ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA

ALKANES ENTRY

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Like a library or most large databases (such as EPA's national STORET water quality database), this document contains information of variable quality from very diverse sources. In compiling this document, mistakes were found in peer reviewed journal articles, as well as in databases with relatively elaborate quality control mechanisms [366,649,940]. A few of these were caught and marked with a "[sic]" notation, but undoubtedly others slipped through. The [sic] notation was inserted by the editors to indicate information or spelling that seemed wrong or misleading, but which was nevertheless cited verbatim rather than arbitrarily changing what the author said.

Most likely additional transcription errors and typos have been added in some of our efforts. Furthermore, with such complex subject matter, it is not always easy to determine what is correct and what is incorrect, especially with the "experts" often disagreeing. It is not uncommon in scientific research for two different researchers to come up with different results which lead them to different conclusions. In compiling the Encyclopedia, the editors did not try to resolve such conflicts, but rather simply reported it all.

It should be kept in mind that data comparability is a major problem in environmental toxicology since laboratory and field methods are constantly changing and since there are so many different "standard methods" published by EPA, other federal agencies, state agencies, and various private groups. What some laboratory and field investigators actually do for standard operating practice is often a unique combination of various standard protocols and impromptu "improvements." In fact, the interagency task force on water methods concluded that [1014]:

> It is the exception rather than the rule that water-quality monitoring data from different programs or time periods can be compared on a scientifically sound basis, and that...
>
> No nationally accepted standard definitions exist for water quality parameters. The different organizations may collect data using identical or standard methods, but identify them by different names, or use the same names for data collected by different methods [1014].

Differences in field and laboratory methods are also major issues related to (the lack of) data comparability from media other than water: soil, sediments, tissues, and air.

In spite of numerous problems and complexities, knowledge is often power in decisions related to chemical contamination. It is therefore often helpful to be aware of a broad universe of conflicting results or conflicting expert opinions rather than having a portion of this information arbitrarily censored by someone else. Frequently one wants to know of the existence of information, even if one later decides not to use it for a particular application. Many would like to see a high percentage of the information available and decide for themselves what to throw out, partly because they don't want to seem uniformed or be caught by surprise by potentially important information. They are in a better position if they can say: "I knew about that data, assessed it based on the following quality assurance criteria, and decided not to use it for this application." This is especially true for users near the end of long decision processes, such as hazardous site cleanups, lengthy ecological risk assessments, or complex natural resource damage assessments.

For some categories, the editors found no information and inserted the phrase "no information found." This does not necessarily mean that no information exists; it simply means that during our efforts, the editors found none. For many topics, there is probably information "out there" that is not in the Encyclopedia. The more time that passes without encyclopedia updates (none are planned at the moment), the more true this statement will become. Still, the Encyclopedia is unique in that it contains broad ecotoxicology information from more sources than many other reference documents. No updates of this document are currently planned. However, it is hoped that most of the information in the encyclopedia will be useful for some time to come even with out updates, just as one can still find information in the 1972 EPA Blue Book [12] that does not seem well summarized anywhere else.

Although the editors of this document have done their best in the limited time available to insure accuracy of quotes as being "what the original author said," the proposed interagency funding of a bigger project with more elaborate peer review and quality control steps never materialized.

The bottom line: The editors hope users find this document useful, but don't expect or depend on perfection herein. Neither the U.S. Government nor the National Park Service make any claims that this document is free of mistakes.

The following is one topic entry (one file among 118). See the file entitled RERENCE for the indentity of numbered references in brackets. See the README file for an introduction, an explanation of how to search and otherwise use this document, the oganization of each entry, information quality, copyright issues, and other entries (other topics) covered.

HOW TO CITE THIS DOCUMENT: As mentioned above, for critical applications it is better to obtain and cite the original publication after first verifying various data quality assurance concerns. For more routine applications, this document may be cited as:

> **Irwin, R.J., M. VanMouwerik, L. Stevens, M.D. Seese**, and **W. Basham.** 1997. Environmental Contaminants Encyclopedia. National Park Service, Water Resources Division, Fort Collins, Colorado. Distributed within the Federal Government as an Electronic Document (Projected public availability on the internet or NTIS: 1998).

