

ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA

MTBE ENTRY

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Like a library or many 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 uninformed 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 without 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 or summaries 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 chemical topic entry (one file among 118). Before utilizing this entry, the reader is strongly encouraged to read the README file (in this subdirectory) for an introduction, an explanation of how to use this document in general, an explanation of how to search for power key section headings, an explanation of the organization of each entry, an information quality discussion, a discussion of copyright issues, and a listing of other entries (other topics) covered.

See the separate file entitled REFERENC for the identity of numbered references in brackets.

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).

MTBE (t-butyl methyl ether, Methyl tertiary butyl ether, Methyl-Tert-Butyl-Ether, CAS number 1634-04-4)

Brief Introduction:

Br. Class: General Introduction and Classification Information:

Three of the more common oxygenated fuel additives that have been used with unleaded gasolines are methanol, ethanol, and methyl tertiary-butyl ether (MTBE) [661]. The most widely used oxygenate is MTBE. Since it has a relatively low heat of vaporization, MTBE improves fuel mixing and atomization during cold operation and consequently reduces emissions. MTBE has been blended into both USA and European gasolines for many years, primarily because it has an extremely high octane value which has enabled it to take the place of lead compounds gradually being phased out [819].

MTBE is the second most commonly manufactured chemical in the U.S. and also the world; it has different physical chemical characteristics and thus cleanup approaches for groundwater must be different than approaches taken for benzene, toluene, xylenes, and other common gasoline contaminants (James Davidson, Alpine Environmental, Fort Collins, CO, personal communication, 1997; for details, see Davidson and Parsons, 1996. Remediating MTBE with current and emerging technologies. Proceedings of the Petroleum Hydrocarbons and Organic Chemicals in Groundwater Conference, November 13-15, 1996, Houston, pages 15-29).

MTBE is a solvent used as a gasoline additive. There has been recent interest in the use of this agent to dissolve gallstones [606].

MTBE is made synthetically from petroleum feedstocks. The choice of which of the compounds, commonly used in oxygenated fuels, to use is dependent on region, cost of production, and availability of raw materials [661].

MTBE is a volatile ether used as an octane booster and oxygenate in unleaded gasoline [597,606,694]. It is the second most common volatile organic compound (VOC) detected in urban wells (second by a small margin to chloroform) [694]. Considered a VOC by EPA [903]. MTBE was the most common VOC contaminant in Denver, Colorado, and New England [694].

MTBE is a Group One pollutant on the 1989 Canadian Priority Substances List, listed under the Canadian

Environmental Protection Act [597].

Br.Haz: General Hazard/Toxicity Summary:

Potential Hazards to Fish, Wildlife, Invertebrates, Plants, and other Non-Human Biota:

There has been more publicity and attention given to this VOC as a potential hazard to humans than to fish or wildlife; thus there is more literature related to humans and the information found on other species is comparatively sparse compared to the more detailed human health literature. The recognition that there may be notable concentrations in the environment is relatively recent. The imbalance in favor of human effects information (and information on human surrogates: rats and mice), as reflected in the sections below, will hopefully be corrected in the future as more ecological effects information becomes available.

Effects of this volatile compound (if any) to non-human biota could possibly result from: A) high concentrations immediately after a spill (before the compound has volatilized into the atmosphere) or B) the indirect impacts of contaminated groundwater. For example, if highly polluted groundwater water comes into surface waters from springs or seeps, local effects may occur in the mixing zone where the groundwater enters surface water.

Effects observed in test animals have included increased absolute and relative liver and kidney weights and increased severity of spontaneous renal lesions (females), increased prostration (females), and swollen periocular tissue (males and females) [893]. For additional details on other effects, see IRIS [893].

Since it is a gasoline additive, this compound often occurs together with PAHs, BTEX compounds, and other compounds found in gasolines, some possibly more carcinogenic and otherwise generally hazardous than this compound.

Highest MTBE concentrations in surface water tend to be in marinas, where 2 cycle engines blow by MTBE along with gasoline. In a marina at California's Lake Shasta, concentrations as high as 84 ppb MTBE have been found along with BTEX concentrations of about 30 ppb (James Davidson, Alpine Environmental, Fort Collins, CO, personal

communication, 1997). These concentrations are less than known toxicity concentrations for fish (see W.Fish section below).

Potential Hazards to Humans:

According to one source, MTBE so far appears to have no adverse human health effects. There is little reason to assume this situation will change since similar ethers have been in commercial and industrial use for many years [661]. MTBE is acutely only slightly toxic. Snamprogetti (1991) determined that MTBE is more toxic than gasoline alone, but the toxicity of gasoline was not altered by adding 10-15% MTBE. Conaway et al. (1985) determined that although the addition of MTBE did not increase acute toxicity of gasoline in rats and mice, it did lengthen barbiturate-induced sleeping time, reduce spontaneous motor activity, and caused slight disturbances in motor coordination [818].

According to another source, MTBE is highest in the blood of humans (gas station workers and commuters, for example) exposed to air concentrations, and a number of human maladies are associated with exposure [694].

Gas station attendants have complained of nausea, dizziness, irritation, and confusion [1000].

However, one source concluded that MTBE posed relatively little danger to either humans or the environment in Canada [964].

Information on human exposure to MTBE is limited. Humans are acutely exposed to MTBE as a part of a medical treatment to dissolve cholesterol gallstones [893]. Injection of the gall bladder with a high dose of MTBE can be associated with several types of health effects (e.g., nausea, vomiting, sleepiness). Minor transient mucosal damage in the gallbladder has been demonstrated with extensive exposure [893].

A case of acute renal failure is reported in one of 8 patients (aged 37-75 yr) with a history of biliary colic and radiolucent gallstones who were given continuous methyl tert-butyl ether (MTBE I) infusion through a catheter, 5-10 ml for 7 hr. Hemolysis due to extravasation of MTBE after leakage alongside the catheter was suspected as the cause of the renal failure. Dialysis over 18 days was required before renal function recovered completely. (Ponchon T et al; Lancet 2, July 30,

1988: 276-277)[609].

Most effects information in EPA's IRIS database relates to inhalation effects on mammalian test species, including [893]:

The inhalation Reference Concentration (RfC) is analogous to the oral RfD and is likewise based on the assumption that thresholds exist for certain toxic effects such as cellular necrosis, but may not exist for other toxic effects such as carcinogenicity. The inhalation RfC considers toxic effects for both the respiratory system (portal-of-entry) and for effects peripheral to the respiratory system (extrarespiratory effects). It is appropriately expressed in units of mg/cu.m. In general, the RfC is an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily inhalation exposure of the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime.

