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Soil quality — Assessment of impact from soil contaminated with petroleum hydrocarbons

Qualité du sol — Évaluation de l'impact du sol contaminé avec des hydrocarbures pétroliers

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation on the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see the following URL: www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 190, *Soil quality*, Subcommittee SC 7, *Soil and site assessment.*

This second edition cancels and replaces the first edition, which has been technically revised.

Introduction

Petroleum hydrocarbons (PHCs) are common environmental contaminants. They are components of crude oil and products derived from it and are consequently found on a variety of sites including refineries, sites where they are used as feedstock (e.g. for manufacture of plastics), manufactured gas production sites, sites where hydrocarbons are used as fuel or lubricants and retail service stations. They may also be present as a result of spills and leaks during transportation or related to vehicle accidents.

Petroleum hydrocarbons can present unacceptable risks to the health and safety of humans, ecological systems, surface water, groundwater resources and to structures and building materials. Measuring the total concentration of petroleum hydrocarbons (TPH) in soil (and pore water and pore gas) does not give a useful basis for the evaluation of the potential risks to man and the environment. The variety of physical-chemical properties, and thus differences in the migration and fate of individual compounds, and the toxicity and carcinogenicity of different fractions and compounds in oil products, need to be taken into account in human health and environmental risk assessments.

Only a limited number of individual compounds can be routinely identified and quantified. It is, consequently, important to adopt methods of analysis that provide information about the amount of different hydrocarbon fractions present, preferably distinguishing between aliphatic and aromatic fractions, and the concentrations of single compounds of particular concern with respect to the potential health and environmental risks that they pose.

Although most petroleum hydrocarbons found in soil are of anthropogenic nature, there are some natural sources of these materials and other organic substances (e.g. peat and coal). The analytical methods historically used for the measurement of total petroleum hydrocarbons (TPH) tend to measure natural materials as TPH. This issue will not be dealt with in this document, except to note that a method which is able to give a more precise determination of the petroleum hydrocarbons is less prone to giving results that can be misinterpreted and potentially lead to unnecessary or unsustainable remedial actions.

The purpose of this document is to give recommendations with respect to the choice of relevant fractions and individual compounds, and to give guidance on the appropriate use of the results. Decisions about which analytical methods to adopt are based primarily on the need to provide the right type and quality of data for use in risk assessments. This requires consideration of how the results of the analysis are most appropriately used in a risk assessment, e.g. how can the fractions be used in exposure models and assessments, and how sufficient it is to analyse soil or necessary to obtain related values in other media as well (pore water and pore gas).

There are five existing International Standards covering the analysis of the range of petroleum hydrocarbons of interest. ISO 16703, ISO 16558-1 and ISO/TS 16558-2 can be used to measure mineral oil (C10 to C40) and ISO 22155 or ISO 15009 to measure volatiles. However, methods need to be able to properly measure the fractions and compounds recommended for determination in this document. ISO/TC190 has thus developed standards for methods of analysis designed to be compatible with the recommendations provided in this document: ISO 16558-1, which describes a method for determination of aliphatic and aromatic fractions of volatile petroleum hydrocarbons, and ISO 16558-2, which describes a method for the determination of aliphatic and aromatic fractions of semi-volatile petroleum hydrocarbons.

Soil quality — Assessment of impact from soil contaminated with petroleum hydrocarbons

1 Scope

This document gives guidelines with regard to the choice of fractions and individual compounds when carrying out analysis for petroleum hydrocarbons in soils, soil materials and related materials, including sediments, for the purpose of assessing risks to human health, the environment and other possible receptors. Since many products based on petroleum hydrocarbons often contain substances that are not hydrocarbons, the recommendations also encompass such compounds where relevant.

This document also includes relevant background information on which the recommendations are based together with guidance on the use of the fractions recommended in the assessment of risk.

This document does not set criteria or guidelines for use as assessment criteria, since this is typically a national or regional regulatory issue. This document also does not include recommendations as to the specific model for the exposure assessment or the specific parameter values to be used; with respect to guidance on this matter, reference is made to ISO 15800.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 11074, *Soil quality — Vocabulary*

ISO 15800, *Soil quality — Characterization of soil with respect to human exposure*

ISO 16558-1, *Soil quality — Risk-based petroleum hydrocarbons — Part 1: Determination of aliphatic and aromatic fractions of volatile petroleum hydrocarbons using gas chromatography (static headspace method)*

ISO 16558-2, *Soil quality — Risk-based petroleum hydrocarbons — Part 2: Determination of aliphatic and aromatic fractions of semi-volatile petroleum hydrocarbons using gas chromatography with flame ionization detection (GC/FID)*

ISO 18400-105, *Soil quality — Sampling — Part 105: Packaging, transport, storage and preservation of samples*

ISO 18512, *Soil quality — Guidance on long and short term storage of soil samples*

ISO 25177, *Soil quality — Field soil description*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 11074, ISO 15800 and ISO 25177 and the following apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— IEC Electropedia: available at http://www.electropedia.org/

— ISO Online browsing platform: available at http://www.iso.org/obp

3.1
aliphatic hydrocarbon
acyclic or cyclic, saturated or unsaturated carbon compound, excluding aromatic compounds

3.2
aromatic hydrocarbon
hydrocarbon of which the molecular structure incorporates one or more planar sets of six carbon atoms that are connected by delocalized electrons, numbering the same as if they consisted of alternating single and double covalent bonds

3.3
boiling point
BP
point at which the vapour pressure of a liquid equals the external pressure acting on the surface of a liquid

Note 1 to entry: It is expressed in degrees Celsius.

3.4
carcinogen
substance that causes the development of malignant cells in animals or humans

3.5
compliance point
location (e.g. soil or groundwater) where the assessment criteria shall be measured and shall not be exceeded

3.6
equivalent carbon number
empirically determined parameter related to the *boiling point* (3.3) of a chemical normalized to the boiling point of the *n*-alkanes or its retention time in a boiling point gas chromatographic (GC) column

3.7
fraction
group of aromatic and/or aliphatic compounds with leaching and volatilization factors that differ by approximately one order of magnitude

3.8
gas chromatography
analytical method that is used to separate and determine the components of complex mixtures based on partitioning between a gas phase and stationary phase

3.9
hydrocarbon
compound of hydrogen and carbon which are the principal constituents of crude oil, refined petroleum products and products derived from the carbonization of coal (at high or low temperature)

3.10
indicator compound
compound chosen to describe properties, primarily toxicity, of a petroleum mixture or *fraction* (3.7)

Note 1 to entry: This method is often used to assess carcinogenic compounds.

3.11
NSO compound
organic compound that contains nitrogen, sulphur and oxygen

Note 1 to entry: NSO compounds occur in organic matter and crude oil. Asphaltenes are examples of NSO compound. NSO compounds can be separated from crude oil by polar solvents such as methanol.

3.12
partitioning
extent to which a compound of a *hydrocarbon* (3.9) mixture separates into different media (or phases) based on its chemical and physical properties and the size and properties of the media in the specific situation

3.13
petroleum hydrocarbon
organic compound comprised of carbon and hydrogen atoms arranged in varying structural configurations which make up the principal constituents of crude oil and petroleum products

Note 1 to entry: Mineral oil is a colloquial term for petroleum hydrocarbons or petroleum products.

