



Background Document

Establishment of a list of Predicted No Effect Concentrations (PNECs) for naturally occurring substances in produced water

(OSPAR Agreement 2014-05)¹

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¹ This Agreement is in English only.

It was agreed that this Background Document would be published on the OSPAR website as an OSPAR Agreement. OIC 2014 agreed to replace Table 1 (PNECs and EQSs for naturally occurring substances found in produced water) in Appendix 5 of the OSPAR RBA Guidelines (Agreement 2012/7) with a link to this Background document

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1 Executive summary

In support of Recommendation 2012/15 for a Risk Based Approach to the Management of Produced Water Discharges from Offshore Installations (OSPAR Agreement: 2012-7) a set of Predicted No Effect Concentrations (PNECs) are compiled for naturally occurring substances as part of the development of these guidelines. The document at hand provides this list of PNECs derived from already established and publicly available values.

First a list of relevant substances is specified. Chapter 3 provides the list of substances and describes the rationale behind choosing the substances. Characteristics of substances (groups) are also presented to some extent in this chapter.

Chapter 4 describes the procedure followed for collecting and selecting PNECs from different sources is described in Chapter 4. In Chapter 5 an overview of all the selected PNECs that are recommended used in the Risk Based Approach (RBA), is provided.

The list of substances and PNECs presented needs periodical updating to include new data or new insights. In some specific cases Contracting Parties (CP) may also want to deviate from the listed PNECs. Chapter 6 presents in which cases the list should be updated and in which cases deviation from selected PNECs is possible.

The document ends with separate fact sheets per substance in Chapter 7. Each fact sheets contains basic information on the specific substances, the selected PNEC and its source and alternative PNECs and their sources.

Appendices containing background information on PNEC derivation principles and their respective interpretation are also provided.

2 Background

2.1 Objective

OSPAR adopted Recommendation 2012/5 for a risk-based approach to the management of produced water discharges from offshore installations and the OSPAR Guidelines in support of Recommendation 2012/5 with effect from 29 June 2012.

Prior to the adoption of the Guidelines a workshop was held to establish a harmonised set of PNEC values for naturally occurring substances typically found in produced water. The list of PNECs resulting for the Workshop was included in the 2012/7 Guidelines. In these guidelines it was stated that more detailed information about the PNEC selection would be outlined in a background document. A draft background document for the establishment of a list of PNECs for naturally occurring substances in produced water was presented at OIC 2013 and the Netherlands, Norway and UK were invited to finalize it for discussion at OIC 2014. When finalised, the background document should be published on the OSPAR website as an OSPAR Agreement. This will need regular updating as a living document. When published, the list of PNECs currently annexed to the RBA Guidelines should be removed.

In the present background document the final set of PNECs is presented and the way these PNEC-values have been determined is described.

3 Selection of produced water substances to be included in a substance based risk assessment approach

3.1 Produced water substances

Produced water consists of formation water (the water naturally present in the reservoir), injection water, and in the case of gas production, condensed water (E&P Forum, 1994). Produced water contains a variety of substances that have been dissolved from the geologic formations including inorganic salts, metals, and organic substances (Røe Utvik, 1999, Neff, 2002). The organic substances include low molecular weight organic acids, phenols, petroleum hydrocarbons, related S-, N-, and O-substituted hydrocarbons and several unidentified polar compounds. The composition of produced water varies from one well to another and changes over the lifetime of the field (Neff, 2002; Røe Utvik, 1999).

Historically, only the amount of dispersed oil is regulated (performance standard of 30 mg/L, OSPAR Rec 2001/1). However, produced water discharges also contain dissolved substances with varying potential to cause environmental harm. PAHs and related cyclic and heterocyclic compounds, alkyl phenols and metals have been highly focused, because of their assumed contribution to ecological effects of produced water (Neff, 2002; Røe, 1998, Røe Utvik & Johnsen, 1999).

Chemical analyses on produced water samples through the years have elucidated which substances are the most relevant regarding potential effects of naturally occurring substances on the marine environment (OGP, 2005). For this reason the United Kingdom (UK) and Norway have developed

extensive guidance on sampling and chemical analysis of potentially harmful substances in produced water from their offshore installations (See Table 1 for an overview of components typically being analyzed in produced water samples). In Norway the oil industry follows the ‘Recommended Guidelines for the sampling of produced water’ (<http://www.norskoljeoggass.no/Global/Retningslinjer/Miljø/085%20-%20Anbefalte%20retningslinje%20for%20prøvetaking%20og%20analyse%20av%20produsert%20van%20n.pdf>) established by the Norwegian Oil & Gas (NOG) in 2003 and revised in 2013 (NOG, 2013). In the UK the guidance ‘Produced Water Sampling and Analysis Guidance Notes’ (https://www.og.decc.gov.uk/en_temp/opa_samp_guide.doc) from the Department of Energy and Climate Change (DECC, 2009) is followed. A detailed description of recommended sampling and analysis procedures for produced water is presented in Roex (2012).

Table 1. Potentially harmful substances typically analyzed to characterize produced water samples.

Substance group	Substances
Metals	arsenic, cadmium, chromium, copper, mercury, lead, nickel and zinc, iron and barium
The monoaromatic hydrocarbons (BTEX)	benzene, toluene, ethylbenzene and xylene
Dispersed oil:	C7-C40 aliphatic hydrocarbons
16 US-EPA Polycyclic Aromatic Hydrocarbons (PAHs)	naphthalene, acenaphthene, acenaphthylene fluorene, anthracene, phenanthrene, fluoranthene, pyrene, benz(a)anthracene, chrysene dibenzo(a)anthracene, benzo (g,h,i)perylene, benzo(a)pyrene, benzo(b)fluoranthene, benzo(k)fluoranthene, indeno(1,2,3,-cd)pyrene
Other PAHs	C1-naphthalenes, C2-naphthalenes, C3-naphthalenes, C1-phenanthrenes, C2-phenanthrenes, C3-phenanthrenes, dibenzothiophene, C1-dibenzothiophenes, C2-dibenzothiophenes, C3-dibenzothiophenes
Phenol/alkylphenols	phenol, C1-alkylphenols, C2-alkylphenols, C3-alkylphenols, C4-alkylphenols, C5-alkylphenols, C6-alkylphenols, C7-alkylphenols, C8-alkylphenols and C9-alkylphenols
Organic acids	formic acid, acetic acid, propionic acid, butyric acid, valeric acid, isobutyric acid and isovaleric acid and naphthenic acids.

Measured concentrations of individual substances in the effluent that potentially cause harm in the receiving environment are a crucial input for a substance based risk assessment. Chemical analyses are part of the data collection (Figure 2, step 1) in the RBA. Information on the concentration of the individual substances in the effluent is used to determine exposure levels (Figure 2, step 3; Exposure Assessment). The results from step 3 will, together with the results from step 2 (Figure 2, Hazard Assessment), in which PNECs for the individual substances are derived, serve as input for the Risk Characterization (Figure 2, step 4).

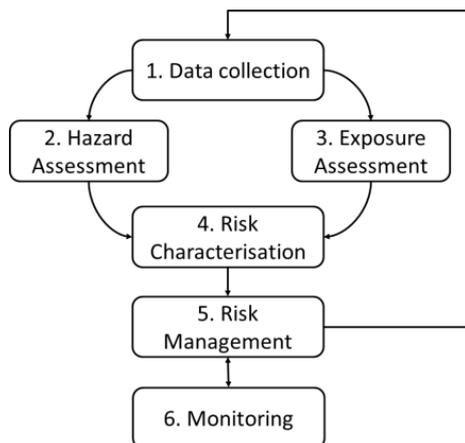


Figure 2. Different steps in the risk based approach.

3.2 Criteria and selection

The Norwegian and UK guidance for sampling and analyzing already provide an overview of potentially harmful substances in produced water. This guidance is used as basis for selecting the naturally occurring substances that should be included in the OSPAR RBA applied to individual produced water substances. In order to identify substances that should be included, the following characteristics, individually or in combination, have been evaluated:

- Whether or not substances have been identified as priority substances (PS) in the European Union’s Water Framework Directive (EU-WFD) and/or the OSPAR list of chemicals for priority action;
- The toxicity, bioavailability and bioaccumulation potential of individual substances;
- The presence and concentration level of individual substances in produced water discharges.

One of the main criteria is whether substances have been categorized as PS in the water policy of the European Union. PS in the EUs water policy are substances identified among those presenting a significant risk to or via the aquatic environment at EU level.

Some PS are identified as priority hazardous substances (PHS) because their persistence, bioaccumulation and/or toxicity (equivalent to substances of very high concern (SVHCs) under REACH). A first list of established Environmental Quality Standards (EQSs) for the PS and some other pollutants within the EU-WFD are listed in the EQS Directive 2008/105/EC; Part A of Annex I (EC, 2008). A review of the EQSs for surface water, sediment or biota and status of existing PS and evaluation of new PS are undertaken at least every four years. The last review was undertaken in 2011, and was recently published in EU DIRECTIVE 2013/39/EU; Part A of Annex II (EC, 2013a).

The substances on the list of chemicals for priority action within OSPAR are those which the OSPAR Commission has to date determined require priority action, due to their persistency, liability to bioaccumulate and toxicity or other equivalent concern. The PS list is based primarily on recommendations from DYNAMEC’s ranking process and expert judgement as to which substances

represent the highest concern due to the amount produced, the degree of hazardous properties and/or the actual occurrence in the marine environment (OSPAR, 2011).

Since 2007, Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) is the legislative framework on chemicals of the European Union (EU). Before REACH came into force, chemicals were regulated by a number of different regulations and directives. For example, the Council Regulation (EEC) No 793/93, also known as the Existing Substances Regulation (ESR) was one of these. Lists of priority substances which require immediate attention because of their potential effects to human health or the environment were established, based on production/imported volumes by different member states were published within the REACH framework. The PSs identified through the Council Regulation, which is relevant in this context, are also identified by WFD and/or OSPAR, with a few exceptions. However, these exceptions are selected by fulfilling the other criteria listed.

3.3 Selected substances

3.3.1 Metals

The presence of metals varies between produced water samples. For most produced waters the concentrations of several metals are higher than concentrations in ambient seawater. For example, some North Sea produced waters contain high concentrations of nickel and copper (Neff, 2002). The metals most frequently present in produced water at elevated concentrations include barium, cadmium, chromium, copper, iron, lead, nickel, and zinc (Neff et al., 1987, OOC, 1997, Røe Utvik, 1999). Arsenic concentrations are usually low, but some produced waters contain elevated concentrations (Frankiewicz et al., 1998). Produced water samples from the Norwegian sector of the North Sea, Gulf of Mexico and Gulf of Thailand contained elevated concentrations of mercury. Elevated concentrations of manganese in Gulf of Mexico were also reported (Frankiewicz et al., 1998; OOC, 1997). In nearly all produced waters discharged to offshore waters to the Gulf of Mexico and the North Sea, elevated levels of zinc compared to concentrations in ambient seawater – by factors ranging from 2 to about 1000 – were reported (Neff, 2002).

Some metals that are in soluble or colloidal forms in produced water, introduced to the oxygenated seawater rich in sulfate, tend to either precipitate or adsorb to suspended particulate matter and form complexes with colloidal or dissolved organic matter and deposit in the surficial sediments, and therefore become non-bioavailable in the water column (Salomons and Føstner, 1984, Schindler and Stumm, 1987; Kuma et al., 1996). Barium, iron and manganese are likely to precipitate rapidly from the produced water plume in the receiving water (DOE, 1997; OOC, 1997; Monnin et al, 1999). The mercury in produced water is also most often in inorganic forms or complexes with organic substances, and particulate forms dominates.

Because the particle size of these precipitated metals is very small, the particulate metals tend to settle slowly out of the water column and accumulate to slightly elevated concentrations in surficial sediment over a large area around the produced water discharge, keeping their concentration in the water column and sediments low.

Since barium, iron and manganese in produced water tend to become non-bioavailable and have low toxic potential, they are not included in the RBA. Mercury, particularly as various organic-mercury

substances, is considered among the most toxic metals to marine organisms. Mercury is identified as a PS under the EU-WFD, together with the metals cadmium, lead and nickel, one of the selection criteria for evaluating substances to be included in the RBA. EQSs are established for all these metals (EC, 2013a). All these metals, except nickel, are also for priority action in OSPAR (OSPAR, 2011). The level of toxicity is another important selection criterion. Therefore are also copper, chromium and arsenic (in the trivalent form of arsenate) included. Zinc is included due to the elevated concentrations in produced waters and it is moderately toxic. Based on these considerations arsenic, cadmium, chromium, copper, mercury, lead, nickel and zinc were identified relevant for inclusion in the RBA.

3.3.2 Monoaromatic hydrocarbons (BTEX)

Monoaromatic hydrocarbons like benzene, toluene, ethylbenzene and xylene, form the bulk of aromatic substances in produced water. These substances are moderately soluble in water, are highly volatile and biodegrade quickly. However, due to high toxicity and relative high concentrations in produced water (especially for gas and condensate producing platforms) these substances are a concern when discharged to the marine environment. Benzene is categorized as a PS and an EQS established under the EU-WFD is available. For toluene and ethylbenzene RARs including PNECs for the marine environment have been prepared by the EU. For xylene no high quality standard is available. However, due to its toxicity and the considerations above, benzene, toluene, ethylbenzene and xylene were identified relevant for inclusion in the RBA.