Alkanes

Brief Introduction:

Br.Class: General Introduction and Classification Information:

Alkanes are a class of aliphatic hydrocarbons characterized by open chains of carbon atoms with only single bonds between adjacent carbon atoms [255]. Alkanes are one of three classes of aliphatic hydrocarbons. Aliphatic hydrocarbons comprise three subgroups: alkanes (paraffin series), characterized by the existence of only single bonds connecting the carbon atoms; alkenes (olefins), which have at least one double bond; and alkynes (acetylenes), which have one or more triple bonds. Alkanes are hydrocarbons often found in conjunction with oil and gas related activities [265].

Heavy alkanes are solids and are often called the paraffin hydrocarbons [255].

Alkanes, n-alkanes, and isoprenoids (saturate hydrocarbon fractions of petroleum hydrocarbons) are valuable for fingerprinting oil sources and tracking weathering [468]. In weathering of oil, alkanes tend to be lost before alkylated PAHs, so some workers use mostly alkylated PAHs to fingerprint (source identify) weathered oil.

The ratio of pristane to heptadecane and phytane to octadecane for a given source of diesel fuel is frequently distinctive enough to enable source identification in a spill investigation [822]. These ratios also increase during biological degradation and are useful in evaluating the age of environmental contamination [822].

Branched alkanes phytane and pristane are produced by plankton from isoprenoids; both are relatively resistant to breakdown and are abundant in new oil sediments. Phytane is more persistent than pristane, so the phytane/pristane ratio is sometimes used to age oil [856].

Simple alkanes include methane (one carbon atom), ethane (two carbon atoms), propane (three carbon atoms), butane (four carbon atoms), pentane (five carbon atoms), hexane (six carbon atoms), heptane (seven carbon atoms), and octane (eight carbon atoms) [751]. Liquefied propane, butane, or a mixture of these is called liquified natural gas (LPG) and transport of LPG is highly regulated by the USDOT as flammable gases [751].

This entry covers un-substituted (parent compound) alkanes, rather than alkanes having chlorine, other halogen, or methyl/alkyl substitutions. Chlorinated or alkyl alkanes tend to be more hazardous, tend to have different fate characteristics, include some hazardous solvents, and such compounds are not covered in this entry. Priority pollutant halogenated alkanes include:

chloromethane
bromoethane
chloroethane
methylene chloride
1,1'-dichloroethane
chloroform
1,2-dichlorethane
1,1,1-trichloroethane
carbon tetrachloride
bromodichloromethane
1,2-dichloropropane
chlorodibromomethane
1,1,2-trichloroethane
bromoform
1,1,2,2-tetrachloroethane

Br.Haz: General Hazard/Toxicity Summary:

Related to environmental or aquatic toxicology, (unsubstituted) alkanes are generally not of much toxicological concern [468]. Other than fire or explosion hazard, the main concern seems to be potential effects on the CNS or as general asphyxiants or irritants [366,480,875]. The same can not be said for the more hazardous halogenated alkanes such as carbon tetrachloride.

As a group the (non-halogenated) alkanes have very low (aquatic) toxicity which is reflected by the low toxicity of n-hexane and n-decane [832]. On the other hand, the aromatic compounds (benzene, naphthalene and benzo(a)pyrene) are described as "relatively toxic" and some aromatics are potentially carcinogenic [832].

Confirming aromatics such as BTEX and PAH compounds rather than alkanes as the usual suspects in contamination effects of petroleum hydrocarbons, a lengthy 1995 textbook on ecotoxicology [834] barely mentions alkanes (nothing about effects) while including long discussions of PAH hazards in the chapter on petroleum hydrocarbons [835]. Little is said relating to alkanes in the chapter on petroleum hydrocarbons, except that alkanes are a part of most petroleum products, with no reference to toxicology or hazard of alkanes [835]. By contrast, almost the entire chapter on ecotoxicology of petroleum hydrocarbons is devoted to various impacts of PAHs, including such things as endocrine disruption of PAHs on fish and birds and impaired immune system effects of PAHs on mammals [835].

