ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA
ENTRY ON ALKYL PAHS (ALKYL HOMOLOGS OF PAHS)

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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 REFERENC for the identity of numbered references in brackets. See the README file for an introduction, an explanation of how to search and otherwise use this document, the organization 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).

PAHs, Alkyl Homologs of

Brief Introduction:

NOTE: This entry provides general information on alkyl homologs of polyaromatic hydrocarbons (PAHs). For information on specific alkyl homologs or specific classes of alkyl homologs, see the appropriate entry listed in the Associated Chemicals section below.

Br.Class: General Introduction and Classification Information:

Aromatic ring structures in petroleum products range from one- to five-ring combinations [773]. Two or more five- or six-member carbon rings are fused together to form polyaromatic hydrocarbons (PAHs). These petroleum PAHs have abundant alkyl group substitution on their ring structures. The alkyl groups generally have one to four saturated carbon atoms, and thus can produce many different structural isomers and homologs for each aromatic hydrocarbon family. The most abundant aromatic hydrocarbon families have two or three fused rings with one to four carbon atom alkyl group substitutions (denoted C1-, C2-, C3-, and C4- by GC/MS/SIM expanded scans [828]). It is important to point out that crude oils contain primarily the alkyl homologs of aromatic compounds and relatively small quantities of the unsubstituted "parent" aromatic structures [773].

C1-, C2-, C3-, or C4- followed by a PAH name (for example, C1-naphthalene) is a naming convention for reporting the total of all detected C1-, C2-, C3-, or C4- alkyl homologs of the noted PAH. For example, C1-naphthalene reported concentrations represent the total concentration of all C1 naphthalenes. C1-compounds differ from C2-compounds in that there is one rather than two carbon groups attached. Groups of alkyl homologs are often analyzed by a GC/MS/SIM expanded scan for polyaromatic hydrocarbons (PAHs) and alkyl PAHs (such as the NOAA Protocol expanded scan [828]).

Br.Haz: General Hazard/Toxicity Summary:

Probably the most important target analytes in natural resource damage assessments for oil spill are PAHs and the homologous series (alkylated) PAHs [468]. Alkylated PAHs are more abundant, persist for a longer time, and are sometimes more toxic than the parent PAHs [468]. Alkyl substitution usually decreases water solubility [754]. They also tend to bioaccumulate to a greater degree [347,885].

Within an aromatic series, acute toxicity increases with increasing alkyl substitution on the aromatic nucleus [851]. For example, there is an increase in toxicity as alkylation of the naphthalene structure increases. The order of most toxic to least in a study using grass shrimp (Palaemonetes pugio) and brown shrimp (Penaeus aztecus) was dimethylnaphthalenes (C2-) > methylnaphthalenes (C1-) > naphthalenes [853]. Since alkyl PAHs are often more abundant in fresh petroleum products than their parent compounds, and the proportion of alkyl PAHs to parent compound PAHs increases as the oil ages, it is very important to analyze oil samples for alkyl PAHs any time that biological effects are a concern.

Although there is less toxicity information available for most of the alkyl PAHs than for their parent compounds, most alkyl PAHs appear to be at least as toxic or hazardous as the parent compound. Thus, for now, risk assessment experts suggest adding (lumping) all alkyl homolog concentrations with its constituent parent concentration, and interpreting that grouped value (Bill Stubblefield, ENSR, Fort Collins, Personal Communication, 1995). For example, add the reported concentrations for C1-, C2-, C3-, and C4-naphthalenes to the reported naphthalene concentration, and interpret that total value against known toxicological effects benchmarks or criteria for naphthalene.

Alkyl- and hydroxy- substituted PAHs tend to have similar phototoxicity potentials compared to the (unsubstituted) parent PAH compounds [888].

