sediment} .

In principle, the same methods as proposed for the derivation of sediment quality standards for organic substances may be used to derive the MPA_{sediment} of metals (i.e. application of assessment factors (see 4.3.2.3), statistical extrapolation by means of species sensitivity distributions (see 4.3.4), or use of ecosystem simulation studies (see 4.3.5)).

If enough data are available to derive the MPA_{sediment} with the SSD approach, this MPA should in addition be derived using the standard TGD assessment factor approach (including the equilibrium partitioning method²⁷; see section 4.3.2.3) on the same database. If ecosystem simulation studies such as micro/mesocosm tests are available, these should also be evaluated and a MPA derived. A comparison of the two, possibly three MPA values should be carried out and a final MPA determined with full justification.

The MPA_{sediment} is added to the locally relevant background concentration in sediment in order to derive the local QS_{sediment} .

- $QS_{\text{sediment}} = C_{\text{background.sediment}} + MPA_{\text{sediment}}$

All MPA_{sediment} that are not derived on the basis of at least 3 long-term tests with sediment organisms representing different life and feeding conditions should only be considered as indicative values and it is not recommended to derive a legally binding MPA_{sediment} if this mentioned minimum data set is not available for the metal in question.

²⁶ For metals the $K_{\text{p,water-SPM}}$ is highly dependent on local water quality conditions. Therefore a MPA referring to SPM as matrix should only be derived on the basis of the locally relevant partition coefficient.

²⁷ In the case of metals, only empirically derived coefficients for the partition between water and sediment (i.e. $K_{\text{water-suspended particulate matter}}$) should be used.

4.4.3 Specific Considerations with Respect to the derivation of MPAs and EQS referring to the protection of Water and Sediment of Transitional, Coastal and Territorial Marine Waters

For metals, it could be required to differentiate between freshwater and marine water in MPA derivation and 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^[3]. This means that the derivation of MPAs addressing the protection of water and sediment in coastal and territorial waters is not possible if there are no effects data for marine organisms available or if it is not possible to determine with high probability that marine organisms might not be more sensitive than freshwater biota.

Toxicity data sets (as well as BCF data) of marine and freshwater organisms may only be combined if no differences in sensitivities of freshwater and saltwater organisms of the same taxonomic groups exist. Otherwise, it is necessary to set specific quality standards referring to freshwater and marine water bodies, respectively.

For the derivation of metal MPAs referring to the protection of the pelagic and benthic communities (i.e. water and sediment) of transitional, coastal and territorial waters, in principle the same approaches as described for the calculation of the quality standards of organic substances in the respective compartments applies (see sections 4.3.2.2 & 4.3.2.4 for the assessment factor method, 4.3.4 including sub-sections for the SSD-approach and 4.3.5 incl. sub-sections for the use of simulated ecosystem studies).

If enough data are available to derive a MPA with the SSD approach, this MPA should in addition be derived using the standard TGD assessment factor approach on the same database. If ecosystem simulation studies such as micro/mesocosm tests are available, these should also be evaluated and a MPA derived following the provisions laid down in section 4.3.5. A comparison of the two, possibly three MPA values should be carried out and a final MPA determined with full justification.

The MPA is added to the relevant background concentration ($C_{\text{background}}$) in order to derive the local QS.

4.4.4 Secondary Poisoning of Predators – Metal Levels in Biota

For metals, in principle the same TGD-based approach should be followed as outlined in section 4.3.2.5 for organic substances.

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 should 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 bioaccumulation factors (BAFs) observed in the field.

4.4.5 Adverse Health Effects upon Ingestion of Fishery Products – Metal Levels in Biota

For metals in principle the same approach is used as outlined in section 4.3.2.6 for organic substances.

Quality standards (i.e. values equivalent to a $QS_{hh.food}$) addressing the protection of human health are already set by Council Regulation (EC) No 466/2001^[17] as maximum levels of cadmium, lead and mercury in seafood. This $EQS_{hh.food}$ is transformed to the corresponding concentration in water, applying the same approach and considerations as described for the transformation of the $QS_{secpois.biota}$ in section 4.3.2.5 of this report.

$$EQS_{hh.food.water} [\mu g/l] = \frac{QS_{hh.food} [\mu g/kg]}{BCF [l/kg] * BMF_1}$$

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

The same approach as described for organic chemicals is followed (see section 4.3.3).

4.4.7 Derivation of MPAs and Environmental Quality Standards Accounting for Acute Effects of Transient Exposure Peaks (MAC-MPA and MAC-EQS)

The added risk approach as outlined in section 4.4 applies also for the derivation of the MAC-EQS of metals. That is, a MAC-EQS is derived and added to the locally relevant natural background concentration in order to establish the local MAC-EQS.

The MAC-MPA for metals may be derived according to the same principles and methodological approaches as described for the derivation of the MAC-EQS of organic substances (see section 4.3.6 including sub-sections).