Crit. Dose: 259 mg/cu.m [Study 1
NOAEL(HEC)] UF: 100 MF: 1 [893].

RfC: 3E+0 mg/cu.m Confidence: Medium
[893].

This compound often makes the news related to potential hazards or groundwater pollution.

The following are news media reports (neither confirmed nor repudiated by the NPS) from Greenwire: Tuesday --- May 13, 1997 --- Vol. 7 --- No. 9:

MTBE: (Industry sponsored study and information release): ADDITIVE DOESN'T CAUSE CANCER IN HUMANS -- STUDY; A new study of lab rodents exposed to "extremely high doses" of the gasoline additive MTBE indicates that previous research showing a correlation between MTBE and tumors in rodents is irrelevant to humans, according to John Kneiss of the Oxygenated Fuels Assn., which partly funded the study.

The study, conducted by the independent Chemical Industry Institute of Toxicology and published in the current issue of

TOXICOLOGY AND APPLIED PHARMACOLOGY, shows that tumors in the rodents' kidneys are attributable to "a unique protein" found in male rats but not in humans, Kneiss said.

To date, more than 70 animal- and human-health studies have indicated that MTBE, "the anti-smog fighter" in reformulated gas, is safe (AP/BOSTON GLOBE online, 5/9).

STATE LAWMAKERS TAKE ACTION AGAINST MTBE: Meanwhile, conservative and environmentalist lawmakers "struck an unusual alliance" yesterday, winning unanimous approval in a California Senate committee of a pair of bills that take a dim view of MTBE.

A bill by state Sen. Richard Mountjoy (R) would fund studies of MTBE by the U. of California. If the studies show MTBE poses "an undue hazard," it could be banned by 3/98. The other bill, offered by state Sen. Tom Hayden (D), is prompted by concerns about MTBE in Santa Monica's groundwater (GREENWIRE, 1/29). Hayden's bill would require the state to clean up MTBE in groundwater and set standards for MTBE in drinking water.

Talk-radio station KSFO in San Francisco "has been touting what its hosts contend are the additive's ill effects." But the Western States Petroleum Assn. yesterday took out a full-page ad in the SACRAMENTO BEE defending MTBE. The ad was endorsed by state air-quality officials, L.A. Mayor Richard Riordan (R) and the state Chamber of Commerce (Dan Morain, L.A. TIMES DC edition, 5/13).

A BAKERSFIELD CALIFORNIAN editorial opposes against an MTBE ban, arguing "the risk from chemicals it replaces is far higher - - as is the risk from not using any form of [reformulated fuels]" (5/8).

Another electronic News Media Report [Greenwire:January 29, 1997, presented for information purposes, neither the accuracy nor the value of this report has been verified]:

SANTA MONICA FILES SUIT OVER MTBE POLLUTION: The city of Santa Monica, CA, on 1/28 filed a lawsuit against Mobil Oil Corp., claiming leaks at a Mobil-owned gas station have contaminated drinking water in municipal wells with the fuel additive MTBE. MTBE, while mixed with gas to reduce smog, is considered a potential carcinogen (GREENWIRE, 1/15). Santa Monica officials say eight or nine oil companies may have contributed to well pollution that has led the city to shut down half of its normal water supply. The discovery of traces of MTBE in lakes and wells in Los Angeles and the San Fernando Valley have "raised new questions" about the dangers of the fuel additive and the difficulty of cleaning it up. John Froines of the U. of California at Los Angeles: "It is a scandal that we have gotten to this point, with millions of pounds of this stuff being manufactured and so little known about its hazards." US EPA officials have admitted the agency has incomplete knowledge of MTBE's health effects, but defend the chemical's continued use. Some EPA officials say the agency did not move faster to determine potential risks from MTBE pollution because it was felt that a federal underground tank cleanup program "would take care of any problems" (Clifford/Helfand, L.A. TIMES DC edition, 1/29).

Additional human health issues related to this topic have been summarized by ATSDR [1000] and Environment Canada [964]. Due to lack of time, not all of the important highlights from these documents have not yet been completely incorporated into this entry.

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

EPA 1996 IRIS [893]: Carcinogenicity Assessment: empty (no information given in this field).

Cancer results in lab animals were mixed [1000]. Additional information related to this topic have been summarized by ATSDR [1000].

This compound has not been treated as a carcinogen for

model calculation purposes in some EPA risk-based (RBC and PRG) models [868,903].

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

When pregnant lab animals breathed MTBE, birth defects occurred only in baby mice [1000].

Exposure by inhalation of male and female rats to MTBE at up to 3400 ppm did not result in adverse effects on reproductive ability, litter size, or pup viability [606,609]. In a more recent report, MTBE did not produce embryotoxic effects in rabbits, even at doses of 8000 ppm, which were maternotoxic [606]. At 4000 and 8000 ppm, MTBE reduced implantations and induced embryotoxic effects in mice [606].

Mated rats and mice were exposed during the period of organogenesis to target concentrations of 0, 250, 1000, and 2500 ppm MTBE. None of the control or test group animals died during the treatment or post treatment periods. No adverse effects of treatment were reflected in maternal parameters or body wt, water consumption, or liver wt or in physical exam data for either species. In rats, no treatment related changes were recorded in the uterine implantation data, fetal size parameters, or fetal sex distribution data. Examination of fetuses for external abnormalities, skeletal malformations, or ossification variations did not reveal changes caused by MTBE exposure [609].

In a single generation reproduction study, male CD rats (15/group) were exposed by inhalation to methyl t-butyl ether (MBE) at nominal concentrations of 0, 250, 1000 or 2500 ppm for 6 hrs/day, 5 days/week for a 12 week pre-mating and post-mating periods. Female CD rats (30/group) were exposed in the same manner for a three-week pre-mating period. The rats were exposed to MBE for 6 hrs/day during mating and exposure of the females continued (6 hrs/day, daily) through gestation days (GD) 0-20 and lactation days 5-21, and for 6 hrs/day during a two-week rest interval before a second mating period, during which the rats were again treated daily. Significant differences were observed between treated and control animals in the following: decreased first litter pup survival (low- and mid-dose groups, Day 0-4), increased second litter pup survival (mid- and high-dose groups, Day 0-7), increased incidence of dilated renal pelves (low- and high dose group F0 females), and increased incidence of alopecia (high-dose group F0 females). No significant differences were observed between treated and control animals in the following: parental mortality,

body weights, mating indices, male fertility indices, pregnancy rates, reproduction indices (gestation length, litter size, litter survival indices), weights of gonads and organs of the male reproductive tract, pup body weights, first litter interval high-dose group pup survival and mid- and low-dose pup survival data for Days 7-21, second litter interval low-dose group pup survival and mid- and high-dose pup survival data for Days 7-21, pup sex ratios, gross examination of pups and dead pups, weights of F0 rat organs, including ovaries (females), testes, epididymides, seminal vesicles and prostate, and histological evaluation of the gonads. [Bio/Dynamics Inc.; A Single Generation Inhalation Reproduction/Fertility Study in Rats With Methyl t-Butyl Ether, Final Report. (1982), EPA Document No. FYI-AX-1182-0219, Fiche No. OTS0000219-0] [609].