3.3.3 Dispersed oil

Measurement of oil in produced water is required by law and globally this parameter is the most important parameter that legally requires to be measured and reported to authorities. Estimating the oil content of produced water depends to a large degree on the method used to determine it. Often the method is set by the regulatory system. For the OSPAR area a performance standard of 30 mg/L for dispersed oil in water has been used and OSPAR has defined reference methods that should be used to measure dispersed oil in water (OSPAR, 2001). Because of the regulatory focus on dispersed oil it is important to include this group of substances in the risk assessment. In addition dispersed oil, that is often present at high concentrations, contains a range of substances that do not easily dissolve and evaporate and are potentially toxic and bioaccumulative (e.g. PAHs and phenols).

3.3.4 Polycyclic aromatic hydrocarbons (PAHs)

Polycyclic aromatic hydrocarbons are, defined as hydrocarbons containing two or more fused aromatic rings, and are the petroleum hydrocarbons of greatest environmental concern in produced water, because of their toxicity and persistence in the marine environment (Neff, 1987).

The 2 ring (naphthalene) and 3 rings (particularly phenanthrene), and their alkyl homologues most often represents more than 95% of total PAHs in produced water (DOE, 1997; OOC, 1997, Røe Utvik, 1999). Most of the PAHs are low molecular weight non-carcinogenic 2 and 3 ring PAHs that are moderately toxic, and includes the following PAHs: naphthalene and naphthalene C1-C3 alkyl homologues, acenaphtene, acenaphtylene, fluorene, anthracene, phenanthrene and phenanthrene C1-C3 alkyl homologues, dibenzothiophene and dibenzothiophene C1-C3 alkyl homologues.

Within the group of 2-3 ring PAHs, naphthalene and anthracene are identified as PSs under the WFD (EC, 2013a), and EQSs are available. Furthermore, acenaphthene, acenaphthylene, fluorene, anthracene and phenanthrene are in addition to anthracene on the OSPAR list for priority action (OSPAR, 2011). Anthracene is identified as a PBT substance (ECHA, 2009), known to be persistent and with bioaccumulation and toxic potential in the aquatic environment. PNECs derived from European and/or national EU-RARs are available for all the remaining 2- and 3-ring PAHs, except for dibenzothiophene and all 2- and 3-ring PAHs C1-C3 alkyl homologues. Naphthalene and naphthalene C1-C3 alkyl homologues are organized in a separate group since they generally are present at relative higher concentrations and has higher aqueous solubility compared to the other PAHs in this group.

The 4 ring PAHs typically characterized in produced water are fluoranthene, pyrene, benz(a)anthracene and chrysene. The high molecular weight 4 ring PAHs generally occurs at lower concentrations than the 2-3 ring PAHs. Typically, the concentrations in produced water are decreasing as the molecular weight increases. The decrease in the aqueous solubility with increasing PAH alkylation, is favoring retention in the oil phase.

Fluoranthene is identified as a PS under the WFD, while the remaining 4 ring PAHs characterized are on the OSPAR list for priority action. All 4 ring PAHs are identified as PBT substances (ECHA, 2009). Because of their high hydrophobicity, they are bioaccumulated efficiently by marine organisms. EQS established under the WFD is available for fluoranthene and PNECs derived from EU-RARs are available for the remaining 4-ring PAHs.

The 5 and 6 ring PAHs typically analyzed in produced water are dibenzo(a,h)anthracene, benzo(g,h,i)perylene, benzo(a)pyrene, benzo(b)fluoranthene, benzo(k)fluoranthene and ideno(1,2,3-cg)pyrene. The high molecular weight 5 and 6 ring PAHs generally occurs at the lowest concentrations in produced water among the PAHs (DOE, 1997; OOC, 1997, Røe Utvik, 1999). They are poorly soluble in produced water and therefore have low bioavailability.

All 5-6 ring PAHs, except dibenzo(a,h)anthracene, are evaluated as PSs under the EU-WFD (EC, 2013a). However, dibenzo(a,h)anthracene is included in the OSPAR priority list (OSPAR, 2011). A single EQS has been derived for the 5-6 ring PAHs, using benzo(a)pyrene to represent the toxicity for the whole group. Benzo(g,h,i)perylene, benzo(a)pyrene and benzo(k)fluoranthene are identified as PBT substances, highly persistent and bioaccumulative, and carcinogenic substances (ECHA, 2009). PNECs or EQSs derived from EU-RARs and the WFD are also available for the individual 5-6 ring PAHs.

Based on the considerations above all measured individual PAHs and PAH alkyl homologues were identified relevant for inclusion in the RBA.

3.3.5 Phenol/alkyl phenols

Alkyl phenols are present in produced water at concentrations higher than those found in ambient water column measurements. The concentration is highly variable, reflecting the variable nature of produced waters, but in general, the lower molecular weight alkyl phenols (C1-C3) occur in higher concentrations than the higher molecular weight (longer chain) alkyl phenols (Thomas et al., 2004). This is largely due to their oil/water partition coefficients. Phenol has the lowest oil/water partition coefficient and highest aqueous solubility (Taylor et al., 1997), so would be expected to be found in the highest concentrations. It is, however, also the most volatile and losses occur via this route.

With increasing alkyl chain length also comes higher toxicity (up to C8), both in terms of acute toxicity but also other chronic measures such as estrogenicity (Routledge and Sumpter, 1997). So, while the longer chain alkyl phenols occur at much lower concentrations, their increased toxicity makes them just as relevant to measure. In fact, of all the alkyl phenols, octylphenol (C8) and nonylphenol (C9) are PS under the water framework directive, and so EQS values are available for these compounds. Alkyl phenols with a greater chain length than C9 are not likely to be present in produced waters due to their partitioning. None of the alkyl phenols are considered to be bioaccumulative.

Based on these considerations all measured alkyl phenol groups were identified to be relevant for an evaluation in the RBA.

3.3.6 Organic acids

A range of carboxylic acids are analyzed in accordance to the UK and Norwegian guidance. Volatile organic acids are present at high levels in produced water at some installations in the North Sea. Small amounts of aromatic acids (e.g. benzoic acid) also may be present (Neff, 2002). However, they contribute little to the marine toxicity of produced water and are irrelevant for risk assessment, because these compounds in general have a low toxicity and are expected to disappear quite rapidly from the water following produced water discharge because they are highly volatile.

4 Selection of PNECs

4.1 Collection of established PNECs

In a substance based risk approach, samples of produced water are chemically analyzed with respect to naturally occurring substances e.g. metals, BTEX, dispersed oil, 16 EPA PAHs, other PAHs and alkyl phenols as described above.

For these substances a representative environmental threshold value (PNEC) should be established. The PNECs will form a harmonized set of PNECs recommended to be used by OSPAR Contracting Parties for the purpose of substance based risk assessments. A prerequisite was that the selected PNECs should preferably be based on existing EQS values or PNECs established (e.g. under the EU-WFD or through EU-RAR studies). The method of EQS and PNECs derivation is described in the Appendix 1.

4.2 Criteria for selecting PNECs

PNECs were selected for each selected naturally occurring substance in produced water. The PNEC derivation should be well documented and should preferably be derived according to the EU technical guidance for derivation of PNECs (ECHA, 2008) or EQSs (EC, 2011). The following criteria were used in the selection of individual PNECs for the purpose of a substance based risk assessment approach:

1. Highest priority was given to the most recent reviewed PNEC or EQS available from reliable sources. For that reason, EQS values established under the EU- WFD, latest reviewed and published in 2013, were preferred before PNECs derived from EU-RARs.

Under the EU-WFD, EQS are listed for a number of priority substances (EC, 2013a). The AA-EQS-values for other surface waters are selected as PNECs. The EQS substance data sheets (EC, 2013b) were used for background information.

2. In the case where there was no EQS established under the EU-WFD, PNECs established in EU-RARs were preferred. Priority was given to final EU-RARs, otherwise draft RARs were used.
3. In case there was no EU-WFD or EU-RAR PNECs available, other international or national PNECs may be applied. Where multiple PNECs exist, the PNEC derived from the most recent data, with background information publicly available was used. In these cases the most recent PNEC was chosen, derived according to the Technical Guidance for deriving Environmental Quality Standards (EC, 2011).

4.3 Surrogate PNECs and grouping

It is anticipated that reliable PNECs will not be available for all components analyzed in the produced water and some components are analyzed in groups (e.g. C1-naphthalenes, C6 phenols, etc.). In case one still would like to include these substances and groups in the substance based risk assessment, it is suggested that available high quality PNECs (from EU-WFD or EU-RARs) could be used to represent the toxicity of substances for which no PNEC is available and groups of substances that are analyzed together.

When selecting a surrogate PNEC to represent the toxicity of another substance the substance for which the PNEC is available should belong to the same category of substances (e.g. PAHs or phenols) and must have the same main mode of toxic action as the substance it will represent. When a PNEC is selected to represent the toxicity of a group of substances that are analyzed together the substance for which the PNEC is available should be among the dominating and most toxic substances from that group, in order not to underestimate the toxicity.

If one also would like to include the analyzed concentrations of groups of for instance alkyl homologues of PAHs, a representative substance from that group with an established PNEC should be selected to represent the toxicity of the group. It is suggested that the representing substance for which the PNEC is available is the generally more toxic, non-alkyl form of the substance group it will represent (e.g. naphthalene to represent C1-C3 alkyl naphthalene).

For alkyl phenols, there are multiple structures possible for each alkyl carbon number, with the number of structures increasing with carbon number (i.e. only one structure for C0 and C1 alkyl phenols, but 4 structures for C2 alkyl phenols and 5 for C3 alkyl phenols etc.). For this reason it is not practical to have a PNEC for each structure, and there is not toxicity data available for all structures. The alkyl phenols are therefore divided into different groups according to chemical structure and related toxic properties. For each group a substance has been selected to represent the toxicity of the whole group. The substance for which the PNEC is available, is the generally more toxic, primary alkyl form of the substance group it will represent (e.g. pentylphenol to represent C5-phenols). The final set of PNECs presented in the next chapter will provide suggestions for these cases.

5 Selected PNECs

The main goal of this report was to establish a list of PNECs for the most common naturally occurring substances in the produced water based on existing EQSs and PNECs, where available. These values are presented in Table 2. Furthermore a suggestion to grouping of substances is provided.

Harmonized use of the list of PNECs enables sharing of information and comparison of the risk assessment results among CPs. This list should be maintained by OSPAR and updated on a regular basis (e.g. every 5-10 years) or as new scientific data and PNECs/EQS become available. The PNEC list does not include man-added chemicals. Derivation of PNECs for man-added chemicals is described separately in paragraph 24 and Appendix 6 of the Guideline.

Table 2. List of PNECs established for naturally occurring substances typically analyzed in produced water.

Substance	PNEC (µg/L)	Source	Additional information
BTEX			
Benzene (and xylene)	8	EC, 2013	It is proposed to apply the PNEC for benzene to represent the toxicity of xylene
Toluene	7.4	EU RAR, 2003	
Ethylbenzene	10	EU RAR, 2007	
Naphthalenes			
Naphthalene (and alkyl homologues)	2	EC, 2013	It is proposed to apply the PNEC for naphthalene to represent the toxicity of C1-C3 alkyl homologues of naphthalene
Polycyclic aromatic hydrocarbons (PAHs)			
2-3 ring PAH			
Acenaphthene	0.38	EU RAR CTPHT, 2008	
Acenaphthylene	0.13	EU RAR CTPHT, 2008	
Fluorene	0.25	EU RAR CTPHT, 2008	
Anthracene (and dibenzothiophene and alkyl homologues)	0.1	EC, 2013	It is proposed to apply the PNEC for anthracene to represent the toxicity of dibenzothiophene and C1-C3 alkyl homologues of dibenzothiophene
Phenanthrene (and alkyl homologues)	1.3	EU RAR CTPHT, 2008	It is proposed to apply the PNEC for phenanthrene to represent the toxicity of C1-C3 alkyl homologues of phenanthrene
4 ring PAHs			
Fluoranthene	0.0063	EC, 2013	The PNEC _{water} is back calculated from food standard applying bioconcentration factor ¹⁾

Pyrene	0.023	EU RAR CTPHT, 2008	
Benz(a)anthracene	0.0012	EU RAR CTPHT, 2008	
Chrysene	0.007	EU RAR CTPHT, 2008	
5-6 ring PAHs			
Dibenzo(a,h)anthracene	0.00014	EU RAR CTPHT, 2008	
Benzo(a)pyrene ² (and Benzo(g,h,i)perylene, Benzo[b]fluoranthene, Benzo[k]fluoranthene and Indeno[1,2,3-cd]pyrene)	0.00017	EC, 2013	It is proposed to apply the PNEC for benzo(a)pyrene to represent the toxicity of benzo(g,h,i)perylene, benzo[b]fluoranthene, benzo[k]fluoranthene and indeno[1,2,3-cd]pyrene. The PNEC _{water} is back calculated from food standard for benzo(a)pyrene applying bioconcentration factor for molluscs ¹⁾
Dispersed oil			
Dispersed oil	70.5	Smit et al., 2009	No official standard available
Metals			
Arsenic	0.6 +Cb ³	UKTAG, 2007	No EU standard available.,
Cadmium	0.2+Cb ³	EC, 2013	
Chromium	0.6+ Cb	UKTAG, 2007	No EU standard available
Copper	2.6	EU RAR, 2008	
Nickel	8.6 +Cb	EC, 2013	
Mercury ⁴	0.05+Cb ³	WFD, 2008	The PNEC does not account for bioaccumulation ¹⁾
Lead	1.3	EC, 2013	
Zinc	3.4+Cb ³	UKTAG, 2012	
Alkyl phenols			
Phenol (and C1-C3 alkyl phenols)	7.7	EU RAR, 2006	Reliable PNECs are not available for individual C0-C3 alkyl phenols. It is proposed to apply the PNEC for phenol to represent the toxicity of all C0-C3 alkyl phenols
Butylphenol (and other C4 alkyl phenols)	0.64	EU RAR, 2008	Reliable PNECs are not available for individual C4 alkyl phenols. It is proposed to apply the PNEC for butylphenol to represent the toxicity of all C4 alkyl phenols
Pentylphenol (and other C5 alkyl phenols)	0.2	EA RAR, 2008	Reliable PNECs are not available for individual C5 alkyl phenols. It is proposed to apply the PNEC for pentylphenol to

			represent the toxicity of all C5 alkyl phenols
Octylphenol (and C6-C8 alkyl phenols)	0.01	EC, 2013	Reliable PNECs are not available for individual C6-C8 alkyl phenols. It is proposed to apply the PNEC for octylphenol to represent the toxicity of all C6-C8 alkyl phenols
Nonylphenol (and other C9 alkyl phenols)	0.3	EC, 2013	Reliable PNECs are not available for individual C9 alkyl phenols. It is proposed to apply the PNEC for nonylphenol to represent the toxicity of all C9 alkyl phenols

Detailed information on substances within the different groups can be found in Appendix 3, Roex, E (2010).