Cycloalkanes are more toxic than alkanes or branched alkanes [878].

In humans, high concentrations of inhaled alkanes can result in anesthetic effects or narcosis [878]. Alkanes are CNS depressants [855]. In fact, gasoline was once evaluated as an anesthetic agent [855]. However, sudden deaths, possibly as a result of irregular heartbeats, have been attributed to those inhaling vapors of hydrocarbons such as those in gasoline [855].

Some alkanes, including common ones like propane and butane are asphyxiants [366,480]. In mammals, alkanes can solubilize fats or mucous membranes and can penetrate myelin sheath nerve fibers [878]. However, high molecular weight alkanes are considered virtually non toxic [878].

Summaries of the hazards to humans and animals of many of the alkane constituents in fuel oils were summarized by the Air Force Installation Restoration Program in 1990; hexane may be the most highly toxic of the alkanes [875]. Many of the alkanes are CNS depressants and general irritants [875].

Br.Car: Brief Summary of Carcinogenicity/Cancer Information:

Presently, studies indicate that none of the alkanes possess carcinogenic properties. /Alkanes/ [Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982. 3177] [366].

However, chlorinated or otherwise halogenated alkanes are another story; several, including carbon tetrachloride, are carcinogenic (see EPA 1996 IRIS data base) [893].

One notable potential hazard for an alkane involves a substituted (alkyl) pentane rather than a typical parent compound found on standard alkane/aliphatic lab scans. Gasoline, along with a diverse group of hydrocarbons, has been shown to induce alpha-2u globulin-mediated nephropathy and renal tumors in male rats [892]. The mechanism for kidney tumors is unique in male rats, involving binding of 2,4,4-trimethyl-2-pentanol (TMPOH), a metabolite of 2,2,4-trimethyl pentane (TMP), to alpha-2u globulin, a substance found only in male rats [892]. See WHO and ATSDR summaries [747,892] for details.

Br.Dev: Brief Summary of Developmental, Reproductive, Endocrine, and Genotoxicity Information:

Presently, studies indicate that none of the alkanes possess teratogenic, or mutagenic properties. /Alkanes/ [Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982. 3177] [366].

The above statement is not true for halogenated alkanes.

Br.Fate: Brief Summary of Key Bioconcentration, Fate, Transport, Persistence, Pathway, and Chemical/Physical Information:

Persistence in biota is low for the n-alkanes but higher for the aromatic hydrocarbons, particularly the PAHs [832]. In both Jet A and JP-8 mixtures, the alkanes degraded faster than alkyl aromatics [878]. Cycloalkanes are more resistant to degradation than alkanes or branched alkanes [878]. Howard et al. summarized fate of many individual alkanes (heptane, decane, etc.) in 1993 [597].

Alkanes of various types of crude oils and various petroleum products were biodegraded faster than the "unresolved fractions" [975]. Different types of crude oils and products biodegraded at different rates in the same environments [975].

Alkyl or halogenated alkanes would be expected to have different fate characteristics than their parent compounds.

Most biodegradation occurs from about one week to many months after the spill [771]. Bacteria generally degrade hydrocarbons according to the following sequence (first to last): n-alkanes > branched alkanes > aromatic hydrocarbons > cyclic alkanes [657].

Evaporative processes begin immediately after oil is discharged into the environment [771]. Some light products (like 1- to 2-ring aromatic hydrocarbons and/or low molecular weight alkanes less than n-C15) may evaporate entirely; a significant fraction of heavy refined oils also may evaporate [657,771].

Synonyms/Substance Identification:

No information found on alkanes as a group.

Associated Chemicals or Topics (Includes Transformation Products):

Those searching the general literature for information on alkanes should also search for the key word aliphatics and key words representing individual alkanes (phytane, etc.).

See also: entries entitled oil spills and petroleum, general.

