ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA

ENTRY FOR 1,1,1-TRICHLOROETHANE

July 1, 1997

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This document was put together by human beings, mostly by compiling or summarizing what other human beings have written. Therefore, it most likely contains some mistakes and/or potential misinterpretations and should be used primarily as a way to search quickly for basic information and information sources. It should not be viewed as an exhaustive, "last-word" source for critical applications (such as those requiring legally defensible information). For critical applications (such as litigation applications), it is best to use this document to find sources, and then to obtain the original documents and/or talk to the authors before depending too heavily on a particular piece of information.

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 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 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).

Trichloroethane, 1,1,1- (1,1,1-Trichloroethane, methyl chloroform, CAS number 71-55-6)

Brief Introduction:

Caution: Although the acronym TCE has sometimes been applied to 1,1,1 Trichloroethane [366], TCE should probably not be encouraged as a synonym for this substance since it is more commonly applied to a related but different VOC: trichoroethylene (see trichloroethylene entry.)

Br.Class: General Introduction and Classification Information:

Trichloroethane, 1,1,1- is a volatile organic compound (VOC) [868,903] which is widely used as a solvent and degreaser [366]. This compound is considered a purgeable halocarbon [1010].

Trichloroethane, 1,1,1- is a colorless, volatile, nonflammable liquid with a sweet, chloroform-like odor [366,369]. It has replaced carbon tetrachloride as a solvent and cleaning agent in many household products including type cleaners, color film cleaners, insecticides, spot removers, cements and adhesives, fabric cleaning solutions, paint removers, and adhesive tape removers [363]. It has also been used as a propellant and as a solvent in pesticides [498].

Trichloroethane, 1,1,1- is one of the more popular solvents of abuse [369]. 1,1,1-Trichloroethane is an indirect food additive for use only as a component of adhesives. (21 CFR 175.105, 4/1/90) [366].

1,1,1-Trichloroethane can exist in the form of a liquid or a vapor, or it can be dissolved to varying amounts in water, food, and other chemicals. As a liquid in an open container, it evaporates quickly and becomes a vapor in the air. This is the most likely way it is found in the environment. 1,1,1-Trichloroethane also can be found in soil and water, and as a vapor in the air at hazardous waste sites [936].

Through air emission, industrial uses release the largest amount of 1,1,1-trichloroethane into the environment [936]. By the year 1996, 1,1,1-trichloroethane will no longer be made in the United States due to its effect on the ozone layer (written Oct, 1993) [936].

Trichloroethane, 1,1,1- is a priority pollutant [446]. It is a toxic pollutant designated pursuant to section 307(a)(1) of the Clean Water Act and is subject to effluent limitations (40 CFR 401.15, 7/1/90 [366].

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 imbalance in favor of human effects information, as reflected in the sections below, will hopefully be corrected in the future as more ecological effects information becomes available.

Effects of this volatile solvent to non-human biota would often result from high concentrations immediately after a spill (before the compound has volatilized into the atmosphere) or be the indirect result of contamination of 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.

1,1,1-Trichloroethane is known from controlled studies in dogs to be a cardiac sensitizer, which involves increasing the sensitivity of the heart to epinephrine with resulting arrhythmias and fibrillation [369]. The cardiac effects of trichloroethane, 1,1,1 may play a role in cases of sudden death from exposure to high concentrations [369].

Animal studies confirm the low hepatotoxicity of 1,1,1-trichloroethane but indicate that cardiac sensitization can occur if exposures are excessive [498].

Many of the chlorinated ethanes (chloroethanes) are toxic, especially those with high chlorination [302]. EPA has a discussion on them in the Gold Book [302].

Potential Hazards to Humans:

Commercial grades of 1,1,1 trichloroethane generally contain inhibitors (see Associated Chemicals section below) to prevent its reaction with metals [369]. Interpretation of any toxicological study on 1,1,1 trichloroethane should take into account any low-level effects which may have been due to the inhibitor rather than to the 1,1,1 trichloroethane itself [369]. Speculation has centered around the possible role of the inhibitors in 1,1,1 trichloroethane in its genotoxicity [369]. Otherwise, 1,1,1 trichloroethane (in humans) is regarded as probably the least toxic of all the chlorinated hydrocarbon solvents [369,498].

Experimental animal data indicate that the toxicity from an acute exposure to 1,1,2-isomer is several times that of the 1,1,1-isomer (International Labour Office. Encyclopedia of Occupational Health and Safety. Vols. I&II. Geneva, Switzerland: International Labour Office, 1983. 2214) [366].

A comprehensive toxicological profile for 1,1,1-trichloroethane, especially as it relates to human health, is available from ATSDR [936]. Due to lack of time, important highlights from this ATSDR document have not yet been completely incorporated into this entry.

However, since there is so much information available related to human health, much of the information summarized below is taken from various government summary sources such as the Hazardous Substances Data Bank [366], EPA IRIS database [893], and the ATSDR Human Toxicology Profile [936].

EPA has a free and informative (several page) health advisory on this compound, available through the Office of Drinking Water, EPA, Washington, D.C. or through NTIS.

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

EPA 1996 IRIS Information [893]:

Evidence for classification as to human carcinogenicity; weight-of-evidence classification

Classification: D; not classifiable as to human carcinogenicity

BASIS: There are no reported human data and animal studies (one lifetime gavage, one intermediate-term inhalation) have not demonstrated carcinogenicity. Technical grade 1,1,1-trichloroethane has been shown to be weakly mutagenic, although the contaminant, 1,4-dioxane, a known animal carcinogen, may be responsible for this response.