¹⁾ For Priority Substances under the WFD with significant bioaccumulation potential or human health effects from consumption of fishery products (e.g. for some PAHs), the $PNEC_{water}$ is derived from food standards applying bioconcentration factors.

²⁾ 5-6 ring PAHs include the carcinogenic substances: benzo[a]pyrene, benzo(g,h,i)perylene, benzo[b]fluoranthene, benzo[k]fluoranthene and indeno[1,2,3-cd]pyrene. It is proposed to apply the PNEC for benzo[a]pyrene for all 5-6 carcinogenic PAHs.

³⁾ Cb: Background concentration ($\mu\text{g/L}$). Site specific background concentrations are preferred. If not available, ranges for background concentrations can be found in the OSPAR background document (OSPAR, 2004).

⁴⁾ For mercury, which has bioaccumulation potential, back calculation from food standards is not possible because bioconcentration factors are highly variable. Therefore the $PNEC_{water}$ for mercury based on aquatic toxicity is proposed (WFD, 2008). The PNEC does not account for bioaccumulation/secondary effects and is therefore not protective for marine mammals and birds

For some PAHs and mercury standards for biota are available and can be used directly to compare with measured biota concentrations.

6 Update and deviation

6.1 Update

The list of proposed PNEC values is not static. It is expected that the EU will regularly update PNECs and EQS or publish new risk assessment reports. As the methods that are used to derive PNECs are using data from laboratory toxicity tests, new test results could potentially result in updated PNECs. Newly available toxicity data that indicate higher sensitivity (i.e. sensitive species or endpoints) might become available that result in a lower threshold value. New toxicity data might also result in an increase of the threshold value if it affects the applied assessment factor (AF) (e.g. mesocosm studies or data becomes available on additional taxonomic groups).

Where species sensitivity distributions (SSDs) have been used for extrapolation, there can sometimes be finely balanced arguments that will argue for changing the size of the AF applied to the HC5 (hazardous concentrations for 5 % of species) to account for uncertainty. For example, where the PNEC for a metal is close to background levels, this would encourage a review of uncertainties and how best to account for them so that a compliance assessment regime for the EQS can be practically implemented.

Other reasons for updating PNECs or EQS can be new evidence for a mode of toxic action that was not previously considered (e.g. new evidence of endocrine disrupting properties) and as a result of scientific and/or political discussions. In addition there might be a need for including new substances previously not considered in the RBA or other new scientific insights.

It is recommended that OSPAR revise the PNEC list of substances regularly in order to implement potential changes to the established PNECs. Update of existing PNECs/EQSs on the list or inclusion of PNECs for new substances should be based on cooperation between the CPs.

6.2 Deviation

The presented PNECs are the result of a process within the EU and can be used in a first tier risk assessment, i.e. a direct comparison between the aqueous concentrations with the generic EQS. This results in a relatively precautionary assessment in which false negatives (Type II errors) are minimised. However, contracting parties have the possibility to deviate from the list of recommended PNECs in higher tiers if there is a scientifically sound rationale for doing so. Deviation needs to be justified by providing all relevant information and documentation that explains why deviation is acceptable.

Two examples are provided here to illustrate when and how deviation from the proposed PNECs can be justified. Situations where deviation is acceptable might, however, not be restricted to these two:

- New toxicity data are available but the EU has not yet updated their guidance;
- Monitoring data indicates that PNECs based on standards for human food consumption are not relevant.

6.2.1 New toxicity data

When a CP has access to new toxicity data that passes the quality criteria from the EU, this CP has the possibility to derive a new PNEC based on this new data and use it before it officially has been updated by the EU. The procedure that is followed to derive this new value must be in line with the methods used by the EU (EC, 2011). Documentation that justifies the deviation needs to contain a detailed description of the toxicity test (incl. test set-up, test species, conditions, results, etc.), explanation on how the result of the test influences the value of the existing PNEC and the derivation procedure and results of the updated PNEC calculation. Since the purpose of this document is to encourage the use of a standard list of PNECs, if a contracting party derives a new PNEC as described, this information should be disseminated to other CPs in order that they too may use the newly established PNEC if they wish in their assessments. This also limits that chance that several contracting parties independently establish new PNECs for the same substance, leading to multiple PNECs for a single substance.

6.2.2 Monitoring data

For fluoranthene and several 4-5 ring PAHs, standards for human food consumption are used to derive the PNEC that is included in the OSPAR recommended list. Contracting parties might have evidence from monitoring data which show that offshore produced water discharges do not result in unacceptable levels in biota when it comes to human consumption. This data can be used to argue for the use of PNECs based on toxicity data instead of food standards for human consumption. A requirement for this is that for these PAHs an alternative high quality PNEC, accepted by the EU, must be available (see PNEC fact sheets if this is the case for the specific PAHs). Documentation that justifies the deviation needs to contain a description of the monitoring data (which species, which measurements, which substances, monitoring protocol, results, etc.) and a rationale why this data proves that potential risks through human food consumption are irrelevant.

7 PNEC fact sheets

A PNEC fact sheet was developed for each substance represented in the list of PNEC values for naturally occurring substances in offshore produced water (Table 2). Each PNEC fact sheet includes information regarding the substance identity, background information regarding the selected PNEC value, literature source etc. The fact sheets are organized into the following main groups of substances: BTEX, naphthalenes, PAHs, metals, dispersed oil and alkyl phenols. Furthermore, the PAHs are further subdivided into 2-3 ring, 4 ring and 5-6 ring PAHs.

7.1 BTEX

7.1.1 Benzene

Chemical identity

Common name	Benzene
Chemical name (IUPAC)	Benzene
Chemical class (when available/relevant)	Aromatic hydrocarbon
Produced water substance group	BTEX
CAS number	71-43-2
EC number	200-753-7
Molecular formula	C ₆ H ₆
Molecular structure	
Molecular weight (g.mol⁻¹)	78.11

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	8
Derived by	EC, 2013 EC, 2005. Benzene EQS fact sheet (15/01/2005)
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/84a49d75-aafb-4ce3-9683-e79c7066aab3/04_Benzene_EQS_Final%20Data%20Sheet.pdf

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	100
Lowest Effect concentration or HC5 value (µg/L)	Chronic NOEC = 800
Species	<i>Pimephales promelas</i>
Marine / Fresh water	Both marine and freshwater species data
Toxic Mode of Action	Non polar narcotics and carcinogenic
Master reference	Russom & Broderius, 1991
Alternative PNEC values/sources available (µg/L)	8 (EU RAR CTPHT, 2008)
PBT substance (Yes or No)	No
Priority substance (Yes or No)	Yes. Included in Annex I EQS Dir. 2013 (EC, 2013) Substance #4
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

EC (2005). Benzene EQS fact sheet (15/01/2005).

https://circabc.europa.eu/sd/d/84a49d75-aafb-4ce3-9683-e79c7066aab3/04_Benzene_EQS_Final%20Data%20Sheet.pdf

EC (2013). DIRECTIVE 2013/39/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL

of 12 August 2013, amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy .

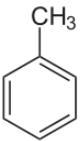
<http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF> European Union Risk Assessment Report: Benzene (2008). CAS No: 71-43-2, EINECS No: 200-753-7. Environment and human health.

EU RAR CTPHT (2008). European Union Risk Assessment Report for Coal-Tar Pitch, High Temperature (CAS-No.: 65996-93-2, EINECS-No.: 266-028-2)(Final report, Environment). Institute for Health and Consumer Protection - European Chemicals Bureau. May, 2008.

Russom, C. L., Broderius, S. J. (1991). A chronic aquatic toxicity database for development of predictive toxicology models for industrial organic chemicals. US EPA, Environmental Research Laboratory-Duluth. Deliverable No. 8477. PPA: L104/G/2013.

7.1.2 Toluene

Chemical identity

Common name	Toluene
Chemical name (IUPAC)	Methylbenzene
Chemical class (when available/relevant)	Aromatic hydrocarbon
Produced water substance group	BTEX
CAS number	108-88-3
EC number	203-625-9
Molecular formula	C ₇ H ₈
Molecular structure	
Molecular weight (g.mol⁻¹)	92.1381

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	7.4
Derived by	EU RAR, 2003
Link	EU RAR 2003

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	100
Lowest Effect concentration or HC5 value (µg/L)	Chronic NOEC = 740
Species	<i>Ceriodaphnia dubia</i>

Marine / Fresh water	Both marine and freshwater species data
Toxic Mode of Action	Non polar narcotics
Master reference	Niederlehner et al., 1998
Alternative PNEC values/sources available (µg/L)	NA
PBT substance (Yes or No)	No
Priority substance (Yes or No)	
Priority hazardous substance (Yes or No)	No

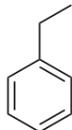
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Niederlehner BR, Cairns J, Smith EP (1998). Modeling acute and chronic toxicity of nonpolar narcotic chemicals and mixtures to *Ceriodaphnia dubia*. Ecotoxicol. Environ. Saf. **39**, 136-146.

7.1.3 Ethylbenzene

Chemical identity

Common name	Ethylbenzene
Chemical name (IUPAC)	Ethylbenzene
Chemical class (when available/relevant)	Aromatic hydrocarbon
Produced water substance group	BTEX
CAS number	100-41-4
EC number	202-849-4
Molecular formula	C ₈ H ₁₀
Molecular structure	
Molecular weight (g.mol ⁻¹)	106.17

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	10
Derived by	EU RAR, 2007
Link	EU RAR 2007

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	100
Lowest Effect concentration or HC5 value (µg/L)	Chronic NOEC= 1000
Species	<i>Ceriodaphnia dubia</i>

Marine / Fresh water	Both marine and freshwater species data
Toxic Mode of Action	Non polar narcotics
Master reference	Niederlehner et al., 1998
Alternative PNEC values/sources available (µg/L)	10 (Smit and Verbruggen, 2011)
PBT substance (Yes or No)	No
Priority substance (Yes or No)	
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

EU RAR (2007). European Union Risk Assessment Report: Ethylbenzene (CAS No: 100-41-4, EINECS No: 202-849-4). Draft April 2007. Environment and human health.

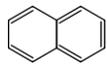
Niederlehner BR, Cairns J, Smith EP (1998). Modeling acute and chronic toxicity of nonpolar narcotic chemicals and mixtures to *Ceriodaphnia dubia*. Ecotoxicol. Environ. Saf. **39**, 136-146.

Smit, C.E and E.M.J. Verbruggen (2011). Environmental risk limits for ethyl-benzene and tributylphosphate in water. RIVM Letter report 601714019/2011.

7.2 Naphthalenes

7.2.1 Naphthalene (incl. C1-C3 alkyl homologues)

Chemical identity

Common name	Naphthalene
Chemical name (IUPAC)	Bicyclo[4.4.0]deca-1,3,5,7,9-pentene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	Naphthalenes
CAS number	91-20-3
EC number	202-049-5
Molecular formula	C ₁₀ H ₈
Molecular structure	
Molecular weight (g.mol ⁻¹)	128.2

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	2
Derived by	EC, 2013 EC, 2011. Naphthalene EQS fact sheet
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/2fc1dfd1-fc77-44af-9d23-2a0c1735ce6d/Naphthalene%20EQS%20dossier%202011.pdf

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	10
Lowest Effect concentration or HC5 value (µg/L)	Chronic LC10 = 20
Species	<i>Onchorhynchus mykiss</i>

Marine / Fresh water	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis
Master reference	Black et al., 1983
Alternative PNEC values/sources available (µg/L)	2.4 (EU RAR, 2003) 2 (EU RAR CTPHT, 2008)
PBT substances (Yes or No)	No
Priority substance (Yes or No)	Yes. Included in Annex I EQS Dir. 2013 (EC, 2013). Substance #22
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Black J.A., Birge W.J., Westerman A.G. and Francis P.C. (1983). "Comparative aquatic toxicology of aromatic hydrocarbons." *Fund. Appl. Toxicol.* 3: 353-358.

E.C. (2010). Draft Technical Guidance Document for deriving Environmental Quality Standards (January 2010 version).

EC (2011). Naphthalene EQS draft fact sheet (dossier 20101221), 01/06/2012.

<https://circabc.europa.eu/sd/d/2fc1dfd1-fc77-44af-9d23-2a0c1735ce6d/Naphthalene%20EQS%20dossier%202011.pdf>

EC (2013). DIRECTIVE 2013/39/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 12 August 2013, amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy .

<http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF>

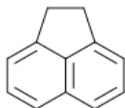
EU RAR (2003). European Union Risk Assessment Report: Naphthalene. European Union Risk Assessment Report: Naphthalene - CAS No: 91-20-3 EINECS No: 202-049-5. Series: 1st Priority List, Volume: 33. European Commission – Joint Research Centre, Institute for Health and Consumer Protection, European Chemicals Bureau (ECB); © European Communities, 2003. The final report is available at the internet site of the European Chemicals Bureau: <http://ecb.jrc.it/existingchemicals/> ⇒ tick ESIS button, then enter CAS or EINECS number of substance.

EU RAR CTPHT (2008). European Union Risk Assessment Report for Coal-Tar Pitch, High Temperature (CAS-No.: 65996-93-2, EINECS-No.: 266-028-2)(Final report, Environment). Institute for Health and Consumer Protection - European Chemicals Bureau. May, 2008.

7.3 2-3 ring PAHs

7.3.1 Acenaphthene

Chemical identity

Common name	Acenaphthene
Chemical name (IUPAC)	1,2-Dihydroacenaphthylene
Chemical class (when available/relevant)	Polyaromatic hydrocarbons (PAHs)
Produced water substance group	PAH 2-3 ring
CAS number	83-32-9
EC number	201-469-6
Molecular formula	C ₁₂ H ₁₀
Molecular structure	
Molecular weight (g.mol ⁻¹)	154.21

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.38
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT, 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	100
Lowest Effect concentration or HC5 value (µg/L)	Chronic EC10 = 38
Species	<i>Pseudokirchneriella subcapitata</i>

Marine / Fresh water data	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis
Master reference	Bisson et al., 2000
Alternative PNEC values/sources available (µg/L)	0.38 (Verbruggen, 2012)
PBT substance (Yes or No)	No
Priority substance (Yes or No)	Yes. Included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Bisson M, Dujardin R, Flammarion P, Garric J, Babut M, Lamy M-H, Porcher J-M, Thybaud É, Vindimian É (2000). *Complément au SEQ-Eau: méthode de détermination des seuils de qualité pour les substances génotoxiques*. Verneuil-en-Halatte, France: Institut National de l'Environnement Industriel et des Risques (INERIS), Agence de l'eau Rhin-Meuse.

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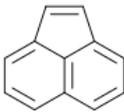
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Verbruggen EMJ (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs) : For direct aquatic, benthic, and terrestrial toxicity . RIVM report 607711007.

7.3.2 Acenaphthylene

Chemical identity

Common name	Acenaphthylene
Chemical name (IUPAC)	Acenaphthylene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 2-3 ring
CAS number	208-96-8
EC number	205-917-1
Molecular formula	C ₁₂ H ₈
Molecular structure	
Molecular weight (g.mol⁻¹)	152.20

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.13
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT , 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	500
Lowest Effect concentration or HCS value (µg/L)	Chronic EC10 = 64
Species	<i>Ceriodaphnia dubia</i>

Marine / Fresh water data	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis
Master reference	Bisson et al., 2000
Alternative PNEC values/sources available (µg/L)	0.13 (Verbruggen, 2012)
PBT substance (Yes or No)	No
Priority substance (Yes or No)	Yes. Included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Bisson M, Dujardin R, Flammarion P, Garric J, Babut M, Lamy M-H, Porcher J-M, Thybaud É, Vindimian É (2000). *Complément au SEQ-Eau: méthode de détermination des seuils de qualité pour les substances génotoxiques*. Verneuil-en-Halatte, France: Institut National de l'Environnement Industriel et des Risques (INERIS), Agence de l'eau Rhin-Meuse.

EU RAR CTPHT (2008). European Union Risk Assessment Report for Coal-Tar Pitch, High Temperature (CAS-No.: 65996-93-2, EINECS-No.: 266-028-2)(Final report, Environment). Institute for Health and Consumer Protection - European Chemicals Bureau. May, 2008.

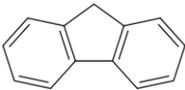
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Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs) : For direct aquatic, benthic, and terrestrial toxicity . RIVM report 607711007.

7.3.3 Fluorene

Chemical identity

Common name	Fluorene
Chemical name (IUPAC)	9H-Fluorene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 2-3 ring
CAS number	86-73-7
EC number	201-695-5
Molecular formula	C ₁₃ H ₁₀
Molecular structure	
Molecular weight (g.mol ⁻¹)	166.22

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.25
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT, 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	100
Lowest Effect concentration value (µg/L)	Chronic EC10 = 25
Species	<i>Ceriodaphnia dubia</i>

Marine / Fresh water	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis
Master reference	Bisson et al., 2000
Alternative PNEC values available (µg/L)	0.30 (Verbruggen, 2012)
PBT substance (Yes or No)	No
Priority substance (Yes or No)	Yes. Included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Bisson M, Dujardin R, Flammarion P, Garric J, Babut M, Lamy M-H, Porcher J-M, Thybaud É, Vindimian É (2000). *Complément au SEQ-Eau: méthode de détermination des seuils de qualité pour les substances génotoxiques*. Verneuil-en-Halatte, France: Institut National de l'Environnement Industriel et des Risques (INERIS), Agence de l'eau Rhin-Meuse.

EU RAR CTPHT (2008). European Union Risk Assessment Report for Coal-Tar Pitch, High Temperature (CAS-No.: 65996-93-2, EINECS-No.: 266-028-2)(Final report, Environment). Institute for Health and Consumer Protection - European Chemicals Bureau. May, 2008.

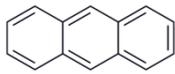
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7.3.4 Anthracene

Chemical identity

Common name	Anthracene
Chemical name (IUPAC)	Anthracene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 2-3 ring
CAS number	120-12-7
EC number	204-371-1
Molecular formula	C ₁₄ H ₁₀
Molecular structure	
Molecular weight (g.mol ⁻¹)	178.2

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.1
Derived by	EC, 2013 EC, 2011. Anthracene EQS fact data sheet
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/60c3c0c0-ea7b-4aa6-81ca-91241a251a79/Anthracene%20EQS%20dossier%202011.pdf

Background information – PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	10
Lowest Effect concentration or HC5 value (µg/L)	Chronic LC50 = 1.0
Species	<i>Daphnia pulex</i>

Marine / Fresh water data	Fresh water species, but both fresh water and marine data collected
Toxic Mode of Action	Non polar narcotics and very phototoxic (photo[induced]toxicity)
Master reference	Allred & Giesy, 1985
Alternative PNEC values/sources available (µg/L)	0.1 (EU RAR CTPHT, 2008) 0.1 (Verbruggen, 2012)
PBT substances (Yes or No)	Fulfilling PBT and vPvB criteria (EQS fact sheet, 2012) and PBT criteria (ECHA, 2009)
Priority substance (Yes or No)	Yes. Included in: - Annex I EQS Dir. 2013 (EC, 2013), Substance #2 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	Yes, included in Annex I EQS Dir. 2013 (EC, 2013). Substance #2

Bibliography, sources and supporting information:

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ECHA (2009). Member State Committee Support Document for identification of *Coal Tar Pitch, High Temperature as a substance of very high concern because of its PBT and CMR properties*, December 2009.
http://echa.europa.eu/documents/10162/13638/svhc_supdoc_pitch_publication_en.pdf

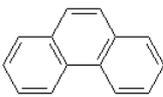
EU RAR CTPHT (2008). European Union Risk Assessment Report for Coal-Tar Pitch, High Temperature (CAS-No.: 65996-93-2, EINECS-No.: 266-028-2)(Final report, Environment). Institute for Health and Consumer Protection - European Chemicals Bureau. May, 2008.
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Verbruggen EMJ (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs): For direct aquatic, benthic, and terrestrial toxicity. RIVM report 607711007.

7.3.5 Phenanthrene (incl. C1-C3 alkyl homologues)

Chemical identity

Common	Phenanthrene
Chemical name (IUPAC)	Phenanthrene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 2-3 ring
CAS number	85-01-8
EC number	201-581-5
Molecular formula	C ₁₄ H ₁₀
Molecular structure	
Molecular weight (g.mol⁻¹)	178.23

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	1.3
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT, 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	10
Lowest Effect concentration or HC5 value (µg/L)	Chronic EC10 = 13
Species	<i>Cerodaphnia dubia</i>

Marine / Fresh water data	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis
Master reference	Bisson et al., 2000
Alternative PNEC values/sources available (µg/L)	1.1 (Verbruggen, 2012)
PBT substance (Yes or No)	Yes, fulfilling the vPvB criteria in the SVHC Support document (ECHA, 2009)
Priority substance (Yes or No)	- Yes. Included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Bisson M, Dujardin R, Flammarion P, Garric J, Babut M, Lamy M-H, Porcher J-M, Thybaud É, Vindimian É (2000). *Complément au SEQ-Eau: méthode de détermination des seuils de qualité pour les substances génotoxiques*. Verneuil-en-Halatte, France: Institut National de l'Environnement Industriel et des Risques (INERIS), Agence de l'eau Rhin-Meuse.

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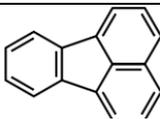
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Verbruggen EMJ (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs): For direct aquatic, benthic, and terrestrial toxicity. RIVM report 607711007.

7.4 4 ring PAHs

7.4.1 Fluoranthene

Chemical identity

Common name	Fluoranthene
Chemical name (IUPAC)	Fluoranthene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 4 ring
CAS number	206-44-0
EC number	205-912-4
Molecular formula	C ₁₆ H ₁₀
Molecular structure	
Molecular weight (g/mol)	202.3

Predicted No Effect Concentration (PNEC)

Quality Standards (QS_{biota}) for protection of human health *via* consumption of fishery product is deemed “critical” for derivation of an Environmental Quality Standard under the Water framework Directive (Fluoranthene EQS fact sheet, 2012). The value is 30 µg/kg_{biota ww} and corresponds to the value of 0.0063 µg/L for both fresh and marine waters and is applied as the PNEC for fluoranthene.

Original data from which QS_{biota} is based on are linked to a virtually safe dose and expressed for an oral cancer risk of 10⁻⁶ based on the read-across between benzo[a]pyrene and fluoranthene.

PNEC value (µg/L)	0.0063
Derived by	EC, 2013 EC, 2011 Fluoranthene EQS fact sheet
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/4336e1e5-ba0c-4545-abee-7743d2085bc3/Fluoranthene%20EQS%20dossier%202011.pdf

Background information – PNEC

Method	According to the Technical Guidance Document on EQS derivation (E.C., 2010), this substance does trigger the bioaccumulation criteria given the high values of log KOW (5.2) and the high value of BCF (7 692). Hence, protection of human health from consumption of fishery product is deemed relevant. The PNEC _{marine water} is derived from back calculation from food quality standard for protection of human health via consumption of fishery products
Assessment factor applied (if relevant)	Not relevant
Lowest Effect concentration or HC5 value (µg/L)	The value is 30 µg/kg _{biota ww} and corresponds to values of 0.0063 µg/L for marine waters ¹ .
Species	-
Marine / Fresh water data	-
Toxic Mode of Action	Non polar narcotics and very phototoxic (photo[induced] toxicity)
Master reference	Baars <i>et al.</i> , 2001
Alternative PNEC values/sources available (µg/L)	0.01 (EU RAR CTPHT, 2008) 0.12 (Verbruggen, 2012)
PBT substances (Yes or No)	Yes, the substance is fulfilling PBT and vPvB criteria in the SVHC Support document (ECHA, 2009)
Priority substance (Yes or No)	Yes. Included in: - Annex I EQS Dir. 2013 (EC, 2013). Substance #15 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

¹: Quality Standard (QS_{biota_hh} for protection of human health *via* consumption of fishery product is deemed the “critical QS” for derivation of an Environmental Quality Standard. The value is 30 µg.kg⁻¹_{biota ww} and corresponds to values of 6.3 10⁻³ µg.l⁻¹ marine waters (and freshwater).

Bibliography, sources and supporting information:

Baars A.J., Theelen R.M.C., Janssen P.J.C.M., Hesse J.M., van Apeldoorn M.E., Meijerink M.C.M., Verdam L. and Zeilmaker M.J. (2001). Re-evaluation of human-toxicological maximum permissible risk levels. RIVM report 711701 025. RIVM, Bilthoven. <http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf>.

EC (2011). Fluoranthene EQS draft fact sheet (dossier 20101221), 01/06/2012.

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EC (2013). DIRECTIVE 2013/39/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 12 August 2013, amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy .

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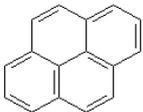
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7.4.2 Pyrene

Chemical identity

Common name	Pyrene
Chemical name (IUPAC)	Pyrene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 4 ring
CAS number	129-00-0
EC number	204-927-3
Molecular formula	C ₁₆ H ₁₀
Molecular structure	
Molecular weight (g.mol⁻¹)	202.25

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.023
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT, 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	10
Lowest Effect concentration or HC5 value (µg/L)	Acute LC50 = 0.23
Species	<i>Mulinia lateralis</i>

Marine / Fresh water data	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis and phototoxic
Master reference	Pelletier et al., 1997
Alternative PNEC values/sources available (µg/L)	0.023 (Verbruggen, 2012)
PBT substance (Yes or No)	Yes, in the PBT/vPvB criteria in the SVHC Support document (ECHA, 2009)
Priority substance (Yes or No)	Yes. Is included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

ECHA (2009). Member State Committee Support Document for identification of *Coal Tar Pitch, High Temperature as a substance of very high concern because of its PBT and CMR properties*, December 2009.

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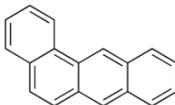
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Pelletier MC, Burgess RM, Ho KT, Kuhn A, McKinney RA, Ryba SA (1997). Phototoxicity of individual polycyclic aromatic hydrocarbons and petroleum to marine invertebrate larvae and juveniles. *Environ Toxicol Chem* 16: 2190-2199.