3.14
polycyclic aromatic hydrocarbon
PAH
compound whose molecules contain two or more simple aromatic rings fused together by sharing two neighbouring carbon atoms

Note 1 to entry: Naphthalene, anthracene, phenanthrene and benzo(a)pyrene.

3.15
surrogate compound
(representative) compound with toxicological and/or properties indicative of a hydrocarbon fraction, which can therefore be used to represent the fraction in an exposure assessment

3.16
total petroleum hydrocarbon
method-defined parameter, depending on the analytical method used to measure it

4 Principle

A petroleum hydrocarbon product typically consists of a mixture of a very large number of individual compounds. When assessing exposure and risk related to a mixture of compounds, such as in a petroleum hydrocarbon product, evaluation has to be made with respect to the migration, fate and toxicity of the different compounds in the mixture and the toxicity of the mixture. During transport in the subsurface, the composition of a mixture may change due to different rates of dissolution, volatilization, retardation, biodegradation, etc. acting on different component compounds. As a result, the toxicity of the resulting mixture may vary with both time and distance from the source zone.

Assessing the potential exposure to a mixture consisting of a large number of compounds is not feasible, neither in relation to the measurement of the concentration of all the compounds, in relation to the evaluation of the resulting mixture (after migration and degradation) in the relevant media (such as in the groundwater or in the indoor air), nor with respect to the resulting toxicity. A method, where only a number of compounds or surrogate compounds are measured and evaluated, is therefore preferable.

On the other hand, it is necessary when choosing the relevant compounds and surrogate compounds (such as relevant fractions of the total oil product) to ensure that the resulting evaluation of either overall exposure or toxicity is a reasonable estimate of the exposure and toxicity related to the oil product as a whole. Furthermore, selection of surrogate compounds should ensure that, if risk-management action is necessary, the risk-management applied for the surrogate is also likely to mitigate the risks associated with other (unquantified) substances present in the mixture.

Studies on migration, fate and toxicity of petroleum hydrocarbons show substantial differences between the properties of individual compounds and fractions of aliphatic and aromatic hydrocarbons. Similar differences exist between hydrocarbon compounds with different carbon content. The choice of surrogate compounds for assessing exposure and toxicity of petroleum hydrocarbons should be based on fractions of the total hydrocarbon mix in a mineral oil product and on individual compounds and fractions with similar properties.

This document gives recommendations about the choice of relevant individual compounds and fractions as a basis for the assessment of risks to humans and the environment at relevant compliance points using established risk assessment models. It should be noted that, for the suggested combination of fractions and singular compounds, it is necessary that comparable analytical methods exist for the suggested fractions, etc. not only for soil but also for water, air and petroleum hydrocarbons present as non-aqueous phase liquids (NAPL) in order to verify exposure assessment calculations and the assumptions employed in the risk assessment model.

As mentioned in the introduction, the choice of fractions and indicator compounds should, apart from the above, be based on the performance characteristics of the possible analytical methods, and on the overall cost of the analysis in relation to the goal of the assessment to be carried out.

5 Relevant fractions and individual compounds

5.1 General

This clause summarizes the recommendations given with respect to relevant petroleum hydrocarbon fractions and individual compounds to measure and use in risk assessment, unless local or national regulations set other requirements. The recommendations are based on the arguments given in the following subclauses.

5.2 Fractions

Where a petroleum hydrocarbon fractionation approach is adopted, it is recommended that the fractions given in Table 1 should be used when measuring and assessing risk related to petroleum hydrocarbons. These fractions will ensure that the calculation of the exposure can be carried out using surrogate physico-chemical properties on the fractions that represent all compounds within the fraction reasonably well, and that toxicity of the compounds within the fractions will be reasonably similar, except for the specific compounds of significant toxicological potency that will have to be assessed also as individual compounds (see 5.3).

Surrogate physico-chemical properties can be set for each of the fractions suggested, either by using a single property for each fraction or by using a set of relevant indicator compounds representing the fraction by set percentages and then using their properties. The first method is the one utilised by Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG)[26]. The other method is used, for instance, in the Danish exposure assessment tool for contaminated soils, JAGG[15]. Some jurisdictions may have specific requirements regarding the properties to be used in risk assessments. If not, it is recommended to use the properties listed in Annex A.

Table 1 — Petroleum hydrocarbon fractions for use in risk assessment related to human health and the environment, based on Equivalent Carbon (EC) number

Aliphatic fractions	Aromatic fractions
>5 to 6	>5 to 7
>6 to 8	>7 to 8
>8 to 10	>8 to 10
>10 to 12	>10 to 12
>12 to 16	>12 to 16
>16 to 35	>16 to 21
>35 to 44	>21 to 35
	>35 to 44
>44 to 70	

NOTE 1 Dependent on the available knowledge concerning the contaminant situation on the site in question, not all fractions can be relevant on a specific site.

NOTE 2 In some countries, assessment criteria are set for some of the suggested fractions, but not all. The use of the auxiliary fractions can still be relevant as a basis for the evaluation of the potential risk at compliance points in other media, e.g. groundwater or indoor air.

5.3 Individual compounds

Since petroleum hydrocarbon mixtures may contain specific compounds with a toxicity that is substantially higher than the other compounds in the fraction it is part of, it is recommended to carry out separate exposure and toxicity assessments of these compounds, unless the initial desk study and conceptual model of the site in question shows that it is not relevant. Table 2 gives the recommended list of specific compounds to include.

Table 2 — Individual compounds to be included in assessments

Benzene	n-hexane
Benzo[a]pyrene	Toluene
Benz[a]anthracene	Ethylbenzene
Benzo[b]fluoranthene	Xylenes
Benzo[k]fluoranthene	Styrene
Benzo[ghi]perylene	Naphthalene
Chrysene	Methylnaphthalenes
Coronene	Anthracene
Dibenz[a,h]anthracene	Fluoranthene
Indeno[1,2,3-c,d]pyrene	Phenathrene
	Pyrene
NOTE The list is not comprehensive.	

NOTE Other PAHs are potentially of concern and can be included if found relevant at the specific site. Some of the listed compounds (e.g. PAH) are not present in certain petroleum hydrocarbon mixtures and can be excluded with appropriate justification.

Other compounds of this type include those containing nitrogen, oxygen and sulphur (NSO-compounds), which can also be found in petroleum hydrocarbon mixtures (e.g. benzo[b]thiophene, carbazole). Many products based on petroleum hydrocarbons also contain additives of different types with purposes specific to the products [e.g. methyl tert-butyl ether (MTBE), ethyl-tert-butylether (ETBE), tert-amyl methyl ether (TAME), ethanol, fatty acid methyl ether (FAME)]. These may have different environmental fate and characteristics, such as a higher solubility, a lower biodegradability or lower olfactory and taste detection thresholds. When choosing the individual compounds to include in an investigation of a specific site, these issues should be taken into account.

It is recommended that the NSO-compounds and additives given in Table 3 are considered, when deciding which compounds should be considered in the risk assessment. Not all compounds may be relevant at all sites or present in all hydrocarbon mixtures.