Water Data Interpretation, Concentrations and Toxicity (All Water Data Subsections Start with "W."):

W.Low (Water Concentrations Considered Low):

No information found on alkanes as a group.

W.High (Water Concentrations Considered High):

No information found on alkanes as a group.

W.Typical (Water Concentrations Considered Typical):

No information found on alkanes as a group.

W.Concern Levels, Water Quality Criteria, LC50 Values, Water Quality Standards, Screening Levels, Dose/Response Data, and Other Water Benchmarks:

W.General (General Water Quality Standards, Criteria, and Benchmarks Related to Protection of Aquatic Biota in General; Includes Water Concentrations Versus Mixed or General Aquatic Biota):

No information found on alkanes as a group.

W.Plants (Water Concentrations vs. Plants):

No information found on alkanes as a group.

W.Invertebrates (Water Concentrations vs. Invertebrates):

NOTE: A frequent experimental difficulty in hydrocarbon toxicity studies is the presence of vapor losses from the hydrocarbon solution during the bioassay, resulting in organism exposure to decreasing concentrations of toxicant. Therefore, truly closed systems (air-tight, with no air space) have sometimes been used for such toxicity tests. Open systems and systems with an air space appear to give less reproducible exposure conditions and, presumably, less reproducible toxicity test results [683]. Although closed system tests have questionable relevance to real world spills, other types of data are hard to find so some closed system results are presented as follows:

Acute toxicity of hydrocarbons to daphnia magna in a closed system [683]:

ALKANES:	LC50 (mg/L)	Predicted LC50 (mg/L)
pentane	135	59
hexane	45	22
octane	3.3	3.3
decane	0.2	0.6

CYCLOALKANES:	LC50 (mg/L)	Predicted LC50 (mg/L)
cyclopentane	150	140
cyclohexane	45	63
methyl cyclohexane	15	24

W.Fish (Water Concentrations vs. Fish):

No information found on alkanes as a group.

W.Wildlife (Water Concentrations vs. Wildlife or Domestic Animals):

No information found on alkanes as a group.

W.Human (Drinking Water and Other Human Concern Levels):

No information found on alkanes as a group.

W.Misc. (Other Non-concentration Water Information):

No information found on alkanes as a group.

Sediment Data Interpretation, Concentrations and Toxicity (All Sediment Data Subsections Start with "Sed."):

Sed.Low (Sediment Concentrations Considered Low):

No information found on alkanes as a group.

Sed.High (Sediment Concentrations Considered High):

No information found on alkanes as a group.

Sed.Typical (Sediment Concentrations Considered Typical):

No information found on alkanes as a group.

Sed.Concern Levels, Sediment Quality Criteria, LC50 Values, Sediment Quality Standards, Screening Levels, Dose/Response Data and Other Sediment Benchmarks:

Sed.General (General Sediment Quality Standards, Criteria, and Benchmarks Related to Protection of Aquatic Biota in General; Includes Sediment Concentrations Versus Mixed or General Aquatic Biota):

No information found on alkanes as a group.

Sed.Plants (Sediment Concentrations vs. Plants):

No information found on alkanes as a group.

Sed.Invertebrates (Sediment Concentrations vs. Invertebrates):

No information found on alkanes as a group.

Sed.Fish (Sediment Concentrations vs. Fish):

No information found on alkanes as a group.

Sed.Wildlife (Sediment Concentrations vs. Wildlife or Domestic Animals):

No information found on alkanes as a group.

Sed.Human (Sediment Concentrations vs. Human):

No information found on alkanes as a group.

Sed.Misc. (Other Non-concentration Sediment Information):

Note: The following case study highlights were copied from NOAA Restoration Guidance Document [622] with permission of Eli Reinharz of the NOAA DART Team.