Pregnant New Zealand white rabbits (15/group) were exposed to 0, 1021, 4058, and 8021 ppm MTBE (0, 3681, 14,630, and 28,918 mg/cu.m) 6 hours/day, during gestational days 6-18. None of the does died, aborted, delivered early, or had to be removed from the study. There were no differences in maternal body weights among the groups. Reduced maternal body weight gain and food consumption were observed during the major period of organogenesis at 4058 and 8021 ppm. However, there were large standard deviations across the groups for body weight gain measurements [893].

Some teratogenicity studies in rats were negative [609].

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

MTBE tends to volatilize quickly; like most ethers it also dissolves readily in water [1000]. Because MTBE has a low octanol:water coefficient and a high solubility, subsurface MTBE will occur predominantly in groundwater (James Davidson, Alpine Environmental, Fort Collins, CO, personal communication, 1997; for details, see Davidson and Parsons, 1996. Remediating MTBE with current and emerging technologies. Proceedings of the Petroleum Hydrocarbons and Organic Chemicals in Groundwater Conference, November 13-15, 1996, Houston, pages 15-29).

MTBE, a gasoline additive designed to reduce air pollution, was detected in almost 80 percent of the wells sampled in the area of Denver, Colorado [690,694]. The wide-spread detections of MTBE suggests a possible nonpoint source of MTBE to Denver's ground water [690,694].

In soils, MTBE will tend to volatilize, but may leach into ground water and may be resistant to biodegradation in the environment [597]. This compound tends to photooxidize and would be expected to be found mostly in air or water, persisting up to 720 days in groundwater [964].

The biodegradability of MTBE in the subsurface is substantially slower than BTEX aromatic fuel components, due in part to the additive's tertiary bonds. It also tends to move faster. Therefore, towards the leading edge of a plume, MTBE's vertical distribution may be slightly deeper (and usually wider horizontally) than BTEX compounds (James Davidson, Alpine Environmental, Fort Collins, CO, personal communication, 1997; for details, see Davidson and Parsons, 1996. Remediating MTBE with current and emerging technologies. Proceedings of the Petroleum Hydrocarbons and Organic Chemicals in Groundwater Conference, November 13-15, 1996, Houston, pages 15-29).

If MTBE is released to soil, it will be subject to volatilization. It will be expected to exhibit very high mobility in soil and, therefore, it may leach to groundwater. It will not be expected to hydrolyze in soil. If MTBE is released to water, it will not be expected to significantly adsorb to sediment or suspended particulate matter, bioconcentrate in aquatic organisms, hydrolyze, directly photolyze, or photooxidize via reaction with photochemically produced hydroxyl radicals in the water, based upon estimated physical-chemical properties or analogies to other structurally related aliphatic ethers [609].

Snow in the Denver area was also reported to be tainted with MTBE [694]. Once in groundwater, MTBE persists longer than benzene, another gasoline component [694].

Environmental Fate/Exposure Summary From HSDB [609]:

t-Butyl methyl ether may be released as a result of its use as an octane booster for unleaded gasoline and its use in the manufacture of isobutene. If t-butyl methyl ether is released to soil, it will be subject to volatilization. It will be expected to exhibit very high mobility in soil and, therefore, it may leach to groundwater. It will not be expected to hydrolyze in soil. If t-butyl methyl ether is released to water, it will not be expected to significantly adsorb to sediment or suspended particulate matter, bioconcentrate in aquatic organisms, hydrolyze, directly photolyze, or photooxidize via reaction with photochemically produced hydroxyl radicals in the water, based upon estimated physical-chemical properties or analogies

to other structurally related aliphatic ethers. t-Butyl methyl ether in surface water will be subject to rapid volatilization with estimated half-lives of 4.1 hr and 2.0 days for volatilization from a river one meter deep flowing 1 m/sec with a wind velocity of 3 m/sec and a model pond, respectively. It may be resistant to biodegradation in environmental media based upon screening test data from a study using activated sludge inocula. Many ethers are known to be resistant to biodegradation. If t-butyl methyl ether is released to the atmosphere, it will be expected to exist almost entirely in the vapor phase based on its vapor pressure. It will be susceptible to photo-oxidation via vapor phase reaction with photochemically produced hydroxyl radicals with an estimated half-life of 5.6 days for this process. Direct photolysis will not be an important removal process since aliphatic ethers do not adsorb light at wavelengths >290 nm. The most probable route of general population exposure to t-butyl methyl ether is probably via inhalation of contaminated air. Exposures through dermal contact may occur in occupational settings. (SRC).

Synonyms/Substance Identification:

2-Methoxy-2-methylpropane [609]
2-Methyl-2-methoxypropane [609]
Ether, tert-butyl methyl [609]
Methyl 1,1-dimethylethyl ether [609]
Methyl tert-butyl ether [609]
Propane, 2-methoxy-2-methyl- [609]
Tert-butyl methyl ether [609]
Methyl-tert-butyl ether [609]
MTBE [609]
T-butyl methyl ether [609]
tert-Butyl methyl ether [607]
2-Methoxy-2-methylpropane [607]
Methyl tert-butyl ether [607]
Methyl tert-butyl ether (DOT) [607]
Methyl 1,1-dimethylethyl ether [607]
Propane, 2-methoxy-2-methyl- (9CI) [607]
UN2398 (DOT) [607]

Molecular Formula [609]:

5-H12-O

Associated Chemicals or Topics (Includes Transformation Products):

See also individual entries for:

Gasoline Additives

Gasoline, General
Gasoline, Unleaded
BTEX
Benzene
Toluene
Ethyl Benzene
Xylene

The compound tert-butyl alcohol (TBA) is the principal metabolite of MTBE [893]. Another metabolite is tertiarybutanol, which has been detected in the tissues of humans using MTBE for gallbladder treatments [964].