It should be noted that other compounds can be relevant at a specific site (e.g. lead additives and fuel dyes). Potentially, there are approximately 14 000 different NSO compounds in crude oil belonging to different heteroatomic classes, e.g. asphaltenes, carboxylic acids and oxygenates. The compounds suggested are typical of NSOs found at fuel and gasoline spill sites and similar.

In the risk assessments based on the fractions and individual compounds measured, the properties listed in Annex A should be used, unless local jurisdictions require otherwise. Since acceptance criteria and guideline values normally are regulated nationally or regionally, this document does not give recommendations with respect to such criteria/guidelines.

Table 3 — List of NSO-compounds and additives to be assessed if relevant

NSO-compounds
Benzo[b]thiophene
Dibenzofurane
Dibenzothiophene
Acridine
Carbazol
Aniline
Dimethyl disulphide
4-methyl aniline
4-methyl quinoline
Thiophene
Quinoline
Additives
Ethyl tert butyl ether (ETBE)
Methyl tert butyl ether (MTBE)
Di-isopropyl ether (DIPE)
Methanol
Ethanol
Butanol
Tert butyl alcohol (TBA)
Fatty acid methyl esters (FAME)
Tertiary amyl methyl ether (TAME)
Amino ethyl ethanolamine
Diethylene triamine (DETA)
Ethylene diamine
Tetraethylenepentamine (TEPA)
1,2-dibromoethane
1,2-dichloroethane

6 Petroleum hydrocarbons in soil

When talking about petroleum hydrocarbons, the difference between the term, petroleum hydrocarbons, as such, and the term, total petroleum hydrocarbons, should be noted. Petroleum hydrocarbons (PHC) typically refer to the hydrogen and carbon containing compounds that originate from crude oil, while total petroleum hydrocarbons (TPH) refer to the measurable amount of petroleum-based hydrocarbons in an environmental matrix and thus to the actual results obtained by sampling and chemical analysis.

TPH is thus a method-defined term. In other words, estimates of TPH concentrations vary depending on the analytical method used to measure them.

NOTE Historically, this has been a significant source of inconsistency, as laboratories have different interpretations of the term TPH. By defining PHC fractions for risk assessment, this document will improve consistency in reporting and PHC risk assessments.

Petroleum hydrocarbons are constituents of crude oil, which, on the other hand, is the basis for the production of a large number of processed hydrocarbons/products. Crude oil contains aliphatic and aromatic hydrocarbons plus NSO compounds, etc. Hydrocarbon products can either be aliphatic or aromatic hydrocarbons or a mixture of both plus the addition of other organic and inorganic compounds (e.g. naturally occurring NSO compounds, additives in fuels and motor oils, dyes etc.). Petroleum hydrocarbons can be grouped according to their structure as shown in Table 4.

Table 4 — Hydrocarbon structural relationship

Hydrocarbons					
Aliphatic hydrocarbons			**Aromatic hydrocarbons**		
Alkanes	**Alkenes**	**Alkynes**	**Mono-aromatics**	**Di-aromatics**	**Cyclo-aromatics**
Cyclo-alkanes					**Polycyclic aromatic hydrocarbons**

Petroleum hydrocarbons are typically found in soils due to spills, leakages and other forms of contamination with different types of mineral oil products, such as gasoline (petroleum), diesel, jet fuel (kerosene), fuel oil, lubricants and solvents. The complexity of the mixture of petroleum hydrocarbons found in soils arises in part from the complexity of the original crude oil itself (which again depends on the location of its origin). In order to satisfy specific needs related to the different commercial products derived from crude oil, the oil is processed, typically by fractionation through distillation and thereafter by a number of thermal and catalytic processes. The distillation fractions are conventionally described by the carbon number range of straight chain *n*-alkanes in the fraction, e.g. C_6 to C_{10}.

Examples of typical products based on petroleum hydrocarbons are given in Table 5 which also shows the carbon number ranges and boiling point ranges of some common petroleum products.

After their release to the environment, the petroleum hydrocarbons partition to different extents between a liquid oil phase (non-aqueous phase liquid) and the soil, water and air phase in the soil matrix. The partitioning is dependent on the physico-chemical properties of the compounds or groups of compounds. In addition, the composition of a petroleum hydrocarbon mix changes over time due to preferential volatilization or dissolution of certain components, or due to the effects of biodegradation, both in the original spill and in the different compartments of the soil matrix. The composition of specific oil contamination in soil will, apart from the properties of the hydrocarbons in the mixture, also depend on soil and water chemistry and degradation of the different compounds.

Suggested physico-chemical properties of different petroleum hydrocarbon compounds to be used in the assessment are given in Annex A It should be noted that some jurisdictions may have specific requirements regarding the properties to be used in risk assessments. Some properties are temperature dependent and it is therefore important that the values used are appropriate for the risk assessment that is to be carried out.

The toxicity to humans and the relevant ecology varies substantially between compounds and thus between different mineral oil products and different migrating streams (mixtures of compounds migrating along different transfer routes, e.g. through vaporisation or leaching). Different petroleum hydrocarbons will also exhibit variously both carcinogenic and direct toxic effects.

An illustration of the relative toxicity of specific petroleum hydrocarbon compounds is given by the list of suggested assessment criteria shown in Annex B. It should be noted that many jurisdictions have specific requirements or recommendations regarding toxicity values to be used in risk assessments.

Table 5 — Typical products based on petroleum hydrocarbons with approximate carbon number and boiling point ranges

Petroleum fuel mixture	Alkane carbon number ranges	Boiling point range °C	Compound classes
Gasoline	C_4 to C_{12}	20 to 200	High concentrations of BTEX compounds[a] Mono-aromatics and branched alkanes Lower concentrations of *n*-alkanes, alkenes, cyclo-alkanes and naphthalenes Very low concentrations of PAHs
Diesel	C_8 to C_{21}	200 to 300	High concentrations of *n*-alkanes Lower concentrations of branched alkanes, cyclo-alkanes, mono-aromatics, naphthalenes and PAHs Very low concentrations of BTEX compounds
Fuel oil	C_{12} to > C_{40}	150 to 700	High concentrations of *n*-alkanes and cyclo-alkanes Lower concentrations of naphthalenes and PAHs Very low concentrations of BTEX compounds
Motor oils	C_8 to > C_{34}	200 to 750	High concentrations of branched alkanes and cyclo-alkanes Very low concentrations of BTEX compounds and PAHs
Crude oil	C_1 to > C_{40}	—	High concentrations of *n*-alkanes, branched alkanes and cyclo-alkanes Lower concentrations of BTEX compounds, PAH without naphthalenes Variable concentrations of NSO compounds

[a] BTEX compounds = benzene, toluene, ethylbenzenes and xylenes.

7 Exposure assessment of petroleum hydrocarbons in soil

7.1 General

With respect to general guidance on human health risk assessment, refer to ISO 15800.