5 Conclusions and Future Steps

The methods proposed in this Manual for the derivation of quality standards addressing objectives of protection such as the integrity of pelagic and benthic communities of inland as well as transitional and marine waters, secondary poisoning and human health including drinking water abstraction are built upon the widely accepted frameworks used in the European Union for the assessment of risks of existing substances and of plant protection products. Where considered useful, additional methods such as the added risk approach have been included in the framework in order to be able to derive quality standards accounting for background levels of naturally occurring substances²⁸. Due to the introduction of the MAC-EQS (maximum acceptable concentration) as a second type of overall quality standard (beside the annual average – AA-EQS), intended to protect aquatic life against adverse effects of transient concentration peaks, the possible impact of the occurrence of acute toxicity is given more relevance as is normally attributed to this issue, at least in the context of the existing substances risk assessment. Further, as best use of the information available should be made in order to calculate realistic quality standards keeping the proportion between the required level of safety and incommensurate discrimination of other societal objectives such as production of goods and services or mobility, the spectrum of approaches that may be used for effects assessment and quality standard derivation has been widened in cases where this appeared reasonable. For example, it is suggested in this Manual that the MAC-EQS may not only be derived by applying an assessment factor on the appropriate toxicity data but to use as well statistical extrapolation (species sensitivity distributions) or observations made in multispecies studies (e.g. mesocosms) if respective data are available. Similarly, guidance is given on how to use and interpret multispecies studies conducted in the context of the plant protection product risk assessment for the purpose of quality standard setting.

The elaboration of quality standards for the Annex X priority substances of the Water Framework Directive clearly showed that the methodological framework presented in this Manual is applicable for the derivation of quality standards. 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 (e.g. in terms of quality) of the available data. For example, toxicity data of saltwater species were in general scarce and the availability of mammalian and avian long-term oral toxicity data as well as information on bioaccumulation will need improvement in order to be able to derive specific quality standards addressing secondary poisoning or protection against adverse health effects due to consumption of fishery products with less uncertainty associated. Data availability was however worst with reference to sediment. Only few standards referring to sediment could be derived on the basis of experimental data. Most values referring to sediment must be calculated with the equilibrium partitioning approach as suggested in the TGD in case of lacking experimental data. Those figures are merely a transformation of the standards

²⁸ However, although the added risk approach is the preferred approach in this manual because of its merits for setting regulatory standards, it will finally be up to the Commission proposal to decide whether the “added risk” approach or the “total risk” approach or a case-by-case decision should be followed for a particular metal.

derived for the protection of the pelagic communities and should be considered tentative. The new EU regulatory framework for chemicals (REACH) might be helpful to improve the data situation substantially in the next couple of years as it will require producers and importers of chemical products as well as (professional) downstream users to create chemical safety reports for their products and to provide within these reports the data necessary to assess the risks exerted by the product and its ingredients during its life-cycle.

Although the proposed methodological framework in its current stage is workable to a satisfactory extent there is, of course, room for improvement. Key future steps could be the development of sediment and biota quality standards for those hydrophobic substances for which monitoring in water is not possible or meaningful. Further, the development of group approaches on the basis of toxic equivalent factors (TEFs) as suggested by the SCTEE ^[19] could result in the implementation of group quality standards taking account of the concomitant presence of several substances of that group. This would lead to a uniform (i.e. simpler) standard for the group while at the same time its quality would be enhanced ²⁹. Similarly, quality standards derived by the proposed methodological framework do not yet account explicitly for a possible combined action of pollutant mixtures because at present there is no consolidated and validated approach to account for combined action of pollutants available that is applicable for quality standard setting³⁰. This aspect should as well be considered in future adaptations of the proposed quality standard setting methodology to scientific progress. Further on, the development or further enhancement of approaches and models to account for water quality parameter dependent speciation, bioavailability and, hence, toxicity of metals such as, e.g., biotic ligand models (BLMs) could lead to better metal quality standards and render the added risk approach needless in order to avoid setting of quality standards below local background concentrations because it would be possible to identify and only consider the (eco)toxicologically relevant metal concentration for effects assessment, no matter which fraction of it is of natural or anthropogenic origin.

²⁹ Possible candidates for development of group standards are, e.g., PAHs, phthalates, halogenated biphenyls, triazine or organophosphate pesticides, chlorophenols, alkylphenols and organotin compounds.

³⁰ Nonetheless, it is assumed that the assessment factors applied in the effects assessment for quality standard setting do cover the possible occurrence of combined action of pollutants in most instances to a great extent.