Case Study: On April 27, 1986 a storage tank at the Texaco Refineria Panama on the Caribbean coast of Panama ruptured, releasing ~240,000 barrels of medium weight crude oil into Cativa Bay. On May 4, a storm broke the containment booms, releasing ~150,000 barrels of oil into the Atlantic Ocean. Winds, tides and rain runoff washed part of the oil onto exposed shorelines. Some of the oil was carried back into Cativa Bay, and some was washed into adjacent embayments with mangrove shorelines. By May 15, oil had spread along the coast and washed across fringing reefs and into mangrove forests and small estuaries. A total of 82 km of coastline (=11 linear km) was oiled to varying degrees. Approximately 75 ha of mangroves, primarily the red mangrove Rhizophora mangle, were killed by the discharge [622].

Oil slicks were observed frequently in Bahia Les Minas during the 4 years following the discharge. The slicks appeared to originate primarily from fringing mangrove areas which had been impacted by the discharge: as dead red mangroves decayed and their wooden structures disappeared, erosion of the associated oiled sediment occurred, releasing trapped oil [622].

Oil was present in mangrove sediments and continued to appear on mangrove roots during the three years following the discharge, with the highest levels of continued oiling occurring in stream habitats and the lowest levels along the open coast [622].

Initial weathering removed labile (unstable) oil components such as n-alkane hydrocarbons from oiled surface sediments within 6 months after the discharge. However, total oil concentrations remained high, up to 20% of dry weight in surface sediments, for at least the first 4 years following the discharge. Residual pools of oil in mangrove sediments were sufficiently fluid to flow out when sediments were cored or disturbed 5 years after the discharge. Most of the oozing oil was highly degraded, but one oiled stream contained a fresh oil residue with a full suite of n-alkanes. Subsequent chemical analysis confirmed that this oil was the crude oil mixture discharged in 1986. Release of oil from pools under and around the collapsed Refineria Panama storage tank and from mangrove sediments caused chronic re-oiling for at least 5 years following the discharge, and undegraded oil residues were found in some heavily oiled sediments 6 years after the discharge. Thus, the discharge site, initially injured by a single point-source of oil, became a chronic source of oil contamination. Hydrocarbon chemistry confirmed the long-term persistence of crude oil in mangrove sediments, with pools of trapped oil maintaining consistent hydrocarbon composition. The frequency and amount of re-oiling differed among habitats. Secondary re-oiling was heaviest in sheltered drainage systems of the mangrove environment, where oil continuously leaked from the sediment, but also occurred along the open coast and along channels. Seasonal variation in weather, water levels and tidal flushing affected the amount of oil released. The greatest amount of re-oiling occurred between February and August 1989 and appeared to be related to the collapse and cutting of dead mangroves and to replanting efforts by the Refineria Panama. It was suggested that the amount of oil released may have begun to decline at the time the monitoring program was terminated 5 years after the discharge, as mangroves became reestablished at oiled sites and developed root mats able to stabilize the substrate [622].

Soil Data Interpretation, Concentrations and Toxicity (All Soil Data Subsections Start with "Soil."):

Soil.Low (Soil Concentrations Considered Low):

No information found on alkanes as a group.

Soil.High (Soil Concentrations Considered High):

No information found on alkanes as a group.

Soil.Typical (Soil Concentrations Considered Typical):

No information found on alkanes as a group.

Soil.Concern Levels, Soil Quality Criteria, LC50 Values, Soil Quality Standards, Screening Levels, Dose/Response Data and Other Soil Benchmarks:

Soil.General (General Soil Quality Standards, Criteria, and Benchmarks Related to Protection of Soil-dwelling Biota in General; Includes Soil Concentrations Versus Mixed or General Soil-dwelling Biota):

No information found on alkanes as a group.

Soil.Plants (Soil Concentrations vs. Plants):

No information found on alkanes as a group.

Soil.Invertebrates (Soil Concentrations vs. Invertebrates):

No information found on alkanes as a group.

Soil.Wildlife (Soil Concentrations vs. Wildlife or Domestic Animals):

No information found on alkanes as a group.

Soil.Human (Soil Concentrations vs. Human):

No information found on alkanes as a group.

Soil.Misc. (Other Non-concentration Soil Information):

No information found on alkanes as a group.

Tissue and Food Concentrations (All Tissue Data Interpretation Subsections Start with "Tis."):

Tis.Plants:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Plants:

No information found on alkanes as a group.