When assessing risk to humans and the environment, a number of aspects should be taken into account within a conceptual site model:

- the existence of plausible source-pathway-receptor linkages;
- the nature of the contaminant source (fuel type; NAPL/dissolved phase; fresh/weathered fuel; high/trace concentration);
- the compounds present in the source material, including appropriate surrogate or indicator compounds;
- the toxicity of the compounds concerned;
- the relevant transport and exposure routes;
- the nature and sensitivity of the receptors present;
- the likely consequences to the receptor(s) arising from the likely exposure to the contaminants.

7.2 Relevant exposure routes for petroleum hydrocarbons

Since petroleum hydrocarbon mixtures typically contain a wide range of compounds with a large variety of properties, many different exposure routes can be relevant for soils contaminated with petroleum hydrocarbons. Examples are given in Table 6.

Table 6 — Examples of exposure routes relevant for soil contaminated with petroleum hydrocarbons

Source (part of soil column)	Pathway (transfer/exposure route)	Receptor
Surface soil[a]	Direct contact, ingestion/absorption Inhalation of fine dry particles Inhalation of volatile compounds Uptake by vegetables Leaching to groundwater	Resident Recreational user Terrestrial ecology Crops and plants Public health Construction worker Water resources
Subsurface soil[b]	Direct contact, ingestion/absorption Inhalation of fine dry particles Inhalation of volatile compounds Vapour intrusion into indoor spaces Uptake by vegetables Leaching to groundwater	Construction worker Resident Terrestrial ecology Crops and plants Public health Building foundations/materials Water resources
Groundwater	Direct contact, ingestion/absorption Vapour intrusion into indoor spaces Groundwater migration towards a drinking water abstraction or towards a surface water body	Resident Water resources Surface water bodies Aquatic ecology

[a] Soil within 0,20 m of the ground surface.

[b] Soil below 0,20 m of the ground surface.

For different petroleum hydrocarbons, not all pathways may be relevant, depending on the properties of the types of petroleum compounds in the product. This can also depend on the weathering of the product in the soil which may cause changes in the composition of the product with time. This should be assessed in the specific case, based on the available information on the products possibly used on the site.

Furthermore, the specific land use should be assessed with the aim of identifying the possible complete exposure pathways on the site. Further guidance on exposure assessment of soils and sites is given in ISO 15800.

7.3 Exposure assessment methods

The exposure assessment on contaminated sites usually involves developing an initial conceptual site model, identifying sources, pathways and potential receptors. If no plausible source-pathway-receptor linkages exist, the assessment may conclude at this stage. However, if plausible source-pathway-receptor linkages are identified, the likely exposure needs to be estimated. At the preliminary stages, the exposure assessment typically takes measured soil concentrations as the starting point and then bases the assessment of impacts encountered in other media (e.g. groundwater, indoor air) on calculations based on mathematical descriptions of the partitioning and transport of the compounds to the relevant point of compliance.

Exposure assessment methods are of two principal types. Either they calculate exposure through different relevant exposure pathways and compare the derived values to specific quality criteria for the media in question (e.g. groundwater); or acceptable concentration levels in the soil are calculated based on summation of impacts through the relevant pathways and the comparison of this sum to an accepted reference dose for the relevant receptors, typically expressed as milligrams per day relative to body weight in kilograms. In either case, it is relevant to calculate partitioning from a measured soil concentration to the relevant compartments (liquid oil, soil, water and air) and transport in this compartment (if relevant). To be able to do this in a meaningful way for petroleum hydrocarbons, the grouping of the individual compounds has to be based on them having similar partitioning and transport properties.

In order to compare the obtained results to a reference dose or a criterion (and to be able to establish such values), it is necessary that the compounds within the group have similar toxicological properties.

7.4 Toxicity assessment methods

In principle, toxicity can be assessed based on the toxicity of a product as a whole, of indicator compound(s) or of fractions of the product. These different assessment methods are illustrated in Table 7. With the whole product method, toxicity criteria for unweathered whole products are typically used. With the indicator method, toxicity of a petroleum hydrocarbon mixture is determined by the toxicity of one or more of the toxic compounds. This method is often used to assess carcinogenic compounds. The fraction method involves dividing petroleum hydrocarbon mixtures into fractions and assigning representative toxicity criteria to each fraction.

Table 7 — Toxicity assessment methods

Method	Toxicity criteria used	Applicable to
Whole product method	Unweathered whole products (Petroleum hydrocarbon mixtures)	e.g. Diesel, JP-4
Indicator method	Toxicity of one or more toxic compounds	Benzene, carcinogenic PAHs
Fraction method	Toxicity criteria assigned to each fraction	Petroleum hydrocarbon mixtures

Information on carcinogenicity typically exists based on investigations of specific compounds (that are also measurable in a petroleum hydrocarbon mix, such as benzene or polycyclic aromatic hydrocarbons). Carcinogenicity varies quite widely between otherwise quite similar compounds. Information on non-carcinogenic effects is not as abundant, but existing research seems to show that the variation is relatively small between similar compounds. This indicates that evaluation of toxicity should be based on a combination of indicator compounds representing the compounds of significant toxicological potency (carcinogenic and directly toxic) and fractions representing a wider range of compounds.

The toxicity evaluation of a single compound or fraction can be combined into an evaluation of the overall toxicity of a petroleum hydrocarbon mixture in a number of ways. It is recommended that the concentrations of specific compounds of significant toxicity should usually be compared to criteria specific to these compounds, and that concentrations of fractions are compared to criteria set specifically for each fraction without subtracting the concentration of possible specific compounds in that fraction, since the specific compounds are assumed to contribute to the toxicity of the fraction.

When assessing the toxicity of a mixture, each fraction should be assessed by itself, if criteria or soil guideline values are given for each fraction. The measured fractions can also be used for the calculation of hazard quotients for each fraction [see Formula (1)]. The sum of all the quotients, typically called a hazard index, represents the overall toxicity of the mixture, since the toxicities of the fractions are assumed to be additive.

Calculation of hazard index

$$I_\mathrm{h} = \sum_{1}^{N} Q_{\mathrm{h},F_i} = \sum_{1}^{N} \frac{\rho_{F_i}}{\mathrm{SGV}_{F_i}} \tag{1}$$

where

I_h	is the hazard index (the overall toxicity of the mixture);
Q_h	is the hazard quotient;
F_i	is the fraction i;
ρ_{F_i}	is the mass concentration of fraction i, in milligrams per kilogram (mg/kg);
SGV_{F_i}	is the soil guideline value for fraction i, in milligrams per kilogram (mg/kg).
N	is the number of fractions

If the hazard index is greater than one, the contamination can pose an unacceptable risk to human health under that exposure scenario, and further evaluation becomes necessary, even if the hazard quotients are all separately below unity.

7.5 Relations between oil fractions in different media related to exposure

Migration of petroleum hydrocarbons through the different environmental compartments varies depending on the physical and chemical properties of the specific compound. The lighter compounds are typically relatively volatile and soluble and will fairly easily be transported away from the original spill with the soil water and soil gas and will also be degraded fairly easily. The heavier and more branched compounds are more strongly bound to the soil particles and are thus more stable, which means they tend to persist in the environment, but are also less likely to be mobile and able to migrate towards distant receptors. Since different mineral oil products consist of different mixtures of petroleum hydrocarbons, these tendencies will also vary between products.