> Cautionary note: Any of the water criteria which have been developed for alkyl PAHs using bioassays performed in the absence of UV light may be under-protective. Phototoxicity of certain PAHs was discovered when organisms which had survived lab exposures to PAHs died quickly after being moved into sunlight. An increase in toxicity due to photo-induced changes is called phototoxicity. For certain PAHs, tests performed in the presence of UV or other solar radiation show greatly increased toxicity to those same organisms at PAH concentrations below maximum solubility [887,888,889,911].

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

No information found. See PAHs entry.

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

No information found. See PAHs entry.

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

Alkylated PAHs generally persist for a longer time than their parent compounds [468]. Alkyl substitution usually decreases water solubility [754]. They also tend to bioaccumulate to a greater degree [347,885]. Of naphthalene and alkyl naphthalenes, the parent compound naphthalene is the first to degrade; so as petroleum products age, the percentage of alkyl PAHs vs. parent PAHs increases, but most standard EPA standard scans (even 8270) do not pick up alkyl naphthalenes [796]. This, coupled with the need for lower detection limits, is one reason the NOAA protocol expanded scan [828] is often recommended rather than the standard EPA scans.

Modification of the basic structure (such as alkylation) causes regular changes to the biological activity. The following rules have been developed [856]:

- Introduction or extension of an alkyl group increases lipophilicity, which often appears as increased absorption.

- Branching of the alkyl chain makes the oxidative metabolism more difficult.

- Cycloalkyl groups increase the absorption rate by facilitating van der Waals bonding.

- Halogen atoms on the carbon skeleton increase lipophilicity. Often they also block sites of hydroxylative metabolism and therefore make the structure more persistent.

- Acylation or alkylation of -OH or -NH groups decreases the polarity. Consequently, absorption properties are changed and the molecule becomes more persistent.

- Metabolic methylation as a rule decreases toxicity of an organic compound but can produce more lipophilic and persistent substances.

Synonyms/Substance Identification:

Alkyl Homologs of PAHs
Alkylated PAHs
Homologous series of PAHs

Associated Chemicals or Topics (Includes Transformation Products):

See also individual entries:

Chrysene, C1-
Chrysene, C2-
Chrysene, C3-
Chrysene, C4-

Dibenzothiophene, C1-
Dibenzothiophene, C2-
Dibenzothiophene, C3-

Fluoranthenes/Pyrenes, C1-

Fluorene, C1-
Fluorene, C2-
Fluorene, C3-

Naphthalene, C1-
Naphthalene, C2-
Naphthalene, C3-
Naphthalene, C4-
Naphthalene, 2,6-Dimethyl
Naphthalene, 1-Methyl
Naphthalene, 2-Methyl
Naphthalene, 1,6,7-Trimethyl
Naphthalene, 2,3,5-Trimethyl

Phenanthrene, 1-Methyl
Phenanthrenes/Anthracenes, C1-
Phenanthrenes/Anthracenes, C2-
Phenanthrenes/Anthracenes, C3-
Phenanthrenes/Anthracenes, C4-
PAHs as a group

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

W.Low (Water Concentrations Considered Low):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

W.High (Water Concentrations Considered High):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

W.Typical (Water Concentrations Considered Typical):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

W.Plants (Water Concentrations vs. Plants):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

W.Invertebrates (Water Concentrations vs. Invertebrates):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

W.Fish (Water Concentrations vs. Fish):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

Sed.Low (Sediment Concentrations Considered Low):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Sed.High (Sediment Concentrations Considered High):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Sed.Typical (Sediment Concentrations Considered Typical):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Sed.Plants (Sediment Concentrations vs. Plants):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Sed.Invertebrates (Sediment Concentrations vs. Invertebrates):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Sed.Fish (Sediment Concentrations vs. Fish):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Sed.Human (Sediment Concentrations vs. Human):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

Soil.Low (Soil Concentrations Considered Low):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Soil.High (Soil Concentrations Considered High):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Soil.Typical (Soil Concentrations Considered Typical):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Soil.Plants (Soil Concentrations vs. Plants):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Soil.Invertebrates (Soil Concentrations vs. Invertebrates):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Soil.Human (Soil Concentrations vs. Human):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