B) Body Burden Residues in Plants: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found on alkanes as a group.

Tis.Invertebrates:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Invertebrates:

No information found on alkanes as a group.

B) Concentrations or Doses of Concern in Food Items Eaten by Invertebrates:

No information found on alkanes as a group.

C) Body Burden Residues in Invertebrates: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found on alkanes as a group.

Tis.Fish:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Fish (Includes FDA Action Levels for Fish and Similar Benchmark Levels From Other Countries):

No information found on alkanes as a group.

B) Concentrations or Doses of Concern in Food Items Eaten by Fish:

No information found on alkanes as a group.

C) Body Burden Residues in Fish: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found on alkanes as a group.

Tis.Wildlife: Terrestrial and Aquatic Wildlife, Domestic Animals and all Birds Whether Aquatic or not:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Wildlife, Domestic Animals, or Birds:

No information found on alkanes as a group.

B) Concentrations or Doses of Concern in Food Items Eaten by Wildlife, Birds, or Domestic Animals (Includes LD50 Values Which do not Fit Well into Other Categories, Includes Oral Doses Administered in Laboratory Experiments):

No information found on alkanes as a group.

C) Body Burden Residues in Wildlife, Birds, or Domestic Animals: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found on alkanes as a group.

Tis.Human:

A) Typical Concentrations in Human Food Survey Items:

No information found on alkanes as a group.

B) Concentrations or Doses of Concern in Food Items Eaten by Humans (Includes Allowable Tolerances in Human Food, FDA, State and Standards of Other Countries):

No information found on alkanes as a group.

C) Body Burden Residues in Humans: Typical, Elevated, or of Concern Related to the Well-being of Humans:

No information found on alkanes as a group.

Tis.Misc. (Other Tissue Information):

No information found on alkanes as a group.

Bio.Detail: Detailed Information on Bioconcentration, Biomagnification, or Bioavailability:

Certain alkanes and other hydrocarbons found in Stoddard solvent can accumulate in the brain or other fatty tissues [960]. While smaller alkanes do not tend to bioaccumulate, larger aromatics and alkanes (including some cycloalkanes) tend to bioaccumulate in fatty tissues [960].

Interactions:

No information found on alkanes as a group.

Uses/Sources:

The major uses of alkanes are to produce energy by the combustion of gas and gasoline, to lubricate as oil and grease, and to serve as chemicals that form alkenes, polymers, and other derivatives [255].

Alkanes are hydrocarbons often found in conjunction with oil and gas related activities [265]. A variety of propane, butane, pentane, hexane, decane, dodecane, tridecane, and tetradecane alkanes are found in water soluble fractions of jet fuels [878].

Naturally occurring (high-molecular-weight) alkanes are found in plants and all marine organisms [878].

Forms/Preparations/Formulations:

Aliphatic Hydrocarbons (AH) of interest in environmental surveys include the following (Tom McDonald, Geochemical and Environmental Research Group, Texas A&M University, Personal Communication):

An aliphatic scan typically includes quantification of the following compounds: n-ClO through n-C34 (n-decane through n-tetratriacontane) plus pristane and phytane:

N-C10, An Alkane.
N-C11, An Alkane.
N-C12, An Alkane.
N-C13, An Alkane.
N-C14, An Alkane.
N-C15, An Alkane.
N-C16, An Alkane.
N-C17, An Alkane
Pristane, An isoprenoid branched-chain C19 hydrocarbon.
N-C18, An Alkane.
Phytane, An isoprenoid branched-chain C20 hydrocarbon.
N-C19, An Alkane.
N-C20, An Alkane.
N-C21, An Alkane.
N-C22, An Alkane.
N-C23, An Alkane.
N-C24, An Alkane.
N-C25, An Alkane.
N-C26, An Alkane.
N-C27, An Alkane.
N-C28, An Alkane.
N-C29, An Alkane.
N-C30, An Alkane.
N-C32, An Alkane.
N-C34, An Alkane.