NOTE 1 Migration of a spill can vary due to a large number of other factors such as the volume and type of PHC released, the site specific hydrogeology, soil and water chemistry, and degradation of the different compounds.

The principal mechanisms that control PHC movement in the subsurface and thus the possible exposure pathways are leaching to the groundwater and volatilization to air. The physico-chemical properties of the PHC compounds that control these processes (e.g. soil-water partition co-efficient, vapour pressure, Henry's law constant) should therefore be similar, when individual compounds are grouped together in fractions to be used for exposure assessments.

Several studies have been carried out with respect to grouping of petroleum hydrocarbons with similar properties (see Bibliography). Evaluations have also been made with respect to how the properties of a group are best represented either by the properties of an indicator compound that, for instance, typically constitutes a large proportion of the group in question, or by averaging the properties for the group. Averaging can also be done in different ways: either by simple average, by weighted average based on composition or by correlation of the properties based on a unifying characteristic (e.g. the equivalent carbon number, EC).

The last method has been used by the Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG) as the basis for dividing petroleum hydrocarbons into groups with similar potential for leaching and volatilization. Their studies showed that correlation with a good fit between leaching properties and the equivalent carbon number could be obtained, if aliphatic and aromatic compounds were evaluated separately. For volatilization, there was not an obvious difference between aliphatics and aromatics.

NOTE 2 The Total Petroleum Hydrocarbon Criteria Working Group was formed in USA in 1993 with the following goal: To develop scientifically defensible information for establishing soil clean-up levels that are protective of human health at hydrocarbon contaminated sites. The group had more than 400 participants from the oil industry, consultants, several state governments and the US EPA. The group has published five reports encompassing their findings and their recommendations.

The equivalent carbon number (EC) of a petroleum hydrocarbon is related to its boiling point, normalised to the boiling point of *n*-alkanes and is correlated with its retention time on a non-polar boiling point gas chromatographic column. For example, benzene's EC number is 6,5 because its boiling point and GC retention time are approximately halfway between those of *n*-hexane (C_6) and *n*-heptane (C_7). Benzene's EC number is higher than that of *n*-hexane because its ring structure results in a higher boiling point although they are both C_6-compounds.

The TPHCWG suggestion for fractionation is based on a division into groups with leaching and volatilization factors that differ by approximately one order of magnitude. The one order of magnitude criterion was chosen after considering the level of uncertainty in performing toxicity and exposure assessments. Suggested transport properties were assigned to each fraction based on the observed correlations with the EC-number. It should be noted that the calculated leaching and volatilization factors are based partly on properties that are estimated based on correlation equations (e.g. the octanol/water partition coefficient, K_{ow}), where the basis for the correlation is not necessarily fully consistent with the range of petroleum hydrocarbons for which it is used, but obviously represents the best available knowledge.

This method of using fractions with quite similar leaching and volatilization behaviour and estimating the relevant transport properties based on the correlation with the fractions, EC numbers, has been further evaluated by the American Petroleum Institute (API). The original version of the TPHCWG methodology did not include hydrocarbons greater than carbon number 35 (EC_{35}). This is appropriate for most refined petroleum products such as gasoline and diesel. However, the concentration of hydrocarbons with carbon numbers greater than 35 (i.e. EC_{35+}) can be as high as 50 % to 60 % in some crude oils. Therefore, API suggested a modification of the method to be able to conduct a risk-based analysis of sites where crude oil was present. This was done by modifying the gas chromatographic technique to quantify hydrocarbons up to EC_{44} Then, the fraction EC_{44+} can be determined by distillation or estimation.

In 2008, the World Health Organization (WHO) published a background document for the development of Guidelines for Drinking-water Quality for petroleum products[38]. WHO recommends use of a fraction approach for the evaluation of exposure from drinking water based on the TPHCWG approach. It gives guidance about tolerable levels of hydrocarbon fractions in drinking-water, in the event of spills of petroleum products, for the following fractions:

— $>EC_5$-EC_6 and $>EC_6$-EC_8 aromatic fraction;

— $>EC_8$-EC_{10}, and$>EC_{10}$-EC_{12} and $>$ EC_{12}-EC_{16} aromatic fraction;

— $>EC_{16}$-EC_{21}, and $>EC_{21}$-EC_{35} aromatic fraction;

— $>EC_5$-EC_6 and $>EC_7$-EC_8 aliphatic fraction;

— $>EC_9$-EC_{10}, $>EC_{10}$-EC_{12}, and EC_{12}-EC_{16} aliphatic fraction;

— PAHs.

Both before and after the suggestions of the TPHCWG and API, other authorities or research bodies have suggested similar methodologies for soil, some with fewer fractions and some with an assumed fixed division between the aromatic and aliphatic fraction (see Annex C). Obviously, a coarser fractionation will give rise to a higher order of magnitude between each end of the value span for the different transport properties of the compounds included in the fraction, and thus a less precise calculation of the partitioning and transport of the fractions.

Some authorities or research bodies suggest supplementing the measured fractions with the measurement of specific compounds, typically with high relative toxicity compared to the fractions that they would otherwise be part of.

To be able to evaluate the appropriateness of suggested fractions, it is necessary to also compare toxicity values within and between the fractions. Studies carried out by RIVM [e.g. Reference (16)] with a higher number of fractions show similar results with respect to maximum permissible concentrations for the sum of fractions comparable to the toxicity studies carried out by the Total Petroleum Hydrocarbon Criteria Working Group, and no great variety between the smaller fractions. This is true for both soil and water. For soils alone, the maximum permissible concentrations are fairly similar between some of the soil fractions, but this is generally not true for the similar fractions in water. This comparison is based on studies evaluating ecological risk. Similar evaluations for human risk have only been carried out for the fractions suggested by the TPHCWG. For human risk, the difference between the fractions is fairly large. On this basis, a smaller number of fractions is not recommended.

Finally, an evaluation of the suggested fractions should be based on a verification of results obtained by calculation of resulting concentrations in different media, based on measured soil concentrations and the suggested fractions, and a comparison with measurements of the same fractions in the different media. This type of verification has unfortunately not been carried out in a systematic way. Verification studies of the use of coarser fractions and no split between aliphatics and aromatics have been carried out by the Danish EPA, showing that these coarser fractions (3 to 4 fractions in all and no split) only gave a relatively good fit between the calculated concentrations based on measured soil concentrations and the measured concentrations in a leaching test carried out on in principle the same soil sample.

8 Issues related to sampling and investigation

8.1 General

Sampling is very critical if volatile compounds are involved, and precautions have to be taken to prevent losses. The methods to prevent losses described in ISO 22155 and ISO 15009 are recommended. The less volatile fractions can be present as homogenous contaminant, but also as patches. A good pre-treatment is necessary to ensure that a representative sample will be measured in the laboratory. Recommended pre- treatment methods are described in ISO 14507[2].

Samples have to be stored and transported cool according to ISO 18512, and analysis shall be commenced as defined in ISO 18400-105. Sample containers for analysis of volatiles shall only be opened and used once in order to avoid that results obtained are compromised by evaporation losses. If it is anticipated that supplementary analysis is likely to be required, two or more samples shall be taken and stored separately.