The trend of thinking towards natural attenuation was given a boost by a Lawrence Livermore National Laboratory (LLNL) report entitled "Recommendations to Improve the Cleanup Process for California's Leaking Underground Fuel Tanks;" which stressed the use of passive bioremediation for petroleum product contaminated soils, whenever possible, based on the relatively low number of cases where drinking water was impacted [969]. EPA has pointed out some limitations of the LLNL report, including the lack of adequate consideration of PAHs, alkyl PAHs, and additives such as MTBE, as well limited consideration of (non-human) exposure pathways and various geologic conditions [969]. A weakness of arguments of those pushing the natural attenuation option is typically that they have not shown that the alkyl PAHs are degrading to the desired low concentrations, because they are not using good PAH expanded scans that cover alkyl PAHs (Roy Irwin, Personal Communication, 1997, See PAH entry).

No other information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Tis.Invertebrates:

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Tis.Human:

A) Typical Concentrations in Human Food Survey Items:

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Tis.Misc. (Other Tissue Information):

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Interactions:

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Uses/Sources:

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Forms/Preparations/Formulations:

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

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

No information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.

Laboratory and/or Field Analyses:

Recommended detection limits:

Most of the PAH methods which have been commonly used historically for routine monitoring, including PAH parent compound standard methods:

EPA 8270 (8270 includes several PAH parent compounds along with a long list of other organics) for solid waste/RCRA applications [1013], and

EPA NPDES method 610 as specified in 40 CFR Part 136 (method 610 includes 16 PAH parent compounds) [1010],

EPA method 625 for Base/Neutral Extractables (method 625 includes several PAH parent compounds along with a long list of other organics) as specified in 40 CFR Part 136 [1010],

do not cover alkyl PAHs. They are all inadequate for generating scientifically defensible information for Natural Resource Damage Assessments [468]. These standard EPA scans do not cover important alkyl PAHs and do not utilize low-enough detection limits. When biological effects, ecological risk assessment, damage assessment, or bio-remediation are being considered, detection limit should be no higher than 1-10 ng/L (ppt) for water and 1 ug/kg (ppb) dry weight for solids such as tissues, sediments, and soil.

Note: Utilizing up to date techniques, many of the better labs can use detection limits of 0.3 to 1 ppb for tissues, sediments, and soils. When no biological resources are at risk, detection limits for solids should nevertheless generally not be above 10 ppb. One reason that low detection limits are needed for PAHs is that so many of the criteria, standards, and screening benchmarks are in the lower ppb range (see various entries on individual PAHs).

In the past, many methods have been used to analyze for PAHs [861,1010,1013]. However, recent (1991) studies have indicated that EPA approved methods used for oil spill assessments (including total petroleum hydrocarbons method 418.1, semivolatile priority pollutant organics methods 625 and 8270, and volatile organic priority pollutant methods 602, 1624, and 8240) are all inadequate for generating scientifically defensible information for Natural

Resource Damage Assessments [468]. These general organic chemical methods are deficient in chemical selectivity (types of constituents analyzed) and sensitivity (detection limits); the deficiencies in these two areas lead to an inability to interpret the environmental significance of the data in a scientifically defensible manner [468].

For risk, damage assessment, drinking water, or to determine if biodegradation has occurred, the NOAA expanded scan for PAHs and alkyl PAHs [828], or equivalent rigorous and comprehensive scans. (such as SW-846 method 8270 modified for Selective Ion Mode detection limits and an equivalent list of parent compound and alkyl PAH analytes), are recommended.