Priority Pollutant Volatile Halogenated Alkanes Include [634]:

chloromethane
bromoethane
chloroethane
methylene chloride

1,1'-dichloroethane
chloroform
1,2-dichlorethane
1,1,1-trichloroethane
carbon tetrachloride
bromodichloromethane
1,2-dichloropropane
chlorodibromomethane
1,1,2-trichloroethane
bromoform
1,1,2,2-tetrachloroethane

The above-listed halogenated compounds are mentioned for overview perspective, but are not the subject of this entry.

Chem.Detail: Detailed Information on Chemical/Physical Properties:

The carbon atoms in alkanes may form continuous or branched chains; branching increases the number of possible isomers, or structural differences, for any one empirical formula [255]. Alkanes have the characteristic ending "ane" and are "relatively" insoluble in water [255]. However, some alkanes are found dissolved in water soluble fractions [878]. Perhaps a more accurate way to describe solubility is to state that alkanes are slightly soluble in water and extremely soluble in fats and oils [878].

Normal, branched, and cyclic alkanes (paraffins) are the most abundant components found in diesel fuel (estimated 65 to 85 percent). Branched alkanes of particular interest include pristane and phytane, which are frequently present at a significant concentration and can be easily identified by gas chromatography [822].

Diesel Range Organic (DRO) component standard and concentrations recommended by State of Wisconsin (Donalea Dinsmore, Wisconsin DNR, personal communication 1997):

Component Concentration	ug/ml
Decane	1000
Dodecane	1000
Tetradecane	1000
Hexadecane	1000
Octadecane	1000
Eicosane	1000
Docosane	1000
Tetracosane	1000
Hexacosane	1000
Octacosane	1000
Total	10,000

Note: The concentration of the Diesel Component Standard may be varied as long as the concentration of each component is the same.

Some states use alkane standards for DRO, while some use diesel fuel itself for calibration. National guidance is in SW-846 [1013]. One of the problems with DRO methods that concentrate on certain alkane standards is that the alkanes come from sources other than diesel, and the continued need to do occasional correlations with more rigorous scans of PAHs and alkyl PAHs.

Fate.Detail: Detailed Information on Fate, Transport, Persistence, and/or Pathways:

The biodegradation of the water soluble fractions of some jet fuels, including several alkanes, was described by Markiewicz in 1994 [878]. In Jet A, monoaromatics degraded faster than the alkanes, while alkyl aromatics were the most persistent [878]. In JP-8, the alkanes degraded faster than aromatics [878]. Persistence in biota is low for the n-alkanes but higher for the aromatic hydrocarbons, particularly the PAHs [832]. The HSDB [366] and Howard [597] are sources of detailed information on the fate of individual alkanes.

Absorption, Distribution and Excretion [366]:

> Purgeable compounds in mother's milk as indicator of environmental pollution, including n-tridecane. [Pellizzar ed et al; Purgeable organic compounds in mother's milk; Bull Environ Contam Toxicol 28(3) 322 (1982)].
>
> Liver, heart, kidneys, muscle and adipose (perirenal and subcutaneous) tissues were collected from 6 animals for analysis of their hydrocarbon composition. Qualitative and quantitative determinations were carried out by gas chromatography and combined gas chromatography-mass spectrometry. Although differing in the proportions, a homologous series of n-alkanes ranging from n-c12 to n-c31 was found in all samples. [Lintas C et al; Distribution of hydrocarbons in bovine tissues; Lipids 14(3) 298 (1979)].

Laboratory and/or Field Analyses:

In response to spills of petroleum fuels, laboratory analysis of individual alkane and aliphatic parent compounds are primarily useful for fingerprinting sources rather than risk assessment. Alkane parent compounds are usually not among the most hazardous (primarily aromatic and alkyl compound) and persistent constituents in these products.

For screening purposes, various total petroleum hydrocarbon and GC\FID methods are used, but most of these do not relate well to risk parameters. TPH analysis 418.1 does not do a good job at picking up alkyl benzenes, nor do most other commonly used methods used to determine total petroleum hydrocarbons. Most TPH methods use standards which tend to favor aliphatic rather than the more hazardous aromatics compounds such as BTEX compounds and PAHs. Modified method 8015 as used in California does a better job at standard BTEX compounds, but it is not clear if it picks up all important alkyl benzenes.