The number and proportion of samples to be analysed for non-fractionated and fractionated determinants will depend on the nature of the site and the exposure pathways relevant. It shall therefore be determined based on the desk study (the conceptual model), the field observations and eventual field test results.

It should be noted that variation between sampling points in the field typically is much larger than the variations due to the uncertainty related to handling of samples and chemical analysis, if standardised methods are used.

8.2 Issues related to analysis

As noted previously, Total Petroleum Hydrocarbons (TPH) refers to the measurable amount of petroleum-based hydrocarbons in an environmental matrix and thus to actual results obtained by sampling and chemical analysis. TPH is thus a method-defined term. In other words, estimates of TPH concentrations will vary depending on the analytical method used to measure it. Based on ISO standards, TPH is the sum of the measurements using ISO 16703, and the aliphatic and aromatic compounds can be measured based on ISO 22155 or ISO 15009.

Determination using GC-FID of the range C_5 to C_{40} on a single extract without clean-up is also used (see examples of clean-up methods below). This latter method has to be considered as a screening technique, because pre-treatment to obtain a representative sample is not usually carried out.

If a petroleum hydrocarbon mixture is split into the aliphatic and the aromatic compounds, the aromatic compounds will typically be more easily defined and described as singular peaks in a chromatogram than the case for individual aliphatics. Identification and measurement of the individual aromatic compounds is thus much easier than identification and measurement of the individual aliphatic compounds, at least for the lighter compounds (C_6 to C_{12}). Determination of the total concentrations of the more volatile aromatic fractions can therefore be achieved by the summation of the concentrations of individual compounds.

Petroleum hydrocarbons can be quantified using methods based on existing ISO standards that measure

a) volatiles (see ISO 22155 or ISO 15009), and

b) the fractions between C_{10} and C_{40} (see ISO 16703).

For volatiles $<C_{10}$, sampling pre-treatment and extraction is used as described in ISO 22155 or ISO 15009. Individual aromatics are measured with GC-MS following the described procedure. Aliphatics are measured as groups by

a) summation of all peaks in the desired range using FID-detection and subtracting the aromatics, or

b) using the MS detector and detection of mass fractions representative for aliphatics.

This method is now standardised as ISO 16558-1.

For the compounds above C_{10} sampling, pre-treatment and extraction is used as described in ISO 16703. The clean-up procedure with Florisil®[1] is not used but instead, a silica gel column is used to split the TPH in an aliphatic and an aromatic fraction. Both fractions are measured using GC-FID and the total concentration of the desired fractions is integrated from the instrument response time graphs. This method is now standardised as ISO 16558-2.

The leaching to groundwater is a potential exposure mechanism; assessment of the site-specific leaching potential may require leaching test procedures to be completed. In such circumstances, laboratory glassware and equipment, which minimises potential for sorption of organic compounds to laboratory consumables should be selected. Furthermore, in the case of volatile PHC compounds, care should be taken to exclude any air-filled headspace in the leaching test procedure. VOCs are liable to partition into the headspace and generate misleading leaching data. With respect to recommendations in relation to choice and execution of leaching tests reference is made to ISO 18772[8] and ISO/TS 21268 (all parts)[9].

NOTE Note that in some environments, Biogenic Organic Compounds (BOC), such as humic and fulvic acids, can be present in significant concentrations and, if using GC-FID without pretreatment with a silica gel column, can be inadvertently interpreted as Petrogenic Hydrocarbons (PHC). Analysis by GCFID without silica gel pre-treatment to remove polar and semi-polar compounds is therefore Total Recoverable Hydrocarbons and not TPH.

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[1] Florisil is a trade name for a prepared diatomaceous substance, mainly consisting of anhydrous magnesium silicate. Florisil, an example of a suitable product available commercially. This information is given for the convenience of users of this document and does not constitute an endorsement by ISO of this product.

Annex A
(informative)

Physico-chemical properties of different petroleum hydrocarbons, etc.

Table A.1 — Physico-chemical properties of different petroleum hydrocarbons, etc.

Compounds	Carbon atoms	EC	MW g/mol	S mg/l	VP kPa	log K_{ow}	BP °C	D_{air} cm^2/s
Aliphatics								
3-Methylpentane	6	5,6	86,18	17,9	25,27	3,6	63,2	$8,0 \times 10^{-2}$
n-Hexane	6	6,00	86,18	9,5	20,08	3,9	68,7	$8,0 \times 10^{-2}$
Methylcyclopentane	6	6,12	84,16	42	18,25	3,37	71,8	$8,1 \times 10^{-2}$
Cyclohexene	6	6,74	82,15	213	11,86	2,86	82,9	$7,8 \times 10^{-2}$
2-Methylhexane	7	6,68	100,21	2,54	8,84	3,71	90	$7,4 \times 10^{-2}$
2,2,4-Trimethylpentane	8	7,04	114,23	2,44	6,56	4,09	99,2	$6,9 \times 10^{-2}$
n-Propylcyclopentane	8	7,10	112,1	2,04	1,62	4,37	101	$7,0 \times 10^{-2}$
Ethylcyclopentane	7	7,34	98,19	0,77	5,32	3,84	103,5	$7,6 \times 10^{-2}$
n-Octane	8	8	114,23	0,66	1,88	5,18	125,6	$6,9 \times 10^{-2}$
2,2,5-Trimethylhexane	9	7,87	128,26	1,15	2,21	5,06	124	$6,6 \times 10^{-2}$
1-Decene	10	9,91	140,27	0,1	0,22	5,31	170,5	$6,3 \times 10^{-2}$
2-Methylnonane	10	9,75	142,29	0,90	0,25	5,18	167,1	$6,2 \times 10^{-2}$
n-Decane	10	10	142,29	0,052	0,19	5,01	174,1	$6,2 \times 10^{-2}$
n-Dodecane	12	12	170,34	0,0037	0,018	6,1	216,3	$5,7 \times 10^{-2}$
n-Tetradecane	14	14	198,40	0,0022	0,0015	7,2	253,5	$5,3 \times 10^{-2}$
n-Pentadecane	15	15	212,42	0,000 076	0,000 46	7,71	270,6	$5,1 \times 10^{-2}$
n-Hexadecane	16	16	226,45	0,000 9	0,00019	8,25	286,8	$4,9 \times 10^{-2}$
Pristane	19	16,63	268,53	0,000 053	0,000 58	9,38	296	$4,5 \times 10^{-2}$
n-Octadecane	18	18	254,50	0,006	0,000 045	9,18	316,3	$4,7 \times 10^{-2}$
n-Eicosane	20	20	282,56	0,0019	$6,1 \times 10^{-7}$	10,16	343	$4,4 \times 10^{-2}$
Heneicosane	21	20,65	296,58	$2,9 \times 10^{-8}$	0,000 012	10,65	356,6	$4,3 \times 10^{-2}$

EC is the equivalent carbon number.
MW is the molecular weight in grams per mol (g/mol).
S is the solubility in water in micrograms per litre (mg/l).
VP is the vapour pressure in kilo Pascal (kPa).
log K_{ow} is the log octanol/water partition coefficient.
BP is the boiling point in degree Celsius (°C).
D_{air} is the diffusion coefficient in air (cm^2/s).