HUMAN CARCINOGENICITY DATA: None.

ANIMAL CARCINOGENICITY DATA: Inadequate.

Mechanism of Action:

An epoxide is the critical genotoxic metabolite derived from vinyl chloride, and it has been easier to demonstrate the formation of reactive epoxides from vinyl chloride than from other solvents such as trichloroethane [494].

Previous IARC Summary and Evaluation [366]:

No data are available in humans. Inadequate evidence of carcinogenicity in animals. OVERALL EVALUATION: Group 3: The agent is not classifiable as to its carcinogenicity to humans. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. S7 73 (1987)].

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

Developmental effects in humans exposed to 1,1,1-trichloroethane have not been verified. Epidemiology studies found no relationship between adverse pregnancy outcomes and maternal exposure to 1,1,1-trichloroethane [936]. Although there are some positive reports of minor developmental effects in experimental animals, 1,1,1-trichloroethane does not appear to be a potent developmental toxicant in animals [936].

Generally the mutagenic activity of trichloroethane, 1,1,1 is weak and sometimes not reproducible [369].

Pregnant mice & rats were exposed to a concentration of 875 ppm. Both were exposed for 7 hr daily periods on days 6 through 15 of gestation. No fetal toxicity or teratogenicity was found (Shepard, T.H. Catalog of Teratogenic Agents. 5th ed. Baltimore, MD: The Johns Hopkins University Press, 1986. 1452) [366].

The body of evidence in animal studies suggests that 1,1,1 trichloroethane is not a reproductive hazard even at high doses [369].

Reproductive effects of 1,1,1-trichloroethane in humans have not been reported [936]. However, testicular degeneration was observed in guinea pigs [936].

A multigeneration reproduction study was modified to incl screening for dominant lethal and teratogenic effects of 1,1,1-trichloroethane in drinking water soln. Male & female icr swiss mice received 1,1,1-trichloroethane at concentrations(s) of 0, 0.58, 1.75, Or 5.83 Mg/ml. These concentrations(s) were designed to yield daily doses of 0, 100, 300, or 1,000 mg/kg. No taste aversion was evident & there appeared to be no dose-dependent effects on fertility, gestation, viability or lactation indices. Pup survival & wt gain were not adversely affected. 1,1,1-Trichloroethane failed to produce significant dominant lethal mutations or teratogenic effects in either of the 2 generations tested (Lane RW et al; Toxicol Appl Pharmacol 63, 3: 409-21, 1982) [366].

The genotoxic effects of 1,1,1-trichloroethane have been studied extensively [936]. Although 1,1,1-trichloroethane was mutagenic in a few assays with Salmonella, induced chromosomal aberrations in a Chinese hamster ovary cell assay, and was positive in most mammalian cell transformation assays, the existing genotoxicity data are largely negative. In addition, positive results may have been produced by stabilizers and not 1,1,1-trichloroethane itself. Therefore, a firm conclusion regarding the genotoxic potential of 1,1,1-trichloroethane in humans is not possible [936].

1,1,1-Trichloroethane was examined for mutagenic activity in Salmonella typhimurium tester strains TA98, TA100, TA1537 and TA1538, both with and without addition of rat liver S9 fraction to provide metabolic activation (Ames Test). Using the plate incorporation technique (dose not stated), all assays were negative (Stanford Research Institute International; Investigations of the Species Sensitivity and Mechanism of Carcinogenicity of Halogenated Hydrocarbons, Final Report, 1984, EPA Document No. 40-8424225, Fiche No. OTS0509408) [366].

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

Spillage, improper disposal, or industrial emissions and consumer use can release large amounts of the chemical into the environment. Contaminated water from landfills and hazardous waste sites may contaminate surrounding soil and nearby surface water or groundwater, but more likely, most of the chemical will eventually evaporate into the air [936].

It is not known how long 1,1,1-trichloroethane lasts in water or soil. From surface waters such as lakes and rivers, where 1,1,1-trichloroethane partially mixes with water, much of it evaporates quickly into the air. It also evaporates into the air from soil surfaces. Water can easily carry 1,1,1-trichloroethane through soil into groundwater, from which it may evaporate and pass through soil as a gas and finally be released to the air. Also, naturally occurring organisms may break down 1,1,1-trichloroethane. One study suggests it takes 200 to 300 days to remove half of the chemical from contaminated groundwater; however, this number may vary widely [936]. See Fate.Detail section below for more details.

Breakdown products include trichloroacetic acid, trichloroethanol, 1,1-dichloroethane, and chloroethane (see Fate.Detail and Associated Chemicals sections below for details).

1,1,1-Trichloroethane will not build up in plants or animals [936].

Food chain concentration potential: None [367].

Because 1,1,1-trichloroethane does not adsorb strongly to soil, it should leach extensively [498].

Environmental Fate/Exposure Summary [366]:

1,1,1-Trichloroethane is likely to enter the environment from air emissions or in wastewater from its production or use in vapor degreasing, metal cleaning, etc. It can also enter the environment in leachates and volatile emissions from landfills. Releases to surface water will decrease in concentrations(s) almost entirely due to evaporation. Spills on land will decrease in concentration almost entirely due to volatilization and leaching. Releases to air may be transported long distances and partially return to earth in rain. In the troposphere, 1,1,1-trichloroethane will degrade very slowly by photooxidation and also slowly diffuse to the stratosphere where photodegradation will be rapid. Major human exposure is from air and drinking water. Exposure can be high near sources of emission or where drinking water is contaminated (SRC)].