Metabolism/Metabolites [609]:

Exposure to methyl tertiary-butyl ether (MTBE) previously been shown to alter various muscle, kidney, and liver metabolic activities. In the present study, the metabolism of MTBE by liver microsomes from acetone- or phenobarbital-treated Sprague-Dawley rats was studied at concn of up to 5 mM MTBE. Equimolar amounts of tertiarybutanol, as measured by head-space gas chromatography, and formaldehyde were formed. The V_{max} for the demethylation increased by 4 fold and 5.5 fold after acetone and phenobarbital treatments, respectively. The apparent K_m value of 0.70 mM using control microsomes was decreased slightly after acetone treatment, but was increased by 2 fold after phenobarbital treatment. The metabolism of MTBE (1 mM) was inhibited by 35% by monoclonal antibodies against p450IIE1, the acetone/ethanol inducible form of cytochrome p450, suggesting a partial contribution by this isozyme. A single 18 hr pretreatment of rats with 1 or 5 ml/kg MTBE (ip) resulted in a 50 fold induction of liver microsomal pentoxyresorufin dealkylase activity but no change in N-nitrosodimethylamine demethylase activity. These trends in activity agreed with immunoblot analysis which showed an elevation in p450IIB1 but no change in p450IIE1 level. [Brady JF et al; Arch Toxicol 64 (2): 157-60 (1990)].

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

W.Low (Water Concentrations Considered Low):

No information found.

W.High (Water Concentrations Considered High):

Groundwater concentrations in (mostly) polluted areas (some impacted by leaking underground tanks) ranged from 0.197 to 236 ppm [597].

Groundwater: t-Butyl methyl ether has been detected at concn up to 50 ppb in the Old Bridge aquifer under an industrial plant in South Brunswick Township, NJ (no sampling dates specified)(1). A contamination abatement system installed at this aquifer, including 7 extraction wells and a water treatment facility, reduced the t-butyl methyl ether concn by an estimated 26%(1). [(1) Althoff WF et al; Groundwater 19: 495-504 (1981)] [609].

Highest concentrations of MTBE in surface waters tends to be in marinas, where 2 cycle engines blow by MTBE along with gasoline. In a marina at California's Lake Shasta, concentrations as high as 84 ppb MTBE have been found along with BTEX concentrations of about 30 ppb (James Davidison, Alpine Environmental, Fort Collins, CO, personal communication, 1997).

W. Typical (Water Concentrations Considered Typical):

Notable amounts of this compound may be found in urban groundwater [694]. The USGS stated that MTBE had been detected in 23 of 29 Denver area wells in typical concentrations of 0.6 ppb [694].

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.

W. Plants (Water Concentrations vs. Plants):

No information found.

W. Invertebrates (Water Concentrations vs. Invertebrates):

No information found.

W. Fish (Water Concentrations vs. Fish):

The 96 hour LC50 for fathead minnows was 673 mg/L [964].

Aquatic toxicity data on MTBE from Environment Canada (mg/L) [560]:

Genus/Species	LC0	24h LC50	96h LC50	LC100
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Golden Orfes	1000	2000
Nitocra Spinipes		> 10000
Rainbow Trout		1300
		1483
Alburnus Alburnus	1700-1800 (static system)	
Fathead Minnow		760

Additional bioassay work on fish was being done by the API and others in 1997 (James Davidson, Alpine Environmental, Fort Collins, CO, personal communication, 1997).

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

No information found.

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

The USGS stated that MTBE had been detected in 23 of 29 Denver area wells in typical concentrations of 0.6 ppb, well below the 20-200 ppb levels being considered by EPA as a national drinking water standard [694].

EPA 1996 IRIS information [893]: No MCL or MCLG information given, no Drinking Water Health Advisories available.

EPA Region 9 Preliminary remediation goals (PRGs) for tap water [868]: 1.8E+02 (180) ug/L. This same value is a Region III RBC level for tapwater [903].

Additional Misc. (Unconfirmed) News Media Information on groundwater standards related to human health, from National Journal's GREENWIRE, The Environmental News Daily, Thursday, June 26, 1997:

CALIFORNIA: SANTA MONICA STRIKES DEAL TO CLEAN UP MTBE: Santa Monica, CA, whose MTBE-contaminated groundwater "may be an omen of the downside of cleaner-burning gasoline," will announce today that it has reached a \$5 million deal with Shell Oil Co. and Chevron Corp. to clean its polluted wells. The agreement, which will save the companies from future litigation costs, stipulates that city wells should have an MTBE limit no higher than 20 parts per billion, much lower than the US EPA's advisory limit of 70 ppb or California's recommended level of 35 ppb. Under the agreement, the companies will begin to clean

the contaminated Charnock well field and fund a three- person scientific advisory panel to oversee the clean up. Santa Monica and the companies will work to bring other site owners into to the deal -- raising the city's chances of quickly restoring its wells. The EPA, which has said the fuel additive is a possible carcinogen, will meet today with city officials and all adjacent site owners to encourage others to enter the deal. MTBE exists in 90% of California's gasoline supply and is responsible for daily removing 520 tons of carbon monoxide from the state's air (Abigail Goldman, Los Angeles Times, 6/26).

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

Highest concentrations in surface water tend to be in marinas, where 2 cycle engines blow by MTBE along with gasoline (see W.High section above).

MTBE tends to head for groundwater due to physical chemical properties (James Davidson, Alpine Environmental, Fort Collins, CO, personal communication, 1997; for details, see Davidson and Parsons, 1996. Remediating MTBE with current and emerging technologies. Proceedings of the Petroleum Hydrocarbons and Organic Chemicals in Groundwater Conference, November 13-15, 1996, Houston, pages 15-29).

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

Sed.Low (Sediment Concentrations Considered Low):

No information found.

Sed.High (Sediment Concentrations Considered High):

No information found.

Sed.Typical (Sediment Concentrations Considered Typical):

No information found.

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.

Sed.Plants (Sediment Concentrations vs. Plants):

No information found.

Sed.Invertebrates (Sediment Concentrations vs. Invertebrates):

No information found.

Sed.Fish (Sediment Concentrations vs. Fish):

No information found.

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

No information found.

Sed.Human (Sediment Concentrations vs. Human):

No information found.

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

No information found.

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

Soil.Low (Soil Concentrations Considered Low):

No information found.

Soil.High (Soil Concentrations Considered High):

No information found.

Soil.Typical (Soil Concentrations Considered Typical):

No information found.

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.

Soil.Plants (Soil Concentrations vs. Plants):

No information found.

Soil.Invertebrates (Soil Concentrations vs. Invertebrates):

No information found.

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

No information found.

Soil.Human (Soil Concentrations vs. Human):

EPA 1995 Region IX Preliminary remediation goals (PRGs) for cancer risk [868]:

Residential Soil: 3.3E+02 mg/kg wet weight
Industrial Soil: 3.4E+03 mg/kg wet weight

NOTE:

- 1) Values are based on a one-in-one million cancer risk.
- 2) PRGs focus on the human exposure pathways of ingestion, inhalation of particulates and volatiles, and dermal absorption. Values do not consider impact to groundwater or ecological receptors.
- 3) PRGs are slightly lower concentrations than EPA Region III RBCs, which consider fewer aspects [903].