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7.4.3 Benz[a]anthracene

Chemical identity

Common name	Benz[a]anthracene
Chemical name (IUPAC)	Benz[a]anthracene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 4 ring
CAS number	56-55-3
EC number	200-280-6
Molecular formula	C ₁₈ H ₁₂
Molecular structure	
Molecular weight (g.mol⁻¹)	228.29

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.0012
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT, 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	1000
Lowest Effect concentration or HC5 value (µg/L)	Acute EC10 = 1.2
Species	<i>Pseudokirchneriella subcapitata</i>

Marine / Fresh water data	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis and phototoxic
Master reference	Bisson et al., 2000
Alternative PNEC values/sources available (µg/L)	0.01 (Verbruggen, 2012) 0.00023 (Verbruggen & van Herwijnen, 2011) - based on human fish consumption
PBT substance (Yes or No)	Yes, in the PBT/vPvB criteria in the SVHC Support document (ECHA,2009)
Priority substance (Yes or No)	Yes. Is included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Bisson M, Dujardin R, Flammarion P, Garric J, Babut M, Lamy M-H, Porcher J-M, Thybaud É, Vindimian É (2000). *Complément au SEQ-Eau: méthode de détermination des seuils de qualité pour les substances génotoxiques*. Verneuil-en-Halatte, France: Institut National de l'Environnement Industriel et des Risques (INERIS), Agence de l'eau Rhin-Meuse.

ECHA (2009). Member State Committee Support Document for identification of *Coal Tar Pitch, High Temperature as a substance of very high concern because of its PBT and CMR properties*, December 2009.

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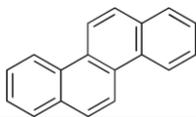
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Verbruggen EMJ (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs): For direct aquatic, benthic, and terrestrial toxicity. RIVM report 607711007.

7.4.4 Chrysene

Chemical identity

Common name	Chrysene
Chemical name (IUPAC)	Chrysene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 4 ring
CAS number	218-01-9
EC number	205-923-4
Molecular formula	C ₁₈ H ₁₂
Molecular structure	
Molecular weight (g.mol ⁻¹)	228.28

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.007
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT, 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	100
Lowest Effect concentration or HC5 value (µg/L)	Acute EC50 = 0.7
Species	<i>Daphnia magna</i>

Marine / Fresh water data	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis and phototoxic
Master reference	Newsted & Giesy, 1987
Alternative PNEC values/sources available (µg/L)	0.007 (Verbruggen, 2012). 0.00023 (Verbruggen & van Herwijnen, 2011) - based on human fish consumption
PBT substance (Yes or No)	Yes, in the PBT/vPvB criteria in the SVHC Support document (ECHA, 2009)
Priority substance (Yes or No)	Yes. Is included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

ECHA (2009). Member State Committee Support Document for identification of *Coal Tar Pitch, High Temperature as a substance of very high concern because of its PBT and CMR properties*, December 2009.

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Newsted JL, Giesy Jr. JP (1987). Predictive models for photoinduced acute toxicity of polycyclic aromatic hydrocarbons to *Daphnia magna*, Strauss (Cladocera, Crustacea). *Environ Toxicol Chem* 6: 445-461.

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Verbruggen EMJ (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs): For direct aquatic, benthic, and terrestrial toxicity. RIVM report 607711007.

7.5 5-6 ring PAHs

Quality Standards (QS_{biota}) for protection of human health *via* consumption of fishery product was deemed “critical” for derivation of an Environmental Quality Standard (EQS) under the Water framework Directive for 5-6 ring PAHs. This includes benzo[a]pyrene (B[a]P), benzo[b]fluoranthene, benzo[k]fluoranthene and indeno[1,2,3-cd]pyrene, known to be carcinogenic substances, in addition to benzo[g,h,i]perylene where no potential for carcinogenicity is demonstrated for (5-6 ring PAH EQS fact sheet, 2012). For the 5-6 ring PAH dibenz[a,h]anthracene, the EQS is based on aquatic toxicity data.

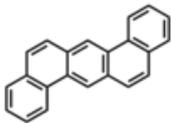
A single Environmental Quality Standards (EQS) has been derived and recommended applied to 5-6 rings PAHs in the review process of the EQS under the European Commission Water framework Directive (2012). The TGD-EQS (E.C., 2010) recommends the use of maximum levels in foodstuffs for benzo[a]pyrene for derivation of a QS_{biota} value. This a QS_{biota} value should be applied as the EQS for compliance with monitored concentrations of benzo[a]pyrene, covering risk to the aquatic environment for the 5-6 ring PAHs as a group. In this case benzo[a]pyrene is used as a marker for the occurrence and effect of carcinogenic polycyclic aromatic hydrocarbons. (B[a]P) is 10 times more potent for carcinogenic effects than the 3 other carcinogenic substances (Baars *et al.*, 2001). This proposed EQS, based on the QS_{biota} value for B[a]P is recommended for comparison with the concentration in biota under the European Commission Water framework Directive (2012).

The monitored maximum concentrations of B[a]P in biota (highest value measured for molluscs) are converted to the corresponding values in seawater by dividing the QS_{biota} value with the bioconcentration factor (BCF) for molluscs. For back calculation of QS_{biota} into water, the B[a]P level of 10 $\mu\text{g}/\text{kg}_{\text{ww}}$ in molluscs is divided by the BCF value of 57 981, corresponding to 0.00017 $\mu\text{g}/\text{L}$ in marine water.

The proposed EQS for B[a]P, is recommended applied as the PNEC for the individual 5-6 ring PAHs, covering the protection of human health and the environment from long term exposure.

7.5.1 Dibenz[a,h]anthracene

Chemical identity

Common name	Dibenzo[a,h]anthracene
Chemical name (IUPAC)	Dibenzo[a,h]anthracene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 5-6 ring
CAS number	53-70-3
EC number	200-181-8
Molecular formula	C ₂₂ H ₁₄
Molecular structure	
Molecular weight (g.mol⁻¹)	278.35

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.00014
Derived by	EU RAR CTPHT, 2008
Link	EU RAR CTPHT , 2008

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	1000
Lowest Effect concentration or HC5 value (µg/L)	Chronic EC10 = 0.14
Species	<i>Pseudokirchneriella subcapitata</i>

Marine / Fresh water data	Both marine and freshwater species data
Toxic Mode of Action	Non-polar narcosis
Master reference	Bisson et al., 2000
Alternative PNEC values/sources available (µg/L)	0.00014 (Verbruggen, 2012).
PBT substance (Yes or No)	No
Priority substance (Yes or No)	Yes. Is included in the OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Bisson M, Dujardin R, Flammarion P, Garric J, Babut M, Lamy M-H, Porcher J-M, Thybaud É, Vindimian É (2000). *Complément au SEQ-Eau: méthode de détermination des seuils de qualité pour les substances génotoxiques*. Verneuil-en-Halatte, France: Institut National de l'Environnement Industriel et des Risques (INERIS), Agence de l'eau Rhin-Meuse.

EU RAR CTPHT (2008). European Union Risk Assessment Report for Coal-Tar Pitch, High Temperature (CAS-No.: 65996-93-2, EINECS-No.: 266-028-2) (Final report, Environment). Institute for Health and Consumer Protection - European Chemicals Bureau. May, 2008.

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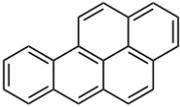
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Verbruggen EMJ (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs): For direct aquatic, benthic, and terrestrial toxicity. RIVM report 607711007.

7.5.2 Benzo[a]pyrene

Chemical identity

Common name	Benzo[a]pyrene
Chemical name (IUPAC)	Benzo[a]pyrene
Chemical class (when available/relevant)	Polycyclic aromatic hydrocarbons (PAH)
Produced water substance group	PAH 5-6 ring
CAS number	50-32-8
EC number	200-028-5
Molecular formula	C ₂₀ H ₁₂
Molecular structure	
Molecular weight (g/mol)	252.3

Predicted No Effect Concentration (PNEC)

The proposed EQS for B[a]P, is recommended applied as the PNEC for the individual 5-6 ring PAHs (benzo[b]fluoranthene, benzo[k]fluoranthene, indeno[1,2,3-cd]pyrene and benzo[g,h,i]perylene), covering the protection of human health and the environment from long term exposure.

PNEC value (µg/L)	0.00017
Derived by	EC, 2013 EC, 2011. 5-6 rings PAH EQS fact sheet
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/4e13a4c4-07b9-4e55-a43d-823e7cd4ce82/PAH%20EQS%20dossier%202011.pdf

Background information – PNEC

Method	<p>According to the Technical Guidance Document on EQS derivation (E.C., 2010), this substance does trigger the bioaccumulation criteria given the high values of log KOW for 5-6 ring PAHs¹ and the high values of BCF, e.g. BCF of 57 981 for B[a]P in molluscs. Hence, protection of human health from consumption of fishery product is deemed relevant.</p> <p>The PNEC_{marine water} is derived from back calculation from food quality standard for protection of human health via consumption of fishery products (QS_{biota}).</p>
Assessment factor applied (if relevant)	Not relevant
Lowest Effect concentration or HC5 value (µg/L)	The value is 10 µg/kg _{biota ww} (molluscs) and corresponds to values of 0.00017 µg/L for marine waters ² based on toxicity of B[a]P.
Species	<i>Molluscs</i>
Marine / Fresh water	-
Toxic Mode of Action	5-6 ring PAHs ¹ are non-polar narcotics and carcinogenic
Master reference	Baars <i>et al.</i> , 2001
Alternative PNEC value/sources based on aquatic toxicity (µg/L)	<p>Benzo[a]pyrene:</p> <p>1) 0.022 (5-6 rings PAH EQS draft fact sheet; dossier 20101221) 2) 0.022 (EU RAR CTPHT, 2008) 3) 0.010 (Verbruggen, 2012).</p> <p>Benzo[b]fluoranthene:</p> <p>1) 0.017 (5-6 rings PAH EQS draft fact sheet; dossier 20101221) 2) 0.0017 (EU CTPHT RAR, 2008) 3) 0.017 (Verbruggen, 2012).</p> <p>Benzo[k]fluoranthene:</p> <p>1) 0.017 (5-6 rings PAH EQS draft fact sheet; dossier 20101221) 2) 0.0017 (EU RAR CTPHT, 2008) 3) 0.017 (Verbruggen, 2012)</p> <p>Indeno[1,2,3-cd]pyrene:</p> <p>1) 0.00027 (EU RAR CTPHT, 2008) 2) 0.00027 (Verbruggen, 2012)</p> <p>Benzo[g,h,i]perylene:</p> <p>1) 0.00082 (5-6 rings PAH EQS draft fact sheet; dossier 20101221) 2) 0.00082 (EU RAR CTPHT, 2008) 2) 0.00082 (Verbruggen, 2012)</p>
Links (alternative PNECS)	<p>EC, 2013. EU RAR CTPHT, 2008 Verbruggen, 2012</p>
PBT substances (Yes or No)	Fulfilling PBT and vPvB criteria for benzo[a]pyrene and benzo[k]fluoranthene and benzo[g,h,i]perylene in the SVHC Support document (ECHA, 2009).

	No information available for benzo[b]fluoranthene and indeno[1,2,3-cd]pyrene (ECHA, 2009)
Priority substance (Yes or No)	Yes. 5-6 ring PAHs ¹ is included in: - Annex I EQS Dir. 2013 (EC, 2013). Substance #28 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	Yes. 5-6 ring PAHs ¹ is included in Annex I EQS Dir. 2013 (EC, 2013). Substance #28

¹ 5-6 ring PAH: Benzo[a]pyrene (B[a]P), benzo[b]fluoranthene, benzo[k]fluoranthene, indeno[1,2,3-cd]pyrene and benzo[g,h,i]perylene.

² Quality Standard (QS_{biota_hh}) for protection of human health *via* consumption of fishery product is deemed the “critical QS” for derivation of an Environmental Quality Standard. The value is 10 µg.kg⁻¹_{ww} (molluscs) and corresponds to values of 0.00017 µg/L marine waters (and freshwater).

Bibliography, sources and supporting information:

Baars A.J., Theelen R.M.C., Janssen P.J.C.M., Hesse J.M., van Apeldoorn M.E., Meijerink M.C.M., Verdam L. and Zeilmaker M.J. (2001). Re-evaluation of human-toxicological maximum permissible risk levels. RIVM report 711701 025. RIVM, Bilthoven. <http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf>.

EC (2011). 5-6 ring PAH EQS draft fact sheet (dossier 20101221), 13/12/2011 <https://circabc.europa.eu/sd/d/4e13a4c4-07b9-4e55-a43d-823e7cd4ce82/PAH%20EQS%20dossier%202011.pdf>

EC (2013). DIRECTIVE 2013/39/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 12 August 2013, amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy .
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http://echa.europa.eu/documents/10162/13638/svhc_supdoc_pitch_publication_en.pdf

EU RAR CTPHT (2008). European Union Risk Assessment Report for Coal-Tar Pitch, High Temperature (CAS-No.: 65996-93-2, EINECS-No.: 266-028-2)(Final report, Environment). Institute for Health and Consumer Protection - European Chemicals Bureau. May, 2008.

OSPAR List of Chemicals for Priority Action (revised 2011).
http://www.ospar.org/content/content.asp?menu=00120000000050_000000_000000

Verbruggen EMJ (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs): For direct aquatic, benthic, and terrestrial toxicity. RIVM report 607711007.