Synonyms/Substance Identification:

1,1,1-TRICHLOORETHAAN (DUTCH) [366]
1,1,1-TRICHLORAETHAN (GERMAN) [366]
1,1,1-TRICLOROETANO (ITALIAN) [366]
METHYLCHLOROFORM [366]
METHYLTRICHLOROMETHANE [366]

TRICHLORO-1,1,1-ETHANE (FRENCH) [366]
TRICHLOROETHANE [366]
TRIELENE [366]
CHLOROFORM, METHYL- [366]
ETHANE, 1,1,1-TRICHLORO- [366]
TCEA [366]
AI3-02061 [366]
Caswell No 875 [366]
ALPHA-TRICHLOROETHANE [366]
AEROTHENE TT [366]
ALGYLEN [366]
ALPHA-T [366]
BALTANA [366]
CF 2 [366]
CHLOROETHENE [366]
CHLOROETHANE-NU [366]
CHLOROTENE [366]
CHLOROTHANE NU [366]
CHLOROTHENE SM [366]
CHLOROTHENE VG [366]
CHLORTEN [366]
CHLORTHANE-NU [366]
CHLORYLEN [366]
GEMALGENE [366]
GENKLENE [366]
ICI-CF 2 [366]
INHIBISOL [366]
Dowclene LS [366]
Chlorothene (Inhibited) [366]
Chlorothene NU [366]
SOLVENT 111 [366]
TRI [366]
TRICHLORAN [366]
NCI-C04626 [366]
Aerothene MM [366]

NOTE: Only a few references ([369]) give TCA as a synonym for 1,1,1 trichloroethane, and many major references do not list TCA as a synonym [365,366]. TCA is more often given as a synonym for several herbicides, so this acronym should be used with caution.

Molecular Formula:
C2-H3-Cl3 [366]

Associated Chemicals or Topics (Includes Transformation Products):

Metabolism/Metabolites [366]:

1. Small percentage of 1,1,1-trichloroethane is metabolized to carbon dioxide, while remainder appears in urine as glucuronide of 2,2,2-trichloroethanol. [International Labour Office. Encyclopedia of Occupational Health and Safety. Vols.

I&II. Geneva, Switzerland: International Labour Office, 1983. 2213].

2. Incubation of chloroethanes, hepatic microsomes, an nadph-generating system & edta results in production of chlorinated metabolites. 1,1,1-Trichloroethane is converted by hepatic microsomal cytochrome p450 to 2,2,2-trichloroethanol. [Ivanetich KM, Van den Honert lh; Carcinogenesis 2 (8): 697-702 (1981)].

3. 1,1,1-Trichloroethane is oxidized by the cytochrome p450 system to metabolites that bind covalently to cellular macromolecules, as evidenced by the dependence of the reaction on reduced nicotinamide adenine dinucleotide phosphate (NAPDPH) and the inhibition by carbon monoxide. [National Research Council. Drinking Water & Health. Volume 5. Washington, D.C.: National Academy Press, 1983. 75].

Impurities [366]:

Stabilizing agents which may be present in small amounts include: glycol diesters, ketones, nitriles, dialkyl sulfoxides, dialkyl sulfides, dialkyl sulfites, tetraethyl lead, nitroaliphatic hydrocarbons, 2-methyl-3-butyn-2-ol, tert-butyl alcohol, 1,4-dioxane, dioxolane, sec-butyl alcohol, and monohydric acetylenic alcohols. [NIOSH; Criteria Document: 1,1,1-Trichloroethane p.11 (1976) DHEW Pub No 76-184].

Chemical was found by gas chromatography to contain 1,2-dichloroethane, 1,1-dichloroethane, chloroform, carbon tetrachloride, trichloroethylene, 1,1,2-trichloroethane, & vinylidene chloride. [Stewart RD et al; Arch Environ Health 19 (4): 467-72 (1969)].

Commercial grades of 1,1,1 trichloroethane generally contain inhibitors to prevent its reaction with metals [369]. These inhibitors include 1,4-Dioxane, dioxilane, epichlorohydrin, and 1,2-epoxybutane [369].

Urinary metabolites (Trichloroacetic acid, one of the strongest organic acids, glucuronate, and trichloroethanol) of 1,1,1 trichloroethane can be detected, and this was judged to be a better indicator of total daily exposure than breath analysis [363,369].

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):

No information found.

W.Typical (Water Concentrations Considered Typical):

Except for spill or industrial locations, surface water concentrations are usually less than 1 ppb [936].