[a] Benzene.

[b] Toluene.

[c] Miscible with water.

NOTE The values given for individual compounds are based on the database in the updated version of the Danish exposure assessment model JAGG[15]. This database was updated in 2008 and 2010 based on a comprehensive literature search. The values for fractions are based on data from the TPHWG reports with updates from References [15], [16] and [19].

Table A.1 *(continued)*

Compounds	Carbon atoms	EC	MW g/mol	S mg/l	VP kPa	log K_{ow}	BP °C	D_{air} cm²/s
n-Pentacosane	25	25	352,69	$2,9 \times 10^{-8}$	$2,0 \times 10^{-7}$	12,62	401,9	$4,0 \times 10^{-2}$
n-Hexacosane	26	26	366,72	0,0017	$6,2 \times 10^{-8}$	13,11	412,2	$3,9 \times 10^{-2}$
n-Octacosane	28	28	394,77	$8,8 \times 10^{-10}$	$2,1 \times 10^{-10}$	14,09	431,6	$3,7 \times 10^{-2}$
n-Triacontane	30	30	422,83	$8,6 \times 10^{-11}$	$3,6 \times 10^{-12}$	15,07	449,7	$3,6 \times 10^{-2}$
n-Dotriacontane	32	32	450,88	$8,3 \times 10^{-12}$	$2,7 \times 10^{-8}$	16,06	467	$3,5 \times 10^{-2}$
Pentatricontane	35	35	492,96	$2,5 \times 10^{-13}$	$7,2x10^{-13}$	17,53	490	$3,3 \times 10^{-2}$
Aromatics								
Benzene	6	6,50	78,10	1790	12,6	2,13	80,1	$8,4 \times 10^{-2}$
Toluene	7	7,58	92,10d	526	3,78	2,73	110,6	$7,7 \times 10^{-2}$
Styrene			104,15	9,600	0,85	3,00		$7,4 \times 10^{-2}$
Ethyl benzene	8	8,5	106,2	169	1,28	3,15	136,1	$7,2 \times 10^{-2}$
m-Xylene	8	8,60	106,2	161	1,10	3,20	139,1	$7,2 \times 10^{-2}$
1,2,4-Trimethylbenzene	9	9,84	120,2	57	0,28	3,63	169,3	$6,8 \times 10^{-2}$
1,3,5-Trimethylbenzene	9	9,62	120,2	48,2	0,33	3,63	164,7	$6,8 \times 10^{-2}$
3-Ethyltoluene	9	9,49	120,2	40	0,40	3,98	161,3	$6,8 \times 10^{-2}$
1,2-Diethylbenzene	10	10,52	134,22	71,1	0,14	3,72	184	$6,4 \times 10^{-2}$
m-cumene	10	10,11	134,22	42,5	0,23	4,5	175,1	$6,4 \times 10^{-2}$
1,2,3,5-Tetramethylbenzene	10	11,19	134,22	27,9	0,066	4,10	198	$6,4 \times 10^{-2}$
Naphthalene	10	11,69	128,18	31	0,011	3,37	218	$6,7 \times 10^{-2}$
1-Methylanthracene	15	11,27	192,26	0,27	0,000 007	3,87	244,7	$6,2 \times 10^{-2}$
2-Ethylnaphthalene	12	12,99	156,23	8,01	0,004 2	4,38	258	$5,9 \times 10^{-2}$
Acenaphthylene	12	15,06	152,2	16,1	0,000 89	3,94	280	$6,0 \times 10^{-2}$
Acenaphthene	12	15,50	154,21	3,92	0,000 29	3,92	277,5	$6,0 \times 10^{-2}$
2,3,5-Trimethylnaphthalene	13	15,96	170,26	4,78	0,000 34	4,78	285	$5,7 \times 10^{-2}$
Fluorene	13	16,55	166,22	1,69	0,000 08	4,18	295	$5,7 \times 10^{-2}$
Phenanthrene	14	19,36	178,24	1,15	0,000 016	4,46	340	$5,7 \times 10^{-2}$
Anthracene	14	19,43	178,24	0,043	$8,7 \times 10^{-7}$	4,45	340	$5,7 \times 10^{-2}$
Pyrene	16	20,8	202,26	0,14	$6,0 \times 10^{-7}$	4,88	404	$5,3 \times 10^{-2}$
Fluoranthene	16	21,85	202,26	0,26	0,000 001 2	5,16	384	$5,3 \times 10^{-2}$

EC is the equivalent carbon number.

MW is the molecular weight in grams per mol (g/mol).

S is the solubility in water in micrograms per litre (mg/l).

VP is the vapour pressure in kilo Pascal (kPa).

log K_{ow} is the log octanol/water partition coefficient.

BP is the boiling point in degree Celsius (°C).

D_{air} is the diffusion coefficient in air (cm²/s).

[a] Benzene.

[b] Toluene.

[c] Miscible with water.

NOTE The values given for individual compounds are based on the database in the updated version of the Danish exposure assessment model JAGG[15]. This database was updated in 2008 and 2010 based on a comprehensive literature search. The values for fractions are based on data from the TPHWG reports with updates from References [15], [16] and [19].

Table A.1 *(continued)*

Compounds	Carbon atoms	EC	MW g/mol	S mg/l	VP kPa	log K_{ow}	BP °C	D_{air} cm^2/s
Chrysene	18	27,41	228,3	0,002	8,3 × 10^{-10}	5,81	448	5,3 × 10^{-2}
Benzo[a]pyrene	20	31,34	252,3	0,001 6	7,3 × 10^{-10}	6,13	495	4,8 × 10^{-2}
Dibenzo(ah)anthracene	22	33,92	278,36	0,002 5	1,3 × 10^{-10}	6,75	524	4,4 × 10^{-2}
Benzo(g,h,i)perylene	22	34,01	276,34	0,000 3	1,3 × 10^{-11}	6,63	520	4,5 × 10^{-2}
Coronene	24	34,01	300,36	0,000 1	2,9 × 10^{-13}	7,64	525	4,3 × 10^{-2}
Indeno(1,2,3-cd)pyrene	22	35,01	276,34	0,000 2	1,7 × 10^{-11}	6,7	536	4,5 × 10^{-2}
Fractions								
Aliphatic >EC5-EC6			86	14	22	3,8	66	8,0 × 10^{-2}
Aliphatic >EC6-EC8			100	5,4	7,5	4,5	95	7,4 × 10^{-2}
Aliphatic >EC8-EC10			140	0,35	0,32	5,2	195	6,2 × 10^{-2}
Aliphatic >EC10-EC12			160	0,026	0,03	6,3	200	5,9 × 10^{-2}
Aliphatic >EC12-EC16			210	0,004 9	0,001	7,7	270	5,1 × 10^{-2}
Aliphatic >EC16-EC35			340	0,000 1	0,000 1	12	380	4,1 × 10^{-2}
Aliphatic >EC35-EC44			490	2,5 × 10^{-13}	7,0 × 10^{-13}	15	490	3,3 × 10^{-2}
Aromatic >EC5-EC7[a]			78	1790	12,6	2,13	80	8,4 × 10^{-2}
Aromatic >EC7-EC8[b]			92	526	3,8	2,73	110	7,7 × 10^{-2}
Aromatic >EC8-EC10			115	95	0,64	3,7	150	7,0 × 10^{-2}
Aromatic >EC10-EC12			145	35	0,089	3,9	200	6,4 × 10^{-2}
Aromatic > EC12-EC16			160	8,2	0,001 4	4,3	275	5,9 × 10^{-2}
Aromatic >EC16-EC21			180	0,75	0,000 02	4,9	350	5,6 × 10^{-2}
Aromatic >EC21-EC35			250	0,04	0,000 000 2	6,4	480	4,8 × 10^{-2}
Aromatic >EC35-EC44			280	0,000 2	1,5 × 10^{-11}	6,7	540	4,5 × 10^{-2}
> EC44-EC70			400	0,000 1	8,5 × 10^{-12}	10	500	4,0 × 10^{-2}
NSO compounds								
Thiophene			84,14	3 010	10,6	1,81	84	9,0 × 10^{-2}
Dimethylsulphide			94,2	3 000	3,8	1,77	109,8	8,5 × 10^{-2}
Aniline			93,13	36 000	0,065	0,9	184,1	8,5 × 10^{-2}
4-methylaniline			107,15	6 500	0,038	1,39	201,4	7,9 × 10^{-2}
Quinoline			129,16	6 110	0,008	2,03	237,1	7,2 × 10^{-2}
Benzo(b)thiophene			134,20	130	0,032	3,12	221	7,1 × 10^{-2}