6 References

- [1] Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy. OJ L 327, 22.12.2000, pp 1- 51
- [2] Final Report of the Study Contract No. B4-3040/2000/30637/MAR/E1: Identification of quality standards for priority substances in the field of water policy. Towards the Derivation of Quality Standards for Priority Substances in the Context of the Water Framework Directive. (04 September 2002)
- [3] Technical Guidance Document on Risk Assessment in Support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European Parliament and the Council Concerning the placing of biocidal products on the market. Part II. European Commission Joint Research Centre, EUR 20418 EN/2, © European Communities 2003. Available at the internet-site of the European Chemicals Bureau: <http://ecb.jrc.it/existing-chemicals/>
- [4] Guidance Document on Aquatic Ecotoxicology in the context of the Directive 91/414/EEC. European Commission Health & Consumer Protection Directorate-General. Sanco/3268/2001 rev.4 (final), 17 October 2002. http://europa.eu.int/comm/food/plant/protection/evaluation/guidance/wrkd0c10_en.pdf
- [5] Bro-Rasmussen, F. et al.: EEC Water Quality Objectives for Chemicals Dangerous to Aquatic Environments (List 1). Reviews of Environmental Contamination and Toxicology Vol. 137, pp.83-110, Springer-Verlag (1994)
- [6] Council Directive 75/440/EEC of 16 June 1975 concerning the quality required of surface water intended for the abstraction of drinking water in the Member States. OJ L 194, 25/07/1975, p. 26-31
- [7] Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption. OJ L 330, 05/12/1998, p. 32-54
- [8] Council Directive 91/414/EEC of 15 July 1991 concerning the placing of plant protection products on the market. OJ L 230, 19/08/1991 p. 1-32
- [9] Council Directive 97/57/EC of 22 September 1997 establishing Annex VI to Directive 91/414/EEC concerning the placing of plant protection products on the market. OJ L 265, 27/09/1997 p. 87-109
- [10] Guidance Document on Higher-tier Aquatic Risk Assessment for Pesticides (HARAP). PJ Campbell et al. (eds.). SETAC-Europe, Brussels 1999. ISBN 90-5607-011-8
- [11] Community-Level Aquatic System Studies – Interpretation Criteria. Proceedings from the CLASSIC Workshop held at the Fraunhofer Institute – Schmallenberg, Germany 30 May – 2 June 1999. JM Giddings et al. (eds.). SETAC Press, 2002. ISBN 1-880611-49-X
- [12] Traas, TP (ed.), 2001: Guidance Document on deriving Environmental Risk Limits. RIVM report 601 501 012. National Institute for Public Health and The Environment (RIVM), Bilthoven, the Netherlands. <http://www.rivm.nl/bibliotheek/rapporten/601501012.pdf>
- [13] Crommentuijn, T, MD Polder, EJ van de Plassche; 1997: Maximum Permissible Concentrations and Negligible Concentrations for metals, taking background concentrations into account. National Institute for Public Health and the Environment, Bilthoven, The Netherlands. RIVM Report no. 601 501 001. <http://www.rivm.nl/bibliotheek/rapporten/601501001.pdf>
- [14] Aldenberg, T, J Jaworska, 2000: Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. Ecotoxicology and Environmental Safety 46: 1-18
- [15] "Bioavailability of Metals in Surface Waters – Integrating Science and Regulations", Workshop, 7-8 February 2002, Ghent, Belgium
- [16] Risk assessment report cadmium metal and cadmium oxide, CAS-Nos.: 1306-19-0 and 7440-43-9, final draft, July 2005. The most recent (draft) report is available at the internet site of the European Chemicals Bureau: <http://ecb.jrc.it/existing-chemicals/> ⇒ tick ESIS button, then enter CAS or EINECS number of substance.
- [17] Commission Regulation (EC) No 466/2001 of 8 March 2001 setting maximum levels for certain contaminants in foodstuffs. OJ L 077 , 16/03/2001 P. 1 – 13

- [18] Cooper, SD and LA Barmuta; 1993: Field Experiments in Biomonitoring. In Freshwater Biomonitoring and Benthic Macroinvertebrates. DM Rosenberg, VH Resh (eds.) pp.399-441, Chapman & Hall, New York
- [19] Opinion of the Scientific Committee on Toxicity, Ecotoxicity and the Environment (SCTEE) on “The Setting of Environmental Quality Standards for the Priority Substances included in Annex X of Directive 2000/60/EC in Accordance with Article 16 thereof”, adopted by the CSTEE during the 43rd plenary meeting of 28 May 2004, European Commission Health & Consumer Protection Directorate General, Brussels.
http://europa.eu.int/comm/health/ph_risk/committees/sct/documents/out230_en.pdf
- [20] Opinion of the Scientific Committee on Toxicity, Ecotoxicity and the Environment (SCTEE) on the “Revision of the 1996 Technical Guidance Document (TGD) in support of Commission Directive 93/67/EEC on risk assessment for new notified substances and Commission Regulation (EC) 1488/94 on risk assessment for existing substances [also being extended to provide guidance on risk assessment for biocides under 98/8/EC (excluding human exposure evaluation)]” submitted for CSTEE opinion on 23 August 2001. Draft revision version on Part 3/B – Environmental Risk Assessment – Marine Part. European Commission Health & Consumer Protection Directorate General, Brussels.
http://europa.eu.int/comm/health/ph_risk/committees/sct/documents/out152_en.pdf
- [21] European Union Risk Assessment Report. Zinc Metal, CAS-No.: 7440-66-6, EINECS-No.: 231-175-3. Part I Environment, Draft Report of 9 February 2004 & Part II Human Health, Final Report. 2nd Priority List, Volume 42 (EUR 21169 EN). The most recent (draft) report is available at the internet site of the European Chemicals Bureau: <http://ecb.jrc.it/existing-chemicals/> ⇒ tick ESIS button, then enter CAS or EINECS number of substance.