Information from HSDB [366]:

DRINKING WATER - 133 United States cities with finished surface water - 0.4 ppb median, 3.3 ppb max; 23 United States cities with finished groundwater - 2.1 ppb median, 3.0 max, 22% of the samples were positive(1). Contaminated drinking water wells in New York, New Jersey, Connecticut and Maine have values of 950-5440 ppb(2). Results of the 1982 EPA Ground Water Supply Survey for 1,1,1-trichloroethane (466 samples) - 5.8% pos, 0.8 ppb median of positives, 18 ppb max(4). As part of EPA's Total Exposure Assessment Methodology (TEAM) study, the concentration of various toxic substances in drinking water of sample populations was measured(3). The mean (maximum) concentrations of 1,1,1-trichloroethane in Bayonne and Elizabeth, New Jersey, an industrial/chemical manufacturing area, was 0.6 (5.3), 0.2 (2.6), and 0.2 (1.6) ppb in the fall 1981, summer 1982, and winter 1983, respectively(3). For comparison the drinking water of a sample of residents of a manufacturing city without a chemical or petroleum refining industry, Greensboro, NC and a small, rural, and agricultural town in North Dakota contained 0.03 (0.05) and 0.04 (0.07) ppb of 1,1,1-trichloroethane, respectively(3). [(1) Coniglio WA et al; EPA Briefing. Criteria and Standards Div. Sci Technol Branch. Exp Assess Proj p. 16 (1980) (2) Brumaster DE; Environ 24: 6-13, 33-6 (1982) (3) Wallace LA et al; Environ Res 43: 290-307 (1987) (4) Contruvo JA; Sci Tot Environ 47: 7-26 (1985)].

GROUNDWATER - Raw groundwater in 13 United States cities - 1.1 ppb median, 13 ppb max, 23% were positive(1). 1,1,1-Trichloroethane has been detected in 18.9% of all groundwater samples analyzed from 178 sites designated as CERCLA (Comprehensive Emergency Response, Compensation and Liability Act) sites by the USEPA monitoring program(2). [(1) Coniglio WA et al; EPA Briefing. Criteria and Standards Div. Sci Technol Branch. Exp Assess Proj p. 16 (1980) (2) Plumb RH Jr; Ground Water Monit Rev 7: 94-100 (1987)].

SURFACE WATER - Raw surface water in 105 United

States cities - 0.2 ppb median, 1.2 ppb max, 12% positive(1). Large study of the Ohio R. Basin in 1980-1981 (4972 samples) reports 33.6% of samples above 0.1 ppb, 3.9% between 1.0 and 0.3% above 10 ppb(2). In a study of 14 heavily industrialized river basins in 1975-1976, 9% of the sites had values above 1 ppb, and 8 ppb was the maximum value measured(3). At industrial sites, mean values are above 10 ppb with maximum values as high as 334 ppb(4). Concentration 20-800 meters away from outfalls of four producing plants and 1 user was 0.1-169 ppm(5). [(1) Coniglio WA et al; EPA Briefing. Criteria and Standards Div. Sci Technol Branch. Exp Assess Proj p. 16 (1980) (2) Ohio River Valley Water Sanit Comm; Assess of Water Qual Cond 1980-81 Cincinnati, OH (1982) (3) Ewing BB et al; Monitoring To Detect Previously Undetected Pollutants In Surface Waters. Appendix: Organic Analysis Data p 1-129 EPA-560/6-77-015A (1977) (4) Pellizzari ED et al; Formulation of Preliminary Assessment of Halogenated Organic Compounds In Man and Environmental Media p. 38-94 EPA-560/13-79-006 (1979) (5) Battelle Columbus Labs; Multimedia Levels Methylchloroform p. 2.1-2.22 EPA-560/6-77-030 (1977)].

SEAWATER: Liverpool Bay seawater averaged <0.25 ppb, 3.3 ppb maximum(1). The mean concentrations(s) of 1,1,1-trichloroethane in arctic seawater collected near Sweden in Aug and Sept 1980 range from about 1.4-1.7 ng/L in the upper 250 meter depths to about 0.4-0.45 ng/L at depths below 1250 meters(2). [(1) Pearson CR, McConnell G; Proc Roy Soc London B 189: 305-32 (1975) (2) Fogelquist E; J Geophys Res 90: 9181-93 (1985)].

RAIN/SNOW - West Los Angeles 26 Mar 82 - 69 parts per trillion(2); La Jolla, Ca - 8.1 parts per trillion (3); an industrial area of England - 0.9 parts per trillion(1). Southern California 6.2 parts per trillion, central California - 0.6 parts per trillion, Alaska 27 parts per trillion (Kawamura K, Kaplan LR; Environ Sci Technol 17: 497-501, 1983) [366].

Average value for 1,1,1-trichloroethane in rain samples from Tokyo, Japan was 369 ng/L between October, 1989 and September, 1990 (Jung et al, 1992) [498].

Effluents Concentrations [366]:

Mean values in raw wastewater of 15 industries range from 3.6 to 38,000 ug/l with the maximum value range from 10 to 1,300,000 ug/l. The highest values were for the metal finishing industry(1). Mean value of treated wastewater for 11 industries 0.6-89 ug/l with maximum values ranging from 0.6 to 7100 ug/l (1). 18-344 ppb outfall from producing plants (2). [(1) USEPA; Treatability Manual page I.12.8-1 to I.12.8-4 EPA-600/2-82-001a (1982) (2) Battelle Columbus Labs; Multimedia levels methylchloroform p 2.1-2.22 (1977)].