7.6 Dispersed oil

Chemical identity

Common name	Dispersed oil
Chemical name (IUPAC)	-
Chemical class (when available/relevant)	-
Produced water substance group	Dispersed oil
CAS number	-
EC number	-
Molecular formula	-
Molecular structure	
Molecular weight (g.mol ⁻¹)	-

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	70.5
Derived by	Smit et al. 2009
Link	http://onlinelibrary.wiley.com/doi/10.1897/08-464.1/abstract

Background information – PNEC

Scholten et al. (1993) collected NOECs for 26 marine organisms for exposures to several types of oil. All exposures experiments focused on whole organism endpoints; reproduction, growth and survival. Description of the test protocol in a peer-reviewed publication, facilitating the quality assurance of the data, was a prerequisite for inclusion of the NOEC in the dataset. From this data set Smit et al (2009) selected NOECs with exposure times exceeding 7 days representing chronic exposure. If more than one NOEC was available per species, the geometric mean of the values was taken to represent the sensitivity of the species. The final set of NOECs used to derive the HC5 included 30 NOECs for 17 marine species from five taxonomic groups. Following the recommendations by Van Straalen and Denneman (1998) the median estimate of the HC5 from the SSD (70.5 µg/L THC) can be regarded as a maximum allowable exposure level for oil.

Method	Species sensitivity distribution
Assessment factor applied (if relevant)	No assessment factor applied
Lowest Effect concentration or HC5 value (µg/L)	-
Species	-
Marine / Fresh water	Marine toxicity data only
Toxic Mode of Action	Non-polar narcosis
Master reference	Smit et al. 2009
Alternative PNEC values available (µg/L)	Several values for dispersed oil are available but this is the only one that is published in a scientific paper
PBT substance (Yes or No)	No
Priority substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Scholten MCTh, Schobben HPM, Karman CC, Jak RG, Van het Groenewoud H. (1993). De berekening van het maximaal toelaatbaar risico niveau van olie en oliecomponenten in water en sediment. TNO Technical Report No. R93/187, Dutch Organisation for Applied Sci

Smit M.G.D., R.K. Bechman A.J. Hendriks S. Bamber, A. Skadsheim, B.K. Larssen, T. Baussant, S.Sanni (2009). Relating biomarkers to whole organism effects using species sensitivity distributions: a pilot study for marine species exposed to oil. Environmental Toxicology and Chemistry. 28:1004-1009.

Van Straalen NM, Denneman CAJ. (1998). Ecotoxicological evaluation of soil quality criteria. Ecotoxicol Environ Saf 18:241-251. Scientific Research (TNO), Den Helder, The Netherlands.

7.7 Metals

Compared with organic compounds, metals have different features, resulting in a different approach with respect to their toxicity than organic compounds. Some of these features hold for the total group of metals, like the aspect of background concentrations and (bio)availability. These two aspects will be discussed in detail in the appendices.

However, a feature like the toxic mode of action of metals, differs between the different metals. Some metals are toxic when they form poisonous soluble compounds. Toxic metals sometimes imitate the action of an essential element in the body, interfering with the metabolic process to cause illness (like Cd acting like the essential element Zn). Certain metals have no biological role, i.e. are not essential minerals, or are toxic when in a certain form. In the case of lead, any measurable amount may have negative health effects. Metals in an oxidation state abnormal to the body may also become toxic: chromium (III) is an essential trace element, but chromium (VI) is a carcinogen. As of the wide range of different modes of action within the group of metals, the mode of action displayed in the factsheets is referring to their own particular mode of action.

7.7.1 Dealing with metals

Unlike most organic substances, metals are neither created nor destroyed by biological or chemical processes. Rather, they are transformed from one chemical form to another. Because metals are naturally occurring, many organisms have evolved mechanisms to regulate their accumulation and storage. Moreover some metals are essential nutrients so, when they are not present in sufficient concentrations, can limit growth, survival and reproduction of the organisms. Excess amounts of certain metals, on the other hand, are potentially toxic.

These features, along with the fact that metals naturally occur as inorganic forms in environmental compartments (e.g. sediments) and are cycled through the biotic components of an ecosystem, complicate the evaluation of toxicity data for inorganic metal substances and have a major influence on the way EQSs for metals are derived.

7.7.2 Total versus dissolved concentrations

When evaluating toxicity data to derive quality standards for metals, total metal concentrations are not usually directly related to ecotoxicological effects because many abiotic and biotic processes can modify the *availability* of metals, even rendering them unavailable for uptake. This means that the fraction available for uptake and toxicity may be a very small part of the total metal present. Due to several physicochemical processes, metals exist in different chemical forms which might differ in (bio)availability. Thus, the (bio)availability of metals in both laboratory tests and in the 'real' environment may be affected by several physicochemical parameters such as the pH, hardness of water and the dissolved organic carbon (DOC). As a default, the water EQS laid is expressed as total concentrations in the whole water sample. By way of derogation from the first subparagraph, in the case of metals, the water EQS refer to the dissolved concentration, i.e. the dissolved phase of a water sample obtained by filtration through a 0,45 µm filter or any equivalent pre-treatment, or, where specifically indicated, to the bioavailable concentration. For the freshwater compartment higher tier

methods are available for appropriate bioavailability modeling. However, these methods are not applicable to marine environments at the moment.

7.7.3 Background concentrations

Preferably, EQS setting is based on the Total Risk Approach (TA), and no explicit account is taken of natural background levels (Cb). However, EQS values below Cb may be generated, especially for metals, if a (too) conservative approach (i.e. a large AF) is used in the derivation, or when the EQS is set using toxicity tests with organisms cultured/tested under conditions of low metal concentrations compared with the Cb (i.e. organisms may have adapted to higher natural concentrations). Setting EQS values below the Cb serves little regulatory purpose. A pragmatic way to overcome this problem is the added risk approach (ARA). This approach accounts for natural background concentrations and avoids setting regulatory standards below the Cb by adding the Maximum Permissible Addition (MPA) to the background concentration Cb. This MPA is the maximum amount of a metal that may be added to the local Cb of this metal without adversely affecting the assessed ecosystem. Contracting Parties may, when assessing the monitoring results against the relevant EQS, take into account natural background concentrations for metals and their compounds where such concentrations prevent compliance with the relevant EQS. Correct determination of the Cb is important in this approach, and this may not be easy to achieve. For some metals, like lead and nickel, it is almost impossible to determine experimentally a 'natural' background concentration in Europe. Due to geochemical differences, the ambient background concentrations will differ in Europe. In addition, since the concentrations that are measured in the environment are the sum of an anthropogenic and a 'natural' source, one cannot simply distinguish the 'natural' part from the anthropogenic part. Hence, background concentrations are not measured, but estimated or determined with other methods. For other metals, like for instance chrome, the incorporation of background concentration is not much use, as "natural concentrations" of these metals in the environment is of anthropogenic origin and natural background levels are negligible.

As background concentrations are often estimated from relatively small datasets, the calculation of Cb should be an iterative process, reviewing the values when new monitoring data become available.

In salt water, concentrations of metals far at sea will normally suffice as Cb, but the Cb may be higher in coastal waters because of the natural input from rivers and settling of particles. The determination of the Cb in coastal waters may be hampered by as rivers are likely to drain pristine areas as well as areas influenced by anthropogenic inputs, and thus a pragmatic approach is needed. As a starting point, the dissolved metal concentration in the coastal water is compared to with the Cb at sea. If these values are equal, then the Cb at sea can also be used for coastal water. If no measurements are available, or if the concentration in coastal waters is higher than at sea, then the Cb in freshwater and at sea are compared. If they are the same, it is reasonable to say that the Cb in coastal waters and estuaries equals the Cb in both fresh water and seas. If the Cb in freshwater differs from the Cb at sea, then the geometric mean if these two values may serve as a Cb for coastal waters. In cases where the Cb is between the Cb in freshwater and the Cb at sea, the Cb for coastal waters is set to the measured value.

In OSPAR (OSPAR, 2004) guidance is given on ambient metal concentrations measured in the OSPAR region. However, these data should be interpreted with care when deriving coastal C_b values, as the range presented for the different metals refer to open ocean ranges which are usually lower than those for coastal waters. It is important to note that preference should be given to values reflecting C_b for coastal zones, and that some might be found in the literature (Laane, 1992; UK NMMP, 2004).

7.7.4 Arsenic

Chemical identity

Chemical name (IUPAC)	Arsenic
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7440-38-2
EC number	231-148-6
Molecular formula	As
Molecular structure	As
Molecular weight (g.mol ⁻¹)	74.92160

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.6 +Cb
Derived by	Lepper et al., 2007
Link	http://a0768b4a8a31e106d8b0-50dc802554eb38a24458b98ff72d550b.r19.cf3.rackcdn.com/scho0407blvu-e-e.pdf

Background information - PNEC

Method	Assessment factor approach The 'added risk' approach is considered appropriate, as arsenic is a naturally occurring substance which organisms will have been exposed to over an evolutionary timescale
Assessment factor applied (if relevant)	10
Lowest Effect concentration or HC5 value (µg/L)	Chronic EC ₁₀ = 6
Species	<i>Strongylocentrosus purpuratus</i>

Marine / Fresh water	Marine
Toxic Mode of Action	Arsenic
Master reference	Garman et al., 1997
Alternative PNEC values/sources available (µg/L)	0.6+Cb (ICPR, 2009)
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

ECHA (2008). Guidance on information requirements and chemical safety assessment. Chapter R.11: PBT Assessment.

http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

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ICPR, 2009. Afleiding van milieukwaliteitsnormen voor Rijnrelevante stoffen [Determination of environmental quality standards for Rhine relevant substances. International Commission for the Protection of the Rhine. Report no. 164] (in Dutch/German/French).

Lepper P, Sorokin N, Maycock D, Crane M, Atkinson C, Hope S-J and Comber S (2007). Proposed EQS for Water Framework Directive

Annex VIII substances: arsenic (total dissolved). Science Report: SC040038/SR3.

<http://a0768b4a8a31e106d8b050dc802554eb38a24458b98ff72d550b.r19.cf3.rackcdn.com/scho0407blvu-e-e.pdf>

7.7.5 Cadmium

Chemical identity

Chemical name (IUPAC)	Cadmium
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7440-43-9
EC number	231-152-8
Molecular formula	Cd
Molecular structure	Cd
Molecular weight (g.mol ⁻¹)	112.41

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.2+Cb
Derived by	EC, 2013 EC, 2005 Cadmium EQS fact sheet
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:P DF https://circabc.europa.eu/sd/d/42a9cfc4-6f5e-41bf-8db2-d5681be56e01/06_Cadmium_EQSdatasheet_310705.pdf

Background information - PNEC

Method	Species sensitivity distribution combined with assessment factor
Assessment factor applied (if relevant)	2
Lowest Effect concentration or HC5 value (µg/L)	HC5 = 0.42
Species	<i>Not relevant</i>

Marine / Fresh water	Marine
Toxic Mode of Action	Cadmium
Master reference	EC (2005)
Alternative PNEC values/sources available (µg/L)	-
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority substance (Yes or No)	Yes. Included in: - Annex I EQS Dir. 2013 (EC, 2013). Substance #6 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	Yes. - Annex I EQS Dir. 2013 (EC, 2013). Substance #6

Bibliography, sources and supportive information:

EC (2005). Environmental Quality Standard fact sheet for cadmium and its compounds.

https://circabc.europa.eu/sd/d/42a9cfc4-6f5e-41bf-8db2-d5681be56e01/06_Cadmium_EQSdatasheet_310705.pdf

EC(2013). DIRECTIVE 2013/39/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 12 August 2013, amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy . <http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF>

EC (2013). DIRECTIVE 2013/39/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 12 August 2013, amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy .

<http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF>

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http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

OSPAR (2011). OSPAR List of Chemicals for Priority Action (revised 2011).

http://www.ospar.org/content/content.asp?menu=00120000000050_000000_000000

7.7.6 Chromium

Chemical identity

Chemical name (IUPAC)	Chromium
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7440-47-3
EC number	231-157-5
Molecular formula	Cr
Molecular structure	Cr
Molecular weight (g.mol ⁻¹)	51.9961

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.6+Cb
Derived by	UKTAG , 2007
Link	http://www.wfduk.org/sites/default/files/Media/chromium.pdf

Background information - PNEC

Method	Assessment Factor Approach A total risk approach is adopted as almost all hexavalent chromium in the environment is of anthropogenic origin and natural background levels are negligible
Assessment factor applied (if relevant)	10
Lowest Effect concentration or HC5 value (µg/L)	Chronic NOEC=6
Species	<i>Nereis arenaceodentata</i>

Marine / Fresh water	Marine
Toxic Mode of Action	Chromium
Master reference	Oshida et al., 1976
Alternative PNEC values/sources available (µg/L)	0.6+Cb (both III+VI chromium) (ICPR, 2009)
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

ECHA (2008). Guidance on information requirements and chemical safety assessment. Chapter R.11: PBT Assessment. http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

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Maycock D, Sorokin N, Atkinson C, Rule K and Crane M, (2007). Proposed EQS for Water Framework Directive Annex VIII substances: chromium(VI) and chromium(III) (dissolved) UK Environment Agency, Science Report: SC040038/SR5, SNIFFER Report: WFD52(v). <http://www.wfduk.org/sites/default/files/Media/chromium.pdf>

Oshida P S, Mearns A J, Reish D J and Word C S (1976). The effects of hexavalent and trivalent chromium on Neanthes arenaceodentata (Polychaeta annelida). Project No. TM225. El Segundo, CA: Southern California Coastal Water Research.