EC is the equivalent carbon number.

MW is the molecular weight in grams per mol (g/mol).

S is the solubility in water in micrograms per litre (mg/l).

VP is the vapour pressure in kilo Pascal (kPa).

log K_{ow} is the log octanol/water partition coefficient.

BP is the boiling point in degree Celsius (°C).

D_{air} is the diffusion coefficient in air (cm^2/s).

[a] Benzene.

[b] Toluene.

[c] Miscible with water.

NOTE The values given for individual compounds are based on the database in the updated version of the Danish exposure assessment model JAGG[15]. This database was updated in 2008 and 2010 based on a comprehensive literature search. The values for fractions are based on data from the TPHWG reports with updates from References [15], [16] and [19].

Table A.1 *(continued)*

Compounds	**Carbon atoms**	**EC**	**MW** g/mol	**S** mg/l	**VP** kPa	**log** K_{ow}	**BP** °C	D_{air} cm^2/s
4-methylquinoline			143,19	480	0,000 8	2,61	262	$6,9 \times 10^{-2}$
Dibenzofuran			168,19	3,1	0,000 33	4,12	287	$6,3 \times 10^{-2}$
Dibenzothiophene			184,25	1,47	0,000 027	4,38	332,5	$6,1 \times 10^{-2}$
Acridine			179,22	38,4	0,000 018	3,4	346	$6,1 \times 10^{-2}$
Carbazole			167,21	1,8	$9,9 \times 10^{-8}$	3,72	354,7	$6,3 \times 10^{-2}$
Additives								
Methanol			32,05	[c]	12,8	−0,8	64,8	$6,0 \times 10^{-2}$
Ethanol			46,08	[c]	7,9	−0,31	78,3	$12,1 \times 10^{-2}$
Butanol			74,14	77 000	0,59	0,88	117,4	$8,1 \times 10^{-2}$
MTBE			88,15	51 000	33	0,94	54	$8,8 \times 10^{-2}$
ETBE			102,2	5 030	20,3	1,89	72	$7,0 \times 10^{-2}$
TAME			102,2	12 000	13,3	1,95	86	$7,0 \times 10^{-2}$
DIPE			102,2	8 800o	10,3	1,52	69	$6,8 \times 10^{-2}$
1,2-Dichloroethane			99,0	8 600	30,3	1,48	83,5	$8,3 \times 10^{-2}$
1,2-Dibromoethane			187,9	4 300	2,3	1,76	131,6	$6,0 \times 10^{-2}$
DETA			103,2	[c]	0,02	−1,3	207	$8,1 \times 10^{-2}$
Diethanolamine			105,1	[c]	0,000 01	−2,18	269	$8,0 \times 10^{-2}$
Triethanolamine			149,2	[c]	0,000 000 4	−2,3	335	$6,0 \times 10^{-2}$
TEPA			189,3	[c]	0,000 000 1	−3,16	340	$12,1 \times 10^{-2}$

EC is the equivalent carbon number.

MW is the molecular weight in grams per mol (g/mol).

S is the solubility in water in micrograms per litre (mg/l).

VP is the vapour pressure in kilo Pascal (kPa).

log K_{ow} is the log octanol/water partition coefficient.

BP is the boiling point in degree Celsius (°C).

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[a] Benzene.

[b] Toluene.

[c] Miscible with water.

NOTE The values given for individual compounds are based on the database in the updated version of the Danish exposure assessment model JAGG[15]. This database was updated in 2008 and 2010 based on a comprehensive literature search. The values for fractions are based on data from the TPHWG reports with updates from References [15], [16] and [19].

Annex B
(informative)

Examples of suggested tolerated concentration in air (TCA) and tolerable daily intake (TDI) values for different specific petroleum hydrocarbons

Table B.1 — Examples of suggested tolerated concentration in air (TCA) and tolerable daily intake (TDI) values for different specific petroleum hydrocarbons

Compound	EC	TCA	TDI
Benzene	6,5	0,03 mg/m^3 to 4,5 mg/m^3 [a]	0,000 4 mg/(kg·d) to 0,004 mg/(kg·d)[b]
Toluene	7,58	0,1 mg/kg·d[c]; 3 mg/m^3	0,2 mg/(kg·d) to 0,43 mg/(kg·d)
Ethylbenzene	8,5	0,077 mg/m^3	0,136 mg/(kg·d)
m-Xylene	8,6	0,2 mg/(kg·d)[c]	0,15 g/(kg·d)
Styrene	8,83	0,8 g/m^3	0,077mg/(kg·d)
Trimethylbenzene	9,62 to 10,06	0,1 mg/(kg·d)[c]	—
Naphthalene	11,69	10 mg/m^3 [a]	0,03 mg/(kg·d)
Phenanthrene	19,36	—	0,02 mg/(kg·d)
Anthracene	19,43	—	0,05 mg/(kg·d)
Benzo[a]pyrene	31,34	0,14 mg/m^3 [a]	0,87 ng/(kg·d)[c]
n-Hexane	6	0,2 g/m^3	0,023 mg/(kg·d)
n-Heptane	7	—	3,1 mg/(kg·d)
n-Octane	8	—	3,1 mg/(kg·d)
Cyclohexane	6,59	0,4 mg/(kg·d)[c]	—
n-Nonane	9,00	5,8 g/m^3	0,3 mg/(kg·d)

[a] Based on an additional cancer risk of 1: 100 000.

[b] e.g. per kg body weight.

[c] TDI, inhalation.