If a Park Service groundwater investigation at Colonial National Historical Park performed in response to contamination by Fuel Oil 5 had utilized EPA semi-volatile scan 8270 or any of the other typical EPA scans (625, etc.) all of which only include parent compounds and typically utilize detection limits in the 170-600 ppb range, the false conclusion reached would have been that no PAHs were present in significant (detection limit) amounts. This false negative conclusion would have been made because the parent compound PAHs present constituted only 7.6% of the PAHs detected in groundwater by the expanded scan [828], and the highest concentration found for any parent compound was 8.4 ppb, far below the detection limits used on the older standard EPA scans. Utilizing the NOAA protocol expanded scan [828], it was determined that 92.4% of the total concentration values of the PAHs detected in groundwater were alkyl PAHs, and that all 39 PAHs and alkyl PAHs were present. Of course, all 39 PAHs were also present in the fresh product, in much higher concentrations, and also having alkyl compounds with the highest percentage of higher values compared to parent compounds.

In a similar vein, if the Park Service sediment investigation at Petersburg National Historical Battlefield (this study was performed in response to contamination by Diesel) had utilized EPA semi-volatile scan 8270 or any of the other typical EPA scans (625, etc.), all of which only include parent compounds and often utilize detection limits no lower than the 170-600 ppb range, the false conclusion reached would have been that only one PAH was present in significant (detection limit) amounts. This false negative conclusion would have been made because the parent compound PAHs present constituted only 2.4% of the PAHs detected in sediments, and the highest concentration found for any parent compound except pyrene was 85.5 ppb, far below the detection limits used on the older standard EPA scans. Pyrene was 185 ppb, which would have been non-detected on many of the EPA scans, but not all. However, utilizing the NOAA protocol expanded scan [828], it was determined that 97.6% of total quantity of PAHs detected in sediments were alkyl PAHs, and that all 39 PAHs and alkyl PAHs were present in these sediments.

When taking sediment samples for toxic organics such as PCBs, PAHs, and organochlorines, one should also routinely ask for total organic carbon analyses so that sediment values may be normalized for carbon. This will allow comparison with the newer EPA interim criteria [86,127]. TOC in sediments influences the dose at which many compounds are toxic (Dr. Denny Buckler, FWS Columbia, personal communication).

In some cases (where the expanded scans are too expensive) an alternative recommendation is that one screen sediments with a size-exclusion high-performance liquid chromatography (HPLC)/fluorescence method. The utility and practicality of the HPLC bile and sediment screening analyses were demonstrated on board the NOAA R/V Mt. Mitchell during the Arabian Gulf Project. Estimates of petroleum contamination in sediment and fish were available rapidly, allowing modification of the sampling strategy based on these results [522].

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 additional discussion in the 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].

In the case of alkyl PAHs, the problem of data comparability in the U.S. has been somewhat less than for other contaminants, since many investigators had standardized on the NOAA expanded scan [828].

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 such as many of the EPA standard scans. This is one reason for using the NOAA expanded scan for PAHs [828]; or method 8270 [1013] modified for Selective Ion Mode (SIM) detection limits (10 ppt for water, 0.3 to 1 ppb for solids) and additional alkyl PAH analytes; or alternative rigorous scans. These types of rigorous scans are less prone to false negatives than many of the standard EPA scans for PAH parent compounds (Roy Irwin, National Park Service, Personal Communication, 1997).

For a much more detailed discussion of the great many different lab and field methods for PAHs in general, see the entry entitled PAHs as a group (file name starting with letter string: PAHS). There the reader will find much more detailed discussions of lab methods, holding times, containers, comparability of data from different methods, field sampling methods, quality assurance procedures, the relationship of various methods to each other, the various EPA standard methods for various EPA programs, the pros and cons of various methods, and additional documentation concerning why many standard EPA methods are inadequate for certain applications. A decision tree key for selecting the most appropriate methods for oil or oil products spills is also provided in the lab section of the PAHs entry. Due to the length of these discussions, they are not repeated here (see PAHs entry).

No other information found; see entries on specific alkyl PAHs and groupings of alkyl PAHs.