In a comprehensive survey of wastewater from 4000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent Guidelines Division of the USEPA, 1,1,1-trichloroethane was identified in discharges of the following industrial category (frequency of occurrence, median concentrations(s) in ppb): timber products (2; 359.7), leather tanning (4; 2.7), iron and steel mfg (6; 34.4), petroleum refining (5; 13.4), nonferrous metals (12; 35.9), paint and ink (36; 9.7), printing and publishing (6; 28.3), ore mining (5; 2.3), coal mining (6; 5.7), organics and plastics (23; 8.5), inorganic chemicals (13; 5.2), textile mills (12; 6.0), plastics and synthetics (12; 1.6), pulp and paper (12; 7.0), rubber processing (10; 24.0), soaps and detergents (1; 26.3), auto and other laundries (10; 6.4), pesticides manufacture (4; 17.0), photographic industries (3; 3.9), pharmaceuticals (20; 3.9), explosives (7; 14.6), plastics mfg (1; 8.3), foundries (5; 54.0), electronics (36; 62.5), electroplating (2; 229.1), organic chemicals (15; 7.2), mechanical products (20; 98.0), transportation equipment (5; 706.3), amusements and athletic goods (4; 33.0), synfuels (8; 6.63), publicly owned treatment works (302; 10.6)(1). The highest effluent concns were 6397 and 6028 ppb in the mechanical products and electronics industry, respectively(1). [(1) Shackelford WM et al; Analyt Chim Acta 146: 15-27 (1983)].

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):

EPA 1996 IRIS Information [893]:

Ambient Water Quality Criteria for Aquatic Organisms

Acute Freshwater: 1.8E+4 ug/L LEC [893].

Chronic Freshwater: None [893].

Acute Marine: 3.12E+4 ug/L LEC [893].

Previous reference gave the same concentration: Marine Acute Criteria: Insufficient data to develop criteria. Lowest Observed Effect Level: 31,200 ug/L [446]. Criteria Federal Register Notice Number: 45 FR 79328 [893].

Marine Chronic: None [893].

Reference: 45 FR 79318 (11/28/80)

Contact: Criteria and Standards Division / OWRS / (202)260-1315

Discussion: The values that are indicated as "LEC" are not criteria, but are the lowest effect levels found in the literature. LECs are given when the minimum data required to derive water quality criteria are not available. [893].

Note: Before citing a concentration as EPA's water quality criteria, it is prudent to make sure you have the latest one. Work on the replacement for the Gold Book [302] was underway in March of 1996, and IRIS is updated monthly [893].

Oak Ridge National Lab, 1994: Ecological Risk Assessment Freshwater Screening Benchmarks for concentrations of contaminants in water [649]. To be considered unlikely to represent an ecological risk, field concentrations should be below all of the following benchmarks [649]:

CAS 71-55-6, TRICHLOROETHANE, 1,1,1- (ug/L):

NATIONAL AMBIENT WATER QUALITY CRITERION - ACUTE: No information found.

NATIONAL AMBIENT WATER QUALITY CRITERION - CHRONIC: No information found.

SECONDARY ACUTE VALUE: 617

SECONDARY CHRONIC VALUE: 62.1

ESTIMATED LOWEST CHRONIC VALUE - FISH: 3493

LOWEST CHRONIC VALUE - DAPHNIDS: 1770

LOWEST CHRONIC VALUE - NON-DAPHNID INVERTEBRATES: No information found.

LOWEST CHRONIC VALUE - AQUATIC PLANTS: > 669,000

ESTIMATED LOWEST TEST EC20 - FISH: 2457

LOWEST TEST EC20 - DAPHNIDS: 1300

SENSITIVE SPECIES TEST EC20: No information found.

POPULATION EC2O: 251

State Water Quality Standards vary widely, with the lowest being New Jersey at 26 ug/L, and many states using 200 ug/L [936].

The Netherlands' Harmonized (between media) Maximum Permissible Concentration (MPC) for this compound in water is 2400 ug/L [655].

Note: Harmonization takes into account whether or not the MPC in one media (such as soil) would lead to exceeding the MPC in another media (such as air, water, or sediment) [655].

The Netherlands' Harmonized (between media) Negligible Concentration (NC) for this compound in water is 1% of the MPC, or 24 ug/L [655].

W.Plants (Water Concentrations vs. Plants):

No information found.

W.Invertebrates (Water Concentrations vs. Invertebrates):

LC50s for Daphnia magna (water flea) were >530 mg/L for a 24-hr exposure, and 5.4 mg/L for a 17-day exposure. The no-observed-effect-concentration (NOEC) for death was 1.3 mg/L for a 17-day exposure [998].

W.Fish (Water Concentrations vs. Fish):

Aquatic toxicity: 75-150 ppm/*/pinfish/Tlm/salt water *Time period not specified [367].

LC50s for Cyprinodon variegatus (sheepshead minnow) were 68 mg/L for a 24-hr exposure, and 71 mg/L for 48-, 72-, and 96-hr exposures. The no-observed-effect-concentration (NOEC) for death was 43 mg/L for a 96-hr exposure [998].

LC50s for Lepomis macrochirus (bluegill) were 40 mg/L for both 24- and 96-hr exposures [998].

LC50s for Oryzias latipes (medaka, high-eyes) were >1000 mg/L for both 24- and 48-hr exposures [998].

Information from HSDB [366]:

LC50 Pimephales promelas (fathead minnow) 52.8 mg/l/96 hr (flow through test) [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 1131].

LC50 Pimephales promelas (fathead minnow) 105 mg/l/96 hr (static test) [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 1131].

LC50 Poecilia reticulata (guppy) 133 ppm/7 day /Conditions of bioassay not specified/ [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 1131].