EPA 1995 Region 3 Risk based concentration (RBC) to protect from transfers to groundwater:

None given [903].

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 and additives such as MTBE, as well limited consideration of (non-human) exposure pathways and various geologic conditions [969].

No other information found.

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.

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

No information found.

Tis.Invertebrates:

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

No information found.

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

No information found.

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

No information found.

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):

For risk to human adults eating fish, separate carcinogenic and non-carcinogenic risk-based fish tissue concentrations were calculated [903]. The following EPA Region III fish tissue risk-based concentration (RBC) benchmark utilizes the lower of the two concentrations (non-carcinogenic), rounded to two significant figures [903]:

RBC = 6.8 mg/Kg wet weight

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

No information found.

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

No information found.

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.

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):

LD50 Rat oral 4.0 ml/kg. /From table/ [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. 2503] [609].

ACUTE TOXICITY: RAT: LD50; ROUTE: Oral; DOSE: 4 gm/kg; [REFERENCE: National Technical Information Service PB87-174603] [607].

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.

Tis.Human:

A) Typical Concentrations in Human Food Survey Items:

No information found.

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):

Oral RfD: 5.0E-03 mg/kg-day

For risk to human adults eating fish, separate carcinogenic and non-carcinogenic risk-based fish tissue concentrations were calculated [903]. The following EPA Region III fish tissue risk-based concentration (RBC) benchmark utilizes the lower of the two concentrations (non-carcinogenic), rounded to two significant figures [903]:

RBC = 6.8 mg/Kg wet weight

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

No information found.

Tis.Misc. (Other Tissue Information):

EPA 1996 IRIS information [893]:

Crit. Dose: 259 mg/cu.m [Study 1 NOAEL(HEC)] UF:
100 MF: 1

RfC: 3E+0 mg/cu.m Confidence: Medium

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

A bioconcentration factor of 1.5 for Japanese carp suggests MTBE will not bioconcentrate in aquatic organisms [597].

If MTBE is released to water, it will not be expected to bioconcentrate in aquatic organisms based upon estimated physical-chemical properties or analogies to other structurally related aliphatic ethers [609].

MTBE and its metabolite tertiary-butanol have been detected in the blood, urine, fatty tissue, and mother's milk of humans using MTBE for gallbladder treatments [964].

Interactions:

Although earlier information suggested that MTBE presence might tend to inhibit biodegradation of BTEX compounds, other information does not support this hypothesis (James Davidison, Alpine Environmental, Fort Collins, CO, personal communication, 1997).

Uses/Sources:

Notable amounts of this compound may be found in urban groundwater [694].

Major Uses [609]:

Octane booster in gasoline. [The Merck Index. 10th ed.

Rahway, New Jersey: Merck Co., Inc., 1983. 866].

Manufacture of isobutene [Sax, N.I. and R.J. Lewis, Sr. (eds.). Hawley's Condensed Chemical Dictionary. 11th ed. New York: Van Nostrand Reinhold Co., 1987. 762].

Unleaded gasoline usually contains additives for octane improvement ... including methyl tert-butyl ether (MTBE). [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. V17 227 (1982)].

Pollution Sources - Artificial Sources [609]:

t-Butyl methyl ether may be released as a result of its use as an octane booster for unleaded gasoline (up to 7% by volume) and its use in the manufacture of isobutene(1,2). [(1) Hawley GG; Condensed Chemical Dictionary 10th ed Van Nostrand Reinhold NY p. 671-2 (1981) (2) Merck; The Merck Index An Encyclopedia of Chemicals, Drugs, and Biologicals 10th ed Rahway, NJ: Merck & Co p. 865-6 (1983)].

Forms/Preparations/Formulations:

No information found.

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

Oxygenates commonly used in Europe are methanol in conjunction with MTBE or tert-butyl alcohol (TBA). Typical oxygenate contents are 3% methanol plus 2% TBA or 5% MTBE. The methanol content in automotive gasolines should not exceed 3%, the MTBE content should not exceed 10%, and the total amount of oxygen should not exceed 2.5% [747].

Solubilities:

Very water soluble (43,000,000 ug/l) (James Davidson, Alpine Environmental, Fort Collins, CO, personal communication, 1997; for details, see Davidson and Parsons, 1996. Remediating MTBE with current and emerging technologies. Proceedings of the Petroleum Hydrocarbons and Organic Chemicals in Groundwater Conference, November 13-15, 1996, Houston, pages 15-29).

Water solubility of 51,000 mg/l at 25 deg C. [Bennett GM, Philip WG; J Chem Soc pp. 1930-7 (1928) [609].

4.8 g/100 g in water [The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 866 [609].

Aqueous Solubility is 40 to 43 g/L at 20 C for freshwater. The solubility of oil in water can be determined by bringing to equilibrium a volume of oil and water, and then analyzing the water phase. Oil's aqueous solubility is expressed as the cumulative concentration of the individually dissolved components. Solubility is significantly reduced by weathering [560].

Very soluble in alcohol, ether [Weast, R.C. (ed.) Handbook of Chemistry and Physics. 69th ed. Boca Raton, FL: CRC Press Inc., 1988-1989.,p. C-177 [609].

Affinity for organic carbon:

Very low (log Koc = 1.01) so its retardation due to absorption onto soil organic matter is very low (James Davidson, Alpine Environmental, Fort Collins, CO, personal communication, 1997; for details, see Davidson and Parsons, 1996. Remediating MTBE with current and emerging technologies. Proceedings of the Petroleum Hydrocarbons and Organic Chemicals in Groundwater Conference, November 13-15, 1996, Houston, pages 15-29).

API GRAVITY (60/60 degrees F) [560]:

NOTE: API gravity = (141.5/specific gravity [60/60 degrees F]) - 131.5, where specific gravity [60/60 degrees F] is the oil density at 60 degrees F divided by the density of water at 60 degrees F.

58.8

DENSITY (g/mL) [560]:

For temperatures of oil (T) between 0 and 30 C:
Density = 0.97871 - 0.000710 T

NOTE: The densities of crude oils and oil products are dependent on the temperature and degree of weathering. The following density values are at "0% Weathering Volume" - in other words, fresh MTBE.