GC/FID is not a good TPH alternative for gasolines, since in typical GC/FID (often modifications of EPA 8015) analyses, PAHs and metals are not covered at all and the lighter (BTEX) hazardous fractions typical of gasolines will be lost in extraction and burning steps.

Although TPH analyses are sometimes done in addition to BTEX analyses in gasoline contaminated soil, the aliphatics emphasized by TPH are not only less hazardous than BTEX compounds, but also less mobile in soil [465], and some are longer lasting. Thus, typically when BTEX compounds have moved out of the soil and into groundwater pathways of concern to humans, some aliphatic compounds may still be in the soil and register in TPH analyses. After additional time, however, the lighter aliphatics in contaminated soils or sediments tend to break down and disappear as reflected by lower TPH values, but the more hazardous and persistent heavy alkyl PAHs remain in the soil and continue to pose a hazard even though TPH 418.1 values have become lower or non detected. The more recent improvements in GC/FID analyses for TPH have somewhat ameliorated but not totally changed this (see TPH entry).

Alkane analyses done for risk or hazard assessments should probably include analyses for alkyl compounds such as 2,2,4-trimethyl pentane (TMP), a compound associated with kidney cancer in male rats [892] (see Br.Hazard section above).

EPA has various alkane-related methods [861], but for risk assessment, alkane methods should usually be supplemented with GC/MS/SIM expanded scans for PAHs and alkyl PAHs [828].

Variation in concentrations of organic contaminants may sometimes be due to the typically great differences in how individual investigators treat samples in the field and in the lab rather than true differences in environmental concentrations. This is particularly true for volatiles and for the relatively lighter semi-volatiles such as the naphthalene PAHs, which are so easily lost at various steps along the way. Contaminants data from different labs, different states, and different agencies, collected by different people, are often not very comparable (see disclaimer section at the top of this entry).

As of 1997, the problem of lack of data comparability (not only for water methods but also for soil, sediment, and tissue methods) between different "standard methods" recommended by different agencies seemed to be getting worse, if anything, rather than better. The trend in quality assurance seemed to be for various agencies, including the EPA and others, to insist on quality assurance plans for each project. In addition to quality control steps (blanks, duplicates, spikes, etc.), these quality assurance plans call for a step of insuring data comparability [1015,1017]. However, the data comparability step is often not given sufficient consideration. The tendency of agency guidance (such as EPA SW-846 methods and some other new EPA methods for bio-concentratable substances) to allow more and more flexibility to select options at various points along the way, makes it harder in insure data comparability or method validity. Even volunteer monitoring programs are now strongly encouraged to develop and use quality assurance project plans [1015,1017].

At minimum, before using contaminants data from diverse sources, one should determine that field collection methods, detection limits, and lab quality control techniques were acceptable and comparable. The goal is that the analysis in the concentration range of the comparison benchmark concentration should be very precise and accurate.

It should be kept in mind that quality control field and lab blanks and duplicates will not help in the data quality assurance goal as well as intended if one is using a method prone to false negatives. Methods may be prone to false negatives due to the use of detection limits that are too high, the loss of contaminants through inappropriate handling, or the use of an inappropriate methods. Some of the simple petroluem hydrocarbon spill scans are also prone to false positives (see TPH entry). This is one reason for using the NOAA expanded scan for PAHs and alkyl PAHs [828] after oil spills rather than relying too heavily on alkane analyses. Rigorous scans for alkyl PAHs are less prone to false negatives in aged oil than analyses for just the alkanes. This is true because alkanes are generally quicker to break down and less hazardous than PAHs and alkyl PAHs (Roy Irwin, National Park Service, Personal Communication, 1997).

See also: Chem.Detail section above.

For a decision process key on how to decide which chemical methods to use in response to oil spills, see PAHs.Gen entry (file).