EC50 Pimephales promelas (fathead minnow) 52.9 mg/l/96 hr (confidence limit not reliable), flow-through bioassay with measured concentrations, 25.5 deg C, dissolved oxygen 5.8 mg/l, hardness 43.8 mg/l CaCO3, alkalinity 42.3 mg/l CaCO3, and pH 7.69. Effect: loss of equilibrium. (Test 1) [Geiger D.L., Poirier S.H., Brooke L.T., Call D.J., eds. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Vol. III. Superior,Wisconsin: University of Wisconsin-Superior, 1986. 29].

LC50 Pimephales promelas (fathead minnow) 52.9 mg/l/96 hr (confidence limit not reliable), flow-through bioassay with measured concentrations, 25.5 deg C, dissolved oxygen 5.8 mg/l, hardness 43.8 mg/l CaCO3, alkalinity 42.3 mg/l CaCO3, and pH 7.69. (Test 1) [Geiger D.L., Poirier S.H., Brooke L.T., Call D.J., eds. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Vol. III. Superior,Wisconsin: University of Wisconsin-Superior, 1986. 29].

LC50 Pimephales promelas (fathead minnow) 42.3 mg/l/96 hr (confidence limit 35.2 -50.7 mg/l), flow-through bioassay with measured concentrations, 25.6 deg C, dissolved oxygen 6.5 mg/l, hardness 46.4 mg/l CaCO3, alkalinity 42.6 mg/l CaCO3, and pH 7.99. (Test 2) [Geiger D.L., Poirier S.H., Brooke L.T., Call D.J., eds. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Vol. III. Superior,Wisconsin: University of Wisconsin-Superior, 1986. 31].

EC50 Pimephales promelas (fathead minnow) 28.8 mg/l/96 hr (confidence limit 23.0 -36.2 mg/l), flow-through bioassay with measured concentrations, 25.6 deg C, dissolved oxygen 6.5 mg/l, hardness 46.4 mg/l CaCO3, alkalinity 42.6 mg/l CaCO3, and pH 7.99. Effect: loss of equilibrium. (Test 2) [Geiger D.L., Poirier S.H., Brooke L.T., Call D.J., eds. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Vol. III. Superior,Wisconsin: University of Wisconsin-Superior, 1986. 31].

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

Oak Ridge National Lab, 1994: Risk Assessment Screening Benchmarks for Wildlife derived from No-Observed-Adverse-Effect (NOAEL) levels (see Tis.Wildlife, B) for these). To be considered unlikely to represent an ecological risk, water concentrations should be below the following benchmarks for each species present at the site [650]:

CAS 71-55-6, 1,1,1-TRICHLOROETHANE

SPECIES	WATER CONCENTRATION (ppm)
Mouse (test species)	0.0000
Short-tailed Shrew	6011.8640
Little Brown Bat	10,390.875
White-footed Mouse	3885.2670
Meadow Vole	6799.9070
Cottontail Rabbit	3222.1030
Mink	3341.2120
Red Fox	2384.5260
Whitetail Deer	1334.1640

Comment: Actually, the number of significant figures for a benchmark value should never be more than one; even if these values have been taken directly from another report, they should be rounded; otherwise the impression is given of a level of accuracy that is simply unwarranted. The uncertainties are too large to justify such a fine distinction (Owen Hoffman, SENES Oak Ridge, Personal Communication, 1997).

Waterfowl toxicity: Data not available [367].

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

EPA 1996 IRIS database information [893]:

Maximum Contaminant Level Goal

Value: 0.2 mg/L [893,952].

Status/Year: Final 1985 Econ/Tech?: No, does not consider economic or technical feasibility Reference: 50 FR 46880 (11/13/85) [893].

Contact: Health and Ecological Criteria Division / (202)260-7571 Safe Drinking Water Hotline / (800)426-4791

Discussion: An MCLG of 200 ug/L for 1,1,1-trichloroethane is proposed based upon a DWEL and an assumed drinking water contribution of 20%. A DWEL of 1.0 mg/L was calculated based on liver toxicity in mice (inhalation study).

Maximum Contaminant Level (MCL)

Value: 0.2 mg/L [893,952].

Status/Year: Final 1987 Econ/Tech?: No, does not consider economic or technical feasibility Reference: technology -- Packed tower aeration; granular activated carbon [893].

Contact: Drinking Water Standards Division / OGWDW / (202)260-7575 Safe Drinking Water Hotline / (800)426-4791 [893].

Discussion: EPA has set an MCL equal to the MCLG [893].

Drinking water equivalent level / lifetime health advisory

DWEL: 1E+0 mg/liter Basis: Oral RfD verified on: 05/15/86 Lifetime HA: 2E-1 mg/liter 20% Exposure by Drinking Water Assumptions: 2 L/day water consumption for a 70-kg adult [893].

According to IRIS 1996, the EPA oral RfD for this substance has been withdrawn pending further review by the RfD/RfC Work Group [893]. However, a 1995 EPA 1996 document listed the oral RfD as 9.0E-02 mg/kg/day [868].

EPA 1995 Region 9 Preliminary remediation goal (PRG) for tapwater, [868]:

1300 ug/L.

Older references:

The national revised primary drinking water maximum contaminant level for 1,1,1-trichloroethane for community water systems is 0.2 mg/l (40 CFR 141.61, 7/1/90, amended by 56 FR 3593, 1/30/91) [366].

Human Health (1E-06 Risk Level for Carcinogens) in ug/L:

Published Criteria for Water and Organisms: 18,400 [446].

Published Criteria for Organisms Only: 1,030,000 [446].