Temp(C) Density (at 0% Weathering Volume)

12	0.7488
15	0.7456
16	0.74
20	0.7404

Density/Specific Gravity [609]:

0.7405 @ 20 DEG C/4 DEG C [Weast, R.C. (ed.) Handbook of Chemistry and Physics. 69th ed. Boca Raton, FL: CRC Press

Inc., 1988-1989.,p. C-177

Additional Physicochemical information from Environment Canada on MTBE [560]:

NOTE: In this section with [560] information, for properties with more than one value, each value came from its own source; in other words, if API Gravity at 60 F was measured several times and several different answers were obtained, all of the answers are provided [560]:

VISCOSITY

NOTE: The viscosities of crude oils and oil products are dependent on the temperature and degree of weathering. The following viscosity values are at "0% Weathering Volume" - in other words, fresh MTBE.

Dynamic Viscosity (mPa.s or cP):

Temp(C)	Dynamic Viscosity (at 0% Weathering Volume)
20	0.35

Kinematic Viscosity (mm²/sec or cSt):

Temp(C)	Kinematic Viscosity (at 0% Weathering Volume)
20	0.47

FIRE AND REACTIVITY

Flash Point (C):

-28

-26

Auto Ignition Temperature (C):

460

435

Explosion Limits of Vapour in Air:

min 1.65

max 8.4

DISTILLATION

NOTE: Distillation data provides an indication of an oil's volatility and relative component distribution.

Final Boiling Point (C)

55.3

55.2

SENSATION

Odor Threshold

Terpene like

OTHER

Reid method Vapor Pressure (kPa):

Temp(C)	Pressure
25	33
53.7	
38	55

Freezing Point (C):
-109

Water Content (Volume %):
< 0.05 Wt%

Information from HSDB [609]:

Color/Form:

Colorless liquid [Sax, N.I. and R.J. Lewis, Sr. (eds.).
Hawley's Condensed Chemical Dictionary. 11th ed. New York: Van
Nostrand Reinhold Co., 1987. 761].

Boiling Point:

55.2 DEG C [Weast, R.C. (ed.) Handbook of Chemistry and
Physics. 69th ed. Boca Raton, FL: CRC Press Inc., 1988-
1989.,p. C-177].

Melting Point:

FP: -109 DEG C [The Merck Index. 10th ed. Rahway, New Jersey:
Merck Co., Inc., 1983. 866].

Molecular Weight:

88.15 [Weast, R.C. (ed.) Handbook of Chemistry and Physics.
69th ed. Boca Raton, FL: CRC Press Inc., 1988-1989.,p. C-177].

Vapor Pressure:

245 mm Hg @ 25 deg C [The Merck Index. 10th ed. Rahway, New
Jersey: Merck Co., Inc., 1983. 866].

Other Chemical/Physical Properties:

Solubility of water in methyl t-butyl ether: 1.5 g/100 g [The
Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc.,
1983. 866].

Research Octane Number 117; Motor Octane Number 101. [Kirk-
Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes
1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. 5(84)
3

Octane blending value: 115-125 (Research), 98-110 (Motor). [Sax, N.I. and R.J. Lewis, Sr. (eds.). Hawley's Condensed Chemical Dictionary. 11th ed. New York: Van Nostrand Reinhold Co., 1987. 762].

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

Environmental Fate [609]:

TERRESTRIAL FATE: If t-butyl methyl ether is released to soil, it will be subject to volatilization based upon a reported Henry's Law constant of 5.87×10^{-4} atm-cu m/mole(1) and vapor pressure of 249 mm Hg at 25 deg C(2). It will be expected to exhibit very high mobility(5, SRC) in soil and, therefore, it may leach to groundwater, based upon an estimated Koc of 11.2(3,4, SRC). It will not be expected to hydrolyze in soil(4). Butyl methyl ether may be resistant to biodegradation in soil based upon screening test data from a study using activated sludge inocula(6, SRC). Many ethers are known to be resistant to biodegradation(7). [(1) Hine J, Mookerjee PK; J Org Chem 40: 292-8 (1975) (2) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds. Am Inst Chem Eng. (1989) (3) Bennett GM, Philip WG; J Chem Soc pp. 1930-7 (1928) (4) Lyman WJ et al; Handbook of Chem Property Estimation Methods NY: McGraw-Hill pp. 4-9, 7-4 (1982) (5) Swann RL et al; Res Rev 85: 17-28 (1983) (6) Fujiwara Y et al.; Yukagaku 33: 111-14 (1984) (7) Alexander M; Biotechnol Bioeng 15: 611-47 (1973)].

AQUATIC FATE: If t-butyl methyl ether is released to water, it will not be expected to significantly adsorb to sediment or suspended particulate matter(1,2, SRC), bioconcentrate in aquatic organisms(1,2, SRC), hydrolyze(2), directly photolyze(3), or photooxidize via reaction with photochemically produced hydroxyl radicals in the water(4), based upon estimated physical-chemical properties or analogies to other structurally related aliphatic ethers(1-3, SRC). t-Butyl methyl ether in surface water will be subject to rapid volatilization(2,5, SRC). Using a reported Henry's Law constant of 5.87×10^{-4} atm-cu m/mole(5), a half-life for volatilization of t-butyl methyl ether from a river one meter deep flowing 1 m/sec with a wind velocity of 3 m/sec has been estimated to be 4.1 hr at 25 deg C(2, SRC). The volatilization half-life from a model pond, which considers the effect of adsorption, has been estimated to be 2.0 days(6). t-Butyl methyl ether may be resistant to biodegradation in environmental media based upon screening test data from a study using activated sludge inocula(7, SRC). Many ethers are known to be resistant to biodegradation(8). [(1) Bennett GM, Philip WG; J Chem Soc pp. 1930-7 (1928) (2) Lyman WJ et al; Handbook of Chem Property Estimation Methods NY: McGraw-Hill pp. 4-9, 5-5, 7-4, 15-16 to

15-29 (1982) (3) Calvert JG, Pitts JNJr; Photochemistry. John Wiley & Sons: NY p. 441-2 (1966) (4) Anbar M, Neta P; Int J Appl Radiation Isotopes 18: 493-523 (1967) (5) Hine J, Mookerjee PK; J Org Chem 40: 292-8 (1975) (6) USEPA; EXAMS II Computer Simulation (1987) (7) Fujiwara Y et al; Yukagaku 33: 111-14 (1984) (8) Alexander M; Biotechnol Bioeng 15: 611-47 (1973)].

ATMOSPHERIC FATE: If t-butyl methyl ether is released to the atmosphere, it will be expected to exist almost entirely in the vapor phase(2) based upon a reported vapor pressure of 249 mm Hg at 25 deg C(3). It will be susceptible to photooxidation via vapor phase reaction with photochemically produced hydroxyl radicals. An atmospheric half-life of 5.6 days at an atmospheric concentration of 5×10^5 hydroxyl radicals per cu cm has been calculated for this process based upon a measured rate constant(1, SRC). Direct photolysis will not be an important removal process since aliphatic ethers do not absorb light at wavelengths >290 nm(4). [(1) Bennett PJ, Kerr JA; J Atmos Chem 10: 29-38 (1990) (2) Eisenreich SJ et al; Environ Sci Technol 15: 30-8 (1981) (3) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds. Am Inst Chem Eng. (1989) (4) Calvert JG, Pitts JNJr; Photochemistry. John Wiley & Sons: NY p. 441-2 (1966)].