7.7.7 Copper

Chemical identity

Chemical name (IUPAC)	Copper
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7440-50-8
EC number	231-159-6
Molecular formula	Cu
Molecular structure	Cu
Molecular weight (g.mol⁻¹)	63.5

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	2.6
Derived by	EU RAR (2008)
Link	http://echa.europa.eu/documents/10162/13630/vrar_effects_part_4_en.rtf

Background information - PNEC

Method	Species sensitivity distribution approach with additional assessment factor
Assessment factor applied (if relevant)	2
Lowest Effect concentration or HC5 value (µg/L)	HC5=5.2
Species	<i>Not relevant</i>

Marine / Fresh water	Marine
Toxic Mode of Action	Copper
Master reference	Van Sprang et al., 2008
Alternative PNEC values available (µg/L)	5 (UK, 2008)
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

ECHA (2008). Guidance on information requirements and chemical safety assessment. Chapter R.11: PBT Assessment.
http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

EU RAR (2008). European Union Risk Assessment Report. Voluntary risk assessment of copper, copper II sulphate pentahydrate, copper(I)oxide, copper(II)oxide, dicopper chloride trihydroxide.

UK (2008). UK Technical Advisory Group on the WFD. Proposals for environmental quality standards for annex VIII substances.

Van Sprang, P., M. Vangheluwe, A. Van Hyfte, D. Heijerick, M. Vandenbroele, F. Verdonck (ARCADIS – EURAS, Belgium) and Kevin Long, (2008). (REGCS), in co-operation with Katrien Delbeke (ECI), Bob Dwyer (ICA) and Bill Adams (Rio Tinto). Chapter 3.2-environmental effects- marine effects. In: EU RAR (2008): European Union Risk Assessment Report. Voluntary risk assessment of copper, copper II sulphate pentahydrate, copper(I)oxide, copper(II)oxide, dicopper chloride trihydroxide. Report available at ECHA website. Accessed on June 7th 2012 at:
http://echa.europa.eu/documents/10162/13630/vrar_effects_part_4_en.rtf.

7.7.8 Nickel

Chemical identity

Chemical name (IUPAC)	Nickel
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7440-02-0
EC number	231-111-4
Molecular formula	Ni
Molecular structure	Ni
Molecular weight (g.mol ⁻¹)	58.6934

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	8.6 +Cb
Derived by	EC, 2013 EC, 2011. Nickel and its compounds EQS fact sheet/dossier
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/1e2ae66f-25dd-4fd7-828d-9fd5cf91f466/Nickel%20EQS%20dossier%202011.pdf

Background information - PNEC

Method	<p>Species sensitivity distribution combined with assessment factor</p> <p>The 'added risk' approach is considered appropriate, as nickel is a naturally occurring substance which organisms will have been exposed to over an evolutionary timescale. However, the concentrations of nickel in marine waters are dependent on natural and anthropogenic conditions: it is almost impossible to determine experimentally a 'natural' background concentration in Europe. Due to geochemical differences, the ambient background concentrations will differ in Europe. In addition, since the concentrations that are measured in the environment are the sum of an anthropogenic and a 'natural' source, one cannot simply distinguish the 'natural' part from the anthropogenic part. Hence, background concentrations are not measured, but estimated or determined with other</p>
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	methods
Assessment factor applied (if relevant)	2
Lowest Effect concentration or HC5 value (µg/L)	HC ₅ = 17.2
Species	Not relevant
Marine / Fresh water	Marine
Toxic Mode of Action	Nickel
Master reference	EC, 2011. Nickel and its compounds, Nickel EQS dossier 2011
Alternative PNEC values/sources available (µg/L)	No
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority substance (Yes or No)	Yes. - Annex I EQS Dir. 2013 (EC, 2013). Substance #23
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

EC (2011). Nickel and its compounds. EQS dossier prepared by the Sub-Group on Review of the Priority Substances List (under WorkingGroup E of the Common Implementation Strategy for the Water Framework Directive).

<https://circabc.europa.eu/sd/d/1e2ae66f-25dd-4fd7-828d-9fd5cf91f466/Nickel%20EQS%20dossier%202011.pdf>

EC (2013). DIRECTIVE 2013/39/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 12 August 2013, amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy .

<http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF>

ECHA (2008). Guidance on information requirements and chemical safety assessment. Chapter R.11: PBT Assessment.

http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

7.7.9 Mercury

Chemical identity

Chemical name (IUPAC)	Mercury
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7439-97-6
EC number	231-106-7
Molecular formula	Hg
Molecular structure	Hg
Molecular weight (g.mol⁻¹)	200.6

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.05+C _b (background concentration) ¹
Derived by	EC, 2013 EC, 2005. Mercury and its compounds EQS fact sheet/dossier
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/ff8e163c-71f6-4fc0-98ef-875a20add4c8/21_Mercury_EQSdatasheet_150105.pdf

¹For Priority Substances under the WFD with significant bioaccumulation potential or human health effects from consumption of fishery products (e.g. for some PAHs), the PNEC_{water} is derived from food standards applying bioconcentration factors. For mercury, which has bioaccumulation potential, back calculation from food standards is not possible because bioconcentration factors are highly variable. Thus, the 2012 revision of the WFD EQS does not include a standard for mercury in other surface waters. Mercury was included in the WFD EQS 2008 for other surface waters at 0.05 µg/l, based on aquatic toxicity. It is proposed to use this value as a PNEC for mercury. Standards for biota are available and can be used directly to compare with measured biota concentrations, therewith taking bioaccumulation into account. In WFD (2008) the EC notes: "If Member States do not apply EQS for biota they shall introduce stricter EQS for water in order to achieve the same level of protection as the EQS for biota set out in Article 3(2) of this Directive. They shall notify the Commission and other Member States, through the Committee referred to in Article 21 of Directive 2000/60/EC, of the reasons and basis for using this approach, the alternative EQS for water established, including the data and the methodology by which the alternative EQS were derived, and the categories of surface water to which they would apply." Since the PNEC does not account for bioaccumulation/secondary poisoning, this PNEC is not protective for (marine) mammals and birds.

Background information - PNEC

Method	Species sensitivity distribution approach with additional assessment factor
Assessment factor applied (if relevant)	3
Lowest Effect concentration or HC5 value (µg/L)	HC5= 0.142
Species	<i>Not relevant</i>
Marine / Fresh water	Freshwater and marine
Toxic Mode of Action	Multiple site of action
Master reference	EC (2005), referring to Slooff et al. (1995)
Alternative PNEC values/sources available (µg/L)	-
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority substance (Yes or No)	Yes. Included in: - Annex I EQS Dir. 2013 (EC, 2013). Substance #21 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	Yes. Included in Annex I EQS Dir. 2013 (EC, 2013). Substance #21

Bibliography, sources and supportive information:

EC (2005): Common Implementation Strategy for the Water Framework Directive. Environmental Quality Standards (EQS). Substance Data Sheet. Priority Substance No. 21. Mercury and its Compounds. CAS-No. 7439-97-6. Final version. Brussels, 15 January 2005. Available at: https://circabc.europa.eu/sd/d/ff8e163c-71f6-4fc0-98ef-875a20add4c8/21_Mercury_EQSdatasheet_150105.pdf

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ECHA (2008): Guidance on information requirements and chemical safety assessment. Chapter R.11: PBT Assessment.
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OSPAR (2011). OSPAR List of Chemicals for Priority Action (revised 2011).
http://www.ospar.org/content/content.asp?menu=00120000000050_000000_000000

Slooff W., Van Beelen P., Annema J.A. & Janus J.A. (1995): Integrated Criteria Document Mercury. RIVM report 601014008.

7.7.10 Lead

Chemical identity

Chemical name (IUPAC)	Lead
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7439-92-1
EC number	231-100-4
Molecular formula	Pb
Molecular structure	Pb
Molecular weight (g.mol⁻¹)	207.2

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	1.3
Derived by	EC, 2013 EC, 2011. Lead and its compounds. EQS dossier.
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/be12c5a9-19b2-40eb-87ce-f62eb3b43b39/Lead%20and%20its%20compounds%20EQS%20dossier%202011.pdf

Background information - PNEC

Method	<p>Species sensitivity distribution approach with additional assessment factor</p> <p>The 'added risk' approach is considered appropriate, as lead is a naturally occurring substance which organisms will have been exposed to over an evolutionary timescale. The concentrations of lead in marine waters are variable and depend on both geogenic and anthropogenic sources. Due to these varying exposure conditions, the ambient background concentrations will differ in Europe. As the concentrations measured in the environment are inevitably the sum of both an anthropogenic and a 'natural' component, it is not possible to differentiate easily between the "natural" and the anthropogenic part. Therefore, background concentrations are not measured, but estimated or determined with other methods</p>
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Assessment factor applied (if relevant)	3
Lowest Effect concentration or HC5 value (µg/L)	HC5 = 3.79
Species	<i>Not relevant</i>
Marine / Fresh water	Marine and freshwater
Toxic Mode of Action	Multiple site of action
Master reference	EC, 2011
Alternative PNEC values/sources available (µg/L)	-
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority substance (Yes or No)	Yes. Included in: - Annex I EQS Dir. 2013 (EC, 2013). Substance #20 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supportive information:

EC (2011). Lead and its compounds. EQS dossier prepared by the Sub-Group on Review of the Priority Substances List (under Working Group E of the Common Implementation Strategy for the Water Framework Directive).

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http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

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SCHER (2011). SCHER (Scientific Committee on Health and Environmental Risks), Opinion on the environmental quality standards – lead, 25 May 2011.

http://ec.europa.eu/health/scientific_committees/environmental_risks/docs/scher_o_136.pdf

7.7.11 Zinc

Chemical identity

Chemical name (IUPAC)	Zinc
Chemical class (when available/relevant)	Metals
Produced water substance group	Metals
CAS number	7440-66-6
EC number	231-175-3
Molecular formula	Zn
Molecular structure	Zn
Molecular weight (g.mol⁻¹)	65.4

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	3.4+Cb (background concentration)
Derived by	UKTAG, 2012
Link	http://www.wfduk.org/sites/default/files/Media/Zinc%20-%20UKTAG.pdf

Background information - PNEC

Method	Species sensitivity distribution approach with additional assessment factor
Assessment factor applied (if relevant)	2
Lowest Effect concentration or HC5 value (µg/L)	HC5=6.76
Species	Not relevant

Marine / Fresh water	Marine
Toxic Mode of Action	Multiple site of action
Master reference	UKTAG (2012)
Alternative PNEC values/sources available (µg/L)	1) 7.8 (JRC, 2010) 2) 3+Cb (ICPR, 2009) 3) 40 (UK, 2008)
PBT substances (Yes or No)	No, the PBT and vPvB criteria of Annex XIII to the Regulation do not apply to inorganic substances but shall apply to organo-metals (ECHA, 2008)
Priority hazardous substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supportive information:

ECHA (2008). Guidance on information requirements and chemical safety assessment. Chapter R.11: PBT Assessment.
http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

ICPR (2009). Afleiding van milieukwaliteitsnormen voor Rijnrelevante stoffen [Determination of environmental quality standards for Rhine-relevant substances. International Commission for the Protection of the Rhine. Report no. 164] (in Dutch/German/French)

JRC (2010) EU Risk Assessment Report Zinc.
<http://publications.jrc.ec.europa.eu/repository/bitstream/111111111/15064/1/lbna24587enn.pdf>

SCHER (2012). SCHER (Scientific Committee on Health and Environmental Risks), Opinion on draft environmental quality standards under the Water Framework Directive – Zinc, 22 March 2012.
http://ec.europa.eu/health/scientific_committees/environmental_risks/docs/scher_o_157.pdf

UK (2008). UK Technical Advisory Group on the WFD. Proposals for environmental quality standards for annex VIII substances.

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<http://www.wfduk.org/sites/default/files/Media/Zinc%20-%20UKTAG.pdf>

7.8 Alkyl phenols

7.8.1 Phenol (incl. C0-C3 alkyl phenols representative)

Chemical identity

Common Name	Phenol
Chemical name (IUPAC)	Phenol
Chemical class (when available/relevant)	Alkyl phenols
Produced water substance group	C0-C3 alkyl phenols
CAS number	108-95-2
EC number	203-632-7
Molecular formula	C ₆ H ₅ OH
Molecular structure	
Molecular weight (g.mol ⁻¹)	94.111

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	7.7
Derived by	EU RAR 2006
Link	http://esis.jrc.ec.europa.eu/doc/risk_assessment/REPORT/phenolreport060.pdf

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	10
Lowest Effect concentration value or HC5 value (µg/L)	Chronic NOEC = 77
Species	<i>Cirrhina mrigala</i>

Marine / Fresh water	Both freshwater and marine, although NOEC used is from a freshwater species. Study concluded that it seems unlikely that long-term tests with representatives of these additional taxonomic groups would result in lower chronic toxicity data than that obtained for fish, so AF of 10 rather than 100 is used.
Toxic Mode of Action	Indirect toxicity, polar narcosis
Master reference	Verma et al., 1984
Alternative PNEC values/sources available (µg/L)	7.7 (Environment Agency UK, 2008)
PBT substances (Yes or No)	No
Priority Substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Environment Agency UK (2008). UK Technical Advisory Group on the Water Framework Directive. Proposals for environmental quality standards for annex viii substances.

http://www.wfduk.org/sites/default/files/Media/Environmental%20standards/Specific%20pollutants%20proposals_Final_010608.pdf

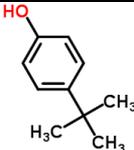
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http://esis.jrc.ec.europa.eu/doc/risk_assessment/REPORT/phenolreport060.pdf

Verma SR, Tonk IP, Gupta AK and Saxena M (1984). Evaluation of an application factor for determining the safe concentration of agricultural and industrial chemicals; Water Res. 18, 111-115.