IRIS Recalculated (9/90) Criteria for Water and Organisms: 3,100 [446].

IRIS Recalculated (9/90) Criteria for Organisms Only: 170,000 [446].

Note: According to EPA staff, the US EPA no longer suggests any RfD generated criteria for 1,1,1 trichloroethane; both 170,000 and 1,030,000 are now considered indefensible (Carl Young, EPA, personal communication, 1994).

Drinking Water MCL: 200 [446].

Criteria Federal Register Notice Number: 45 FR 79328

Note: Before citing a concentration as EPA's water quality criteria, it is prudent to make sure you have the latest one. Work on the replacement for the Gold Book [302] was underway in March of 1996, and IRIS is updated montly [893].

Acceptable Daily Intake [366]:

9.4 mg/l based upon a low dose of 375 mg/kg [USEPA; Drinking Water Criteria Document for 1,1,1-Trichloroethane (Draft) p.VIII-12 (Jan 85)].

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

No information found.

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):

Liverpool Bay marine sediment <5.5 ppb (1). Average background concentration in sediment (St. Francis National Forest) 0.45 ppb (2). [(1) Pearson CR, McConnell G; Proc Roy Soc London B 189:305-32 (1975) (2) Battelle Columbus Labs; Multimedia Levels Methylchloroform p 2.1-2.22 EPA-560/6-77-030 (1977) [366].

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):

Oak Ridge National Lab, 1994: Risk Assessment Screening Benchmarks for Sediment Concentrations. To be considered unlikely to represent an ecological risk, field concentrations should be below all of the following benchmarks in mg/kg (ppm) dry weight [652]:

ESTIMATED EQUIVALENT SEDIMENT QUALITY CRITERION at 1% Organic Carbon: 0.179

> Comment: Actually, the number of significant figures for a benchmark value should never be more than one; even if these values have been taken directly from another report, they should be rounded; otherwise the impression is given of a level of accuracy that is simply unwarranted. The uncertainties are too large to justify such a fine distinction (Owen Hoffman, SENES Oak Ridge, Personal Communication, 1997).

The Netherlands' Harmonized (between media) Maximum Permissible Concentration (MPC) for this compound in sediments is 13 mg/kg [655].

> Note: Harmonization takes into account whether or not the MPC in one media (such as soil) would lead to exceeding the MPC in another media (such as air, water, or sediment) [655].

The Netherlands' Harmonized (between media) Negligible Concentration (NC) for this compound in sediments is 1% of the MPC, or 0.13 mg/kg [655].

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):

Soil concentrations were summarized by ATSDR in 1994 [936]. In relatively clean areas, 0.06 ppb was found [936].

Soil.High (Soil Concentrations Considered High):

Soil concentrations were summarized by ATSDR in 1994 [936]. In polluted areas, up to 230,000 ppb were found [936].

Soil.Typical (Soil Concentrations Considered Typical):

Soil around production plants and user industry 0.06-0.94 ppb; average background concentration in soil (St. Francis National Forest) 0.42 ppb (Battelle Columbus Labs; Multimedia Levels Methylchloroform p 2.1-2.22 EPA-560/6-77-030 (1977) [366].

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):

The Netherlands' Harmonized (between media) Maximum Permissible Concentration (MPC) for this compound in soil is 13 mg/kg [655].

Note: Harmonization takes into account whether or not the MPC in one media (such as soil) would lead to exceeding the MPC in another media (such as air, water, or sediment) [655].

The Netherlands' Harmonized (between media) Negligible Concentration (NC) for this compound in soil is 1% of the MPC, or 0.13 mg/kg [655].

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 1996 National Generic Soil Screening Level (SSL) designed to be conservative and protective at the majority of sites in the U.S. but not necessarily protective of all known human exposure pathways, land uses, or ecological threats [952]:

SSL = none given for ingestion pathway [952].

SSL = 1200 mg/kg for inhalation pathway [952].

SSL = 0.1 to 2 mg/kg for protection from migration to groundwater at 1 to 20 Dilution-Attenuation Factor (DAF) [952].

EPA 1995 Region 9 Preliminary remediation goals (PRGs), 1995 [868]:

Residential Soil: 3000 mg/kg wet wt.
Industrial Soil: 3000 mg/kg wet wt.

NOTE:
1) 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.
2) Values are based on a non-carcinogenic hazard quotient of one.
3) PRGs for residential and industrial landuses 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:

0.9 mg/Kg dry weight [903].

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

No 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:

<9.4-35 ppb (in analytical work CCl_4 was not separable from 1,1,1-trichloroethane) in marine algae (Pearson CR, McConnell G; Proc Roy Soc London B 189:305-32, 1975) [366].

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:

See Tis.Fish, C) below.

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):

EPA 1995 Region 3 Risk based concentration (RBC) for fish tissue to protect human health:

120 mg/Kg [903].

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:

Fish/Seafood Concentrations [366]:

Three species of fish, mollusks in Irish Sea - 2-16 ppb(1). Flesh of nine samples of various fish from Liverpool Bay and Thames Estuary - 0-5 ppb, gut contained up to 26 ppb (2). Marine invertebrates in bays and estuaries of Great Britain - 0-34 ppb (2). [(1) Dickson AG, Riley JP; Marine Pollut Bull 7:167-70 (1976) (2) Pearson CR, McConnell G; Proc Roy Soc London B 189:305-32 (1975)].