Biodegradation [609]:

No data concerning the biodegradation of t-butyl methyl ether in environmental media were located. An activated sludge aqueous screening study found that the compound was biodegraded very slowly with a 1% theoretical biological oxygen demand being measured after 21 days incubation(1). These screening test results suggest that t-butyl methyl ether may be resistant to biodegradation in the environment(SRC). Studies of three biological treatment processes indicated that most of the compound could be removed from wastewater by treatment, but it was not determined whether the removal was due to biological activity or to some other processes such as volatilization or adsorption(2). The percentages of the compound removed by a conventional activated sludge process, an activated sludge process supported by powder activated carbon treatment (PACT), and the PACT-process in combination with wet-air regeneration of activated carbon containing surplus sludge were: 85%, 94%, and 95%, respectively(2). Many ethers are known to be resistant to biodegradation(3). [(1) Fujiwara Y et al; Yukagaku 33: 111-4 (1984) (2) Van Luin AB, Teurlinckx LVM; Manage Haz Toxic Wastes Proc Int Congr p. 476-85 (1987) (3) Alexander M; Biotechnol Bioeng 15: 611-47 (1973)].

Abiotic Degradation [609]:

The rate constant for the vapor phase reaction of t-butyl methyl ether with photochemically produced hydroxyl radicals

has been measured to be 2.84×10^{-12} cu cm/molecule-sec at 25 deg C(1) which corresponds to an atmospheric half-life of 5.6 days at an atmospheric concentration of 5×10^5 hydroxyl radicals per cu cm(SRC). Addition of t-butyl methyl ether to a simultaneously mixture increased the amount of ozone formed and NO consumed(4). Hydrolysis is not expected to be significant under normal environmental conditions (pH 5-9)(2). Direct photolysis will not be an important removal process since aliphatic ethers do not absorb light at wavelengths >290 nm(3). [(1) Bennett PJ, Kerr JA; J Atmos Chem 10: 29-38 (1990) (2) Lyman WJ et al; Handbook of Chem Property Estimation Methods NY: McGraw-Hill p. 7-4 (1982) (3) Calvert JG, Pitts JNJr; Photochemistry. John Wiley & Sons: NY p. 441-2 (1966) (4) Carter WPL, Atkinson R; Environ Sci Technol 21: 670-9 (1987)].

Environmental Transport Soil Adsorption/Mobility [609]:

Based upon a reported water solubility of 51,000 mg/L at 25 deg C(1), a Koc of 11.2 has been estimated using a recommended regression equation(2). Based upon this estimated Koc, t-butyl methyl ether will be expected to exhibit very high mobility in soil(3). t-Butyl methyl ether, therefore, may leach through soil to groundwater if it does not volatilize or biodegrade first(SRC). [(1) Bennett GM, Philip WG; J Chem Soc pp. 1930-7 (1928) (2) Lyman WJ et al; Handbook of Chem Property Estimation Methods NY: McGraw-Hill p. 4-9 (1982) (3) Swann RL et al; Res Rev 85: 17-28 (1983)].

Volatilization from Water/Soil [609]:

The half-life for volatilization of t-butyl methyl ether from a river one meter deep flowing 1 m/sec with a wind velocity of 3 m/sec is estimated to be 4.1 hr at 25 deg C(1,SRC) based on a reported Henry's Law constant of 5.87×10^{-4} atm-cu m/mole(2). The volatilization half-life from a model pond, which considers the effect of adsorption, has been estimated to be 2.0 days(3,SRC). Based upon the Henry's Law constant and a reported vapor pressure of 249 mmHg at 25 deg C(4), t-butyl methyl ether will be subject to volatilization from surfaces and near-surface soil(SRC). [(1) Lyman WJ et al; Handbook of Chem Property Estimation Methods Environ Behavior of Org Compounds NY: McGraw-Hill pp. 15-16 to 15-29 (1982) (2) Hine J, Mookerjee PK; J Org Chem 40: 292-8 (1975) (3) USEPA; EXAMS II Computer Simulation (1987) (4) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds. Am Inst Chem Eng. (1989)].

Laboratory and/or Field Analyses:

MTBE is used in the lab extraction procedures for analysis of several pesticides [861]. Therefore, MTBE may be a lab contaminant.

Detection limits should be as low as possible to avoid false negatives and no higher than comparison benchmarks or criteria. USGS can achieve water detection limits of 0.1 ug/L or less for this compound using advanced methods such as USGS 1996 Custom Method 9090.

A standard TPH (Total Petroleum Hydrocarbon) analysis (EPA method 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 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.

A modified (improved by internal standards, oven temperature profile and use of High resolution GC/MS - HRGC/MS) EPA method 8270 has been used to provide better results for MTBE, BTEX, and naphthalene compounds [801]. Using this method combined with cluster techniques can help fingerprint fresh gasolines, but with aged gasolines, some volatiles (including C2-benzenes, C1-naphthalenes, and C3 benzenes) were so standardized by refining and others (standard BTEX compounds, parent naphthalene) had changed so much with aging, that the only isomeric group which seemed to have relatively reliable fingerprinting for unleaded gasolines potential was C8 alkanes [801].

Gasoline components showing up in GC chromatograms (whether state of the art GC/MS based on improved EPA Method 8270 [801] or more primitive GC/FID or GC/PID [804]) can be divided into three groups [801,804]:

The first third includes relatively low boiling point (very volatile) lighter hydrocarbons such as some alkanes [804] and MTBE [801].

The second third includes the still volatile but somewhat heavier BTEX hydrocarbons [801,804].

The third third includes the heaviest (molecular weight greater than 110) and less volatile PAHs and alkyl PAHs [804] such as naphthalene and alkyl naphthalenes [801].

As gasoline spills age, the first third degrades first and the third third last, so as volatile MTBE and BTEX compounds disappear from soil (and appear in groundwater and air) the heavier PAHs become a greater % of the remaining petroleum contamination in soil [804].