7.8.2 Butylphenol (C4 alkyl phenols representative)

Chemical identity

Common Name	4-tert-butylphenol
Chemical name (IUPAC)	4-tert-butylphenol
Chemical class (when available/relevant)	Alkyl phenols
Produced water substance group	C4 alkyl phenols
CAS number	98-54-4
EC number	202-679-0
Molecular formula	C ₁₀ H ₁₃ OH
Molecular structure	
Molecular weight (g.mol ⁻¹)	150.217

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.64
Derived by	EU RAR, 2008
Link	http://esis.jrc.ec.europa.eu/doc/risk_assessment/REPORT/4tertbutylphenolreport404.pdf

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	500
Lowest Effect concentration or HC5 value (µg/L)	Chronic NOEC = 320
Species	<i>Selenastrum capricornutum</i>

Marine / Fresh water	Freshwater
Toxic Mode of Action	Polar narcosis, possible endocrine activity
Master reference	NIVA, 2001
Alternative PNEC values/sources available (µg/L)	-
PBT substances (Yes or No)	No
Priority Substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

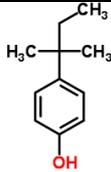
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7.8.3 Pentyl phenol (C5 alkyl phenols representative)

Chemical identity

Common Name	Pentylphenol
Chemical name (IUPAC)	4-tert-pentylphenol
Chemical class (when available/relevant)	Alkyl phenols
Produced water substance group	C5 alkyl phenols
CAS number	80-46-6
EC number	201-280-9
Molecular formula	C ₁₁ H ₁₅ OH
Molecular structure	
Molecular weight (g.mol ⁻¹)	164.244

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.2
Derived by	EA RAR, 2008
Link	http://publications.environment-agency.gov.uk/PDF/SCH00208BNQR-E-E.pdf

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	500
Lowest Effect concentration or HC5 value (µg/L)	Chronic NOEC 100
Species	<i>Oryzias latipes</i>

Marine / Fresh water	Freshwater
Toxic Mode of Action	Polar narcosis, reproductive effects
Master reference	Seki et al., 2003.
Alternative PNEC values/sources available (µg/L)	-
PBT substances (Yes or No)	No
Priority Substance (Yes or No)	No
Priority hazardous substance (Yes or No)	No

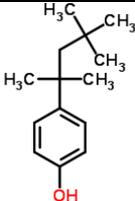
Bibliography, sources and supporting information:

Seki M, Yokota H, Matsubara H, Maeda M, Tadokoro H & Kobayashi K (2003). Fish full life-cycle testing for the weak estrogen 4-tert-pentylphenol on medaka (*Oryzias latipes*). *Environ Toxicol Chem*, 22, 1487–1496.

UK Environment Agency RAR (2008). 4-tert-pentylphenol (<http://publications.environment-agency.gov.uk/PDF/SCHO0208BNQR-E-E.pdf>).

7.8.4 Octylphenol (C6-C8 alkyl phenols representative)

Chemical identity

Common Name	4-tert-octylphenol
Chemical name (IUPAC)	1,1,3,3-tetramethylbutylphenol
Chemical class (when available/relevant)	Alkyl phenols
Produced water substance group	C6-C8 alkyl phenols
CAS number	140-66-9
EC number	205-426-9
Molecular formula	C ₁₄ H ₂₁ OH
Molecular structure	
Molecular weight (g.mol ⁻¹)	206.323

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.01
Derived by	EC, 2013. EC, 2005. Octylphenol EQS fact sheet/dossier
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/38053232-85b7-4668-895b-22bf91aca0e3/25_Octylphenols_EQSdatasheet_310705.pdf

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	500
Lowest Effect concentration or HC5 value (µg/L)	Chronic NOEC = 6.1
Species	<i>Oncorhynchus mykiss</i>

Marine / Fresh water	Freshwater
Toxic Mode of Action	Polar narcosis, reproductive effects
Master reference	Analytical Bio-Chemistry Laboratories , 1986
Alternative PNEC values/sources available (µg/L)	0.0122 (UK EA RAR, 2005)
PBT substances (Yes or No)	No
Priority Substance (Yes or No)	Yes. Included in: - Annex I EQS Dir. 2013 (EC, 2013). Substance #25 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	No

Bibliography, sources and supporting information:

Analytical Bio-Chemistry Laboratories (1986). Inc.:Early life stage toxicity of para-tert.-octylphenol to rainbow trout (*Salmo gairdneri*) in a flow-through system, unpublished test report No. 34452, December 1986, within; IUCLID 1996 datasheet: 4(1,1,3,3-tetramethyl)phenol. International uniform chemical information database. http://esis.jrc.ec.europa.eu/doc/IUCLID/data_sheets/140669.pdf.

UK EA RAR (2005): Environmental Risk Evaluation Report: 4-tert-octylphenol. ISBN: 1 84432 410 9. <http://publications.environment-agency.gov.uk/PDF/SCHO0405BIYZ-E-E.pdf>

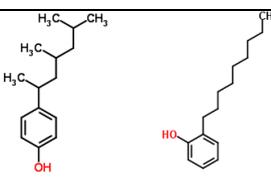
EC (2005). Octylphenol EQS fact sheet. https://circabc.europa.eu/sd/d/38053232-85b7-4668-895b-22bf91aca0e3/25_Octylphenols_EQSdatasheet_310705.pdf

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7.8.5 Nonylphenol (C9 alkyl phenols representative)

Chemical identity

Common name	Nonylphenol
Chemical name (IUPAC)	Nonylphenol (many isomers, so precise name cannot be specified)
Chemical class (when available/relevant)	Alkyl phenols
Produced water substance group	C9 alkyl phenols
CAS number	2515-52-3
EC number	246-672-0
Molecular formula	C ₁₅ H ₂₃ OH
Molecular structure	 <p>CAS Number covers a range of isomers</p>
Molecular weight (g.mol ⁻¹)	220.350

Predicted No Effect Concentration (PNEC)

PNEC value (µg/L)	0.3
Derived by	EC, 2013 EC, 2005. Nonylphenol EQS fact sheet/dossier
Links	http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF https://circabc.europa.eu/sd/d/af1b09f2-ff9a-46f6-ba2d-d4bc2adfee0/24_Nonylphenol_EQSdatasheet_310705.pdf

Background information - PNEC

Method	Assessment factor approach
Assessment factor applied (if relevant)	10
Lowest Effect Concentration or HC5 value (µg/L)	Chronic EC10=3.3
Species	<i>Scenedesmus subspicatus</i>

Marine / Fresh water	Fresh (marine also available, results show similar sensitivity)
Toxic Mode of Action	Polar narcosis and reproductive effects
Master reference	Kopf W. (1997)
Alternative PNEC values/sources available (µg/L)	0.33 (EU RAR, 2002)
PBT substances (Yes or No)	No
Priority Substance (Yes or No)	Yes. Included in: - Annex I EQS Dir. 2013 (EC, 2013). Substance #24 - OSPAR List of chemicals for Priority Action, 2011
Priority hazardous substance (Yes or No)	Yes, included in Annex I EQS Dir. 2013 (EC, 2013). Substance #24

Bibliography, sources and supporting information:

EU RAR (2002). EU risk assessment report 4-nonylphenol http://esis.jrc.ec.europa.eu/doc/risk_assessment/REPORT/4-nonylphenol_nonylphenolreport017.pdf

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9 Appendix 1

9.1 Environmental Quality Standards derived under the Water Framework Directive

The Water Framework Directive (WFD) established a framework for protection of all surface waters and ground waters, with an obligation to prevent any deterioration of status, and to achieve good status, as a rule by 2015. The overall good status is reached for a certain water body if both ecological and chemical status is classified as good (EC, 2000). Environmental Quality Standards (EQSs) are defined as “the concentration of a particular pollutant or group of pollutants in water, sediment or biota which should not be exceeded in order to protect human health and the environment” (WFD article 2 (35)). EQSs are tools used for assessing the chemical status of water bodies that should protect freshwater and marine ecosystems from possible adverse effects of chemicals as well as human health via drinking water or ingestion of food originating from aquatic environments.

EQSs are established at EU level by the EQS Directive (EC, 2013) for 45 priority substances and 8 other pollutants within the WFD (listed in Part A of Annex I of EQS Directive). The EQS Directive (EC, 2013) has established the maximum acceptable concentration (MAC-QS) and/or annual average concentration (AA-EQS) for these substances, and if met, allows the chemical status of the water body to be described as ‘good’. EQS values have been established both for inland (freshwater) waters and coastal (marine) waters.

EQSs are therefore key tools in assessing and classifying chemical status and can therefore affect the overall classification of a water body under the WFD. In addition, EQSs will be used to set discharge permits to water bodies, so that chemical emissions do not lead to EQS exceedance within the receiving water.

EQSs for the substances identified by the EU as Priority Substances (PSs) and Priority Hazardous Substances (PHSs) are derived at a European level and apply to all Member States. The Guidance Document No. 27 “Technical Guidance for Deriving Environmental Quality Standards” (EC, 2011) was used to support derivation of EQSs for the priority substances (new and existing) presenting significant risk to or via the aquatic environment. As far as possible, the technical guidance for EQSs is consistent with the guidance for effects assessments performed for chemical risk assessment under REACH (ECHA, 2008). The Predicted No Effect Concentrations (PNECs) derived from this process are normally adopted as EQSs because the assessments and associated data will have undergone thorough peer review. Or at least the data which the PNECs are based on have been used as basis for establishing EQS under the WFD. However, it is important to highlight some conceptual differences between EQS derivation and the estimation of a PNEC from chemical risk assessment. This will be discussed in chapter 9.3.

The list of priority substances (2013/39/EU) is required reviewed under the WFD at least every four years among others including a review of the existing priority substances and EQSs for surface water, sediment and biota. The background information on the setting of the Environmental Quality Standard is available through “substance data sheets”, derived for each substance. The substance

data sheets are available by CIRCA (Communication & Information Resource Centre Administrator) on the internet (<http://circa.europa.eu/>) or via the WFD website from the European Union. http://ec.europa.eu/environment/water/water-dangersub/lib_pri_substances.htm.

9.1.1 Derivation of EQS values

The goal of EQS setting is to protect both environmental compartments, in this case marine ecosystems, from possible adverse effects of chemicals, as well as human health via ingestion of food originating from the marine environment. Therefore several types of receptors are considered, namely the pelagic and benthic communities in marine ecosystems, the top predators of these ecosystems and human health. Not all receptors need to be considered for every substance. This depends on the environmental fate and behavior of the substance. For instance, if a substance does not have the potential to bioaccumulate, there is no risk of secondary poisoning and so a biota standard is not needed. Where several assessments are performed, the lowest (most stringent) of the thresholds is selected as an “overall” EQS.

Several steps are involved in the process of deriving an EQS for a certain chemical:

1. First an assessment is made of the receptors and compartments at risk
2. Next, data concerning the physicochemical properties and ecotoxicity of a substance are collated and used as input to a standard-setting process.
3. The toxicity data from laboratory (or mesocosm and field studies) are extrapolated to threshold concentrations using deterministic or probabilistic methods. The deterministic approach takes the lowest credible toxicity datum and applies an AF (Assessment Factor) between 1 and 10.000 to extrapolate to an E QS, the AF allowing for the uncertainties in the available data. Probabilistic methods involve Species Sensitivity Distribution (SSD) modeling in which all reliable toxicity (usually NOEC) data are ranked and a model is fitted. From this, the concentration protecting a certain proportion of species is estimated, mostly 95%, named the HC5.

Next a threshold concentration is selected that applies to the water column, sediment and biota. Key assumptions and uncertainties are addressed, and an overall EQS is selected.

Detailed information about the derivation of EQS values can be found in the Technical Guidance for Deriving Environmental Quality Standards (EC, 2011).

9.2 PNECs derived under the Risk Assessments under Existing Substances Regulations (ESR)

For some industrial chemicals, detailed evaluations and risk assessments already have been carried out in accordance with Council Regulation (EEC) 793/931 on the evaluation and control of the risks of “existing” substances (EC, 2003), and published in Risk Assessment Reports. As noted, the effects assessments conducted for chemical and pesticide risk assessments share many of the same principles and practices as those used to estimate an EQS and provide guidance on the use of such

assessments as a basis for deriving EQSs. As mentioned, the PNECs derived from this process are based on toxicity data, have undergone thorough peer review and are published on the internet by the European Commission

The recently published EU-RARs are available from the ESIS (European chemical Substances Information System) database on the internet (<http://esis.jrc.ec.europa.eu/>).

9.3 Differences between WFD and REACH

EQS are tools used for the assessment of the chemical status for example water bodies, whereas the PNEC is part of the risk assessment of a single chemical. Some conceptual differences exist between EQS derivation and estimation of a PNEC:

- Within the derivation of an EQS, all receptors and routes (water, sediment, top predators, and human health) are taken into account. This is a feature that does not normally apply to derivation of a PNEC value.
- Whereas there are opportunities to refine a PNEC in the light of new data, mostly provided by the manufacturer(s) of the chemical this is often not the case in EQS derivation.
- An exceedance of the EQS will not normally trigger a refinement of the standard.
- An underlying requirement of the WFD is to protect the most sensitive waters in Europe. For example for metals, there is therefore a requirement to protect a higher portion of water bodies than for PNECs estimated as part of a risk assessment.
- Where SSD modeling has been used for extrapolation, there may be a difference in the size of the assessment factor applied to the HC5 to account for uncertainty.

In spite of these differences, the process of deriving both is the same. As far as possible, the technical guidance for EQS derivation under the WFD is consistent with the guidance for effects assessments performed for chemical risk assessment under REACH. Therefore where the term EQS is used, it could also be substituted for PNEC.