If used as a measure of BTEX, the more lengthy scan referred to as standard EPA 8240 method often needs to "enhanced" by the inclusion of analytes that would be expected in specific situations. For example, for tanks leaking gasoline and diesel, one should include rigorous analyses for alkyl benzenes (like alkyl PAHs, alkyl benzenes are more resistant to degradation than parent compounds), MTBE and BTEX compounds, 1,2 Dichloroethane, alkyl lead isomers, and other compounds consistent with 1995 risk assessment needs. Enhanced 8240 scans are available from various commercial

labs (Gregory Douglas, Arthur D. Little, Inc., Cambridge, Massachusetts, personal communication, 1995).

Using a modified EPA method 8240 (about \$200 per water sample in 1995), analyses can be done for the following volatile and gasoline additive compounds:

Alkyl benzenes common in oils:

isopropyl benzene:	detection limit (dl): 1 ppb
n-propyl benzene:	dl 1 ppb
1,3,5-trimethyl:	dl 1 ppb
1,2,4-trimethyl:	dl 1 ppb
tert-butyl	dl 1 ppb
sec-butyl	dl 1 ppb
n-butyl	dl 1 ppb
MTBE	dl 1 ppb
BTEX	dl 0.5 ppb
1,2-DCA	dl 0.5 ppb

Contaminants data from different labs, different states, and different agencies, collected by different people, are often not very comparable (see also, 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 to 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 quality assurance problems due to the use of detection limits that are too high, the loss or addition of contaminants through inappropriate handling, or the use of inappropriate methods.

Description of Custom Method 9090: Basic Description of the Method (Brooke Connor, USGS Water Quality Lab, Denver, Personal Communication, 1996):

Tue, 14 May 1996 From: "John S Zogorski, Supervisory Hydrologist, Rapid City, SD" Custom Method 9090: Basic Description of the Method, Identification and Quantification Strategy, and Data Transfer.

General Description of the Method: Custom method 9090 uses capillary column gas chromatography / mass spectrometry (GC/MS) to identify and quantitate 87 analytes, and to tentatively identify unknowns. The method is intended to identify and measure low concentrations of VOCs that may occur in the environmental settings sampled in the NAWQA program, and which may be associated with either point and non-point sources, especially in urban areas. Fifty-five of the analytes included on 9090 are referred to as NAWQA VOC target analytes and were selected because of their known human health concern (A or B carcinogens), aquatic toxicity, frequency of occurrence, and/or emerging chemicals with a potential for wide-scale use and significance. Custom method 9090 builds on the same VOC analytical technology, GC/MS, that has been used at the NWQL and elsewhere for many years, and which is considered the conventional approach for high-quality analysis of VOCs in water....Persons unfamiliar with the GC/MS method for VOCs may wish to refer to 2 recent reports: Rose, D.L., and M.P. Schroeder, 1995, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory -- Determination of volatile organic compounds in water by purge and trap capillary gas chromatography/mass spectrometry: U.S. Geological Survey Open-File Report 94-708, 26 p. Raese, J.W., D.L Rose, and M.W. Sandstrom, 1995, U.S. Geological Survey Laboratory Method for Methyl tert-Butyl Ether and Other Fuel Oxygenates: U.S. Geological Survey Fact Sheet 219-95, 4 p.

Standard methods 8240 have been described by EPA [861]:

Note: 8240 is being replaced by 8260 in the third update of SW-846 [1013].

OSW 8240A S Volatile Organics - Soil, GCMS 73 SW-846
GCMS ug/kg EQL Method 8240A "Volatile Organics by Gas Chromatography/Mass Spectrometry (GC/MS): Packed Column Technique" The volatile compounds are introduced into the gas chromatograph by the purge and trap method or by direct injection (in limited applications) [861]. The components are separated via the gas chromatograph and detected using a mass spectrometer, which is used to provide both qualitative and quantitative information [861]. The chromatographic conditions, as well as typical mass spectrometer operating parameters, are given [861]. If the above sample introduction techniques are

not applicable, a portion of the sample is dispersed in methanol to dissolve the volatile organic constituents [861]. A portion of the methanolic solution is combined with organic-free reagent water in a specially designed purging chamber [861]. It is then analyzed by purge and trap GC/MS following the normal water method [861]. The purge and trap process - An inert gas is bubbled through the solution at ambient temperature, and the volatile components are efficiently transferred from the aqueous phase to the vapor phase [861]. The vapor is swept through a sorbent column where the volatile components are trapped [861]. After purging is complete, the sorbent column is heated and backflushed with inert gas to desorb the components, which are detected with a mass spectrometer [861].

OSW 8240A W Volatile Organics - Water, GCMS 73 SW-846
GCMS ug/L EQL Method 8240A "Volatile Organics by Gas Chromatography/Mass Spectrometry (GC/MS): Packed Column Technique" The volatile compounds are introduced into the gas chromatograph by the purge and trap method or by direct injection (in limited applications) [861]. The components are separated via the gas chromatograph and detected using a mass spectrometer, which is used to provide both qualitative and quantitative information [861]. The chromatographic conditions, as well as typical mass spectrometer operating parameters, are given [861]. If the above sample introduction techniques are not applicable, a portion of the sample is dispersed in methanol to dissolve the volatile organic constituents [861]. A portion of the methanolic solution is combined with organic-free reagent water in a specially designed purging chamber [861]. It is then analyzed by purge and trap GC/MS following the normal water method [861]. The purge and trap process - An inert gas is bubbled through the solution at ambient temperature, and the volatile components are efficiently transferred from the aqueous phase to the vapor phase [861]. The vapor is swept through a sorbent column where the volatile components are trapped [861]. After purging is complete, the sorbent column is heated and backflushed with inert gas to desorb the components, which are detected with a mass spectrometer [861].

OSW 8270A S Semivolatiles - Soil 228 SW-846
CGCMS ug/kg EQL Method 8270A "Semivolatile Organic compounds by Gas Chromatography/Mass Spectrometry (GC/MS): Capillary Column Technique" A table of analyte specific sample preparation procedures that may be used is given in this method [861]. The two procedures that cover most of the analytes are 3510 and 3580 [861]. Prior to using this method, the samples should be prepared for chromatography using the appropriate sample preparation and cleanup methods [861]. This method

describes chromatographic conditions that will allow for the separation of the compounds in the extract [861].

OSW 8270A W Semivolatiles - Water 228 SW-846
CGCMS ug/L EQL Method 8270A "Semivolatile Organic
compounds by Gas Chromatography/Mass Spectrometry
(GC/MS): Capillary Column Technique" A table of analyte
specific sample preparation procedures that may be used
is given in this method [861]. The two procedures that
cover most of the analytes are 3510 and 3580 [861].
Prior to using this method, the samples should be
prepared for chromatography using the appropriate sample
preparation and cleanup methods [861]. This method
describes chromatographic conditions that will allow for
the separation of the compounds in the extract [861].

Additional information related to lab methods for MTBE has been summarized by ATSDR [1000].