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):

Oak Ridge National Lab, 1994: Risk Assessment Screening Benchmarks for Wildlife derived from No-Observed-Adverse-Effect (NOAEL) levels (mg contaminant per kg body weight per day). To be considered unlikely to represent an ecological risk, wet-weight field concentrations should be below the following (right column) benchmarks for each species present at the site [650]:

CAS 71-55-6, 1,1,1-TRICHLOROETHANE

SPECIES	NOAEL (mg/kg/day)	FOOD CONCENTRATION (ppm)
Mouse (test species)	1000.0000	0.0000
Short-tailed Shrew	1322.6100	2204.3500
Little Brown Bat	1662.5400	4987.6200
White-footed Mouse	1165.5800	7541.9880
Meadow Vole	927.2600	8159.8880
Cottontail Rabbit	311.4700	1577.0630
Mink	330.7800	2414.4530
Red Fox	201.3600	2013.6000
Whitetail Deer	87.3700	2837.0140

Comment: Actually, the number of significant figures for a benchmark value should never be more than one; even if these values have been taken directly

> from another report, they should be rounded; otherwise the impression is given of a level of accuracy that is simply unwarranted. The uncertainties are too large to justify such a fine distinction (Owen Hoffman, SENES Oak Ridge, Personal Communication, 1997).

Information from HSDB [366]:

> LD50 Mouse (female) single oral 11.24 g/kg [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 1131].
>
> LD50 Rabbit (female) single oral 5.66 g/kg [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 1131].
>
> LD50 Guinea pig (male) single oral 9.47 g/kg [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 1131].
>
> Groups of 50 male & 50 female B6C3F1 mice, 5 wk of age, were given technical-grade 1,1,1-trichloroethane containing about 3% para-dioxane & 2% minor impurities in corn oil by gavage on 5 days/wk for 78 wk. Initially the high & low doses for both male & female mice were 4000 & 2000 mg/kg body wt/day; during the 10th wk ... these doses were increased to 5000 & 2500 mg/kg body wt/wk; at wk 20 they were increased to 6000 & 3000 mg/kg body wt/day & maintained at these levels to the end of the study. Time-weighted avg doses for high- & low-dose mice were 5615 & 2807 mg/kg body wt/day, respectively. A group of 20 male & 20 female untreated mice were used as controls; no vehicle-control animals were used. In males, 10/20 of the unmatched controls, 21/50 of the low-dose group, & 25/50 of the high-dose group had died within 1 yr after the start of the experiment; in females, the corresponding figures were 1/20, 9/50 & 20/50. At 90 wk, 15 low-dose males, 11 high-dose males, 23 low-dose females & 13 high-dose females were still alive. All animals were killed at 95 wk. Almost all organs, & tissues with macroscopically visible lesions, were exam histologically. Three out of 49 males in high-dose group developed liver-cell adenomas & 1 a hepatocellular carcinomas. No liver

tumors occurred in controls. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V20 521 (1979)].

Groups of 50 male & 50 female Osborne-Mendel rats, 7 wk of age, received technical-grade 1,1,1-trichloroethane containing 3% para-dioxane & 2% minor impurities in corn oil by gavage on 5 days a wk for 78 wk at 2 dose levels: 750 mg/kg body wt/day & 1500 mg/kg body wt/day. A group of 20 male & 20 female untreated rats served as matched controls. The animals were killed 110 wk after the start of treatment. Both males & females given the test chemical exhibited early mortality when compared with the untreated controls: only 3% of treated rats survived to termination of experiment. A few tumors not considered to be related to treatment were observed. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V20 523 (1979)].

Rats given 1500 & 750 mg/kg/day orally from 7-117 wk of age developed nasal discharge, wheezing, urine staining on abdominal fur, & hunched appearance. Tumors observed were not attributed to 1,1,1-trichloroethane. [Carcinog Tech Rep Ser- Natl Cancer Inst (US): 70 PAGES (1977) ISS NCI-CG-TR-3].

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

Irish Sea and North Sea - fresh and saltwater birds - 2.4 to 26 ppb, grey seal - 2.5 to 7.2 ppb. Frodsham Marsh, England - shrew -2.6 to 7.8 ppb(1). /Methyl chloroform (Battelle Columbus Laboratories; Multimedia levels methyl chloroform. EPA-560/6-77-030 p 5-3, 1977) [366].

<16-30 ppb grey seal blubber, <2.3-7 ppb common shrew, <1.1-4.7 ppb in flesh or organs of fresh- and seawater birds (in analytical work CCl4 was not separable from 1,1,1-trichloroethane)(Pearson CG, McConnell G; Proc Roy Soc London B 189: 305-32, 1975) [366].

Tis.Human:

A) Typical Concentrations in Human Food Survey Items:

Food concentrations were summarized by ATSDR in 1994 [936].

5-10 ng/g oils and fats; 1-4 ng/g fruits and vegetables; 2-7 ng/g meat, tea, bread (1). 1,1,1-Trichloroethane was not found in samples of wheat, corn, oats, corn meal or corn grits(2). Of the 9 samples of intermediate grain-based food analyzed, it was found in 3, namely, yellow corn meal (3.8 ppb), fudge brownie mix (3.0 ppb), and yellow cake mix (0.74 ppb)(1). [(1) McConnell G et al; Endeavor 34:13-8 (1975) (2) Heikes DL, Hopper ML; J Assoc Off Anal Chem 69: 990-8 (1986)] [366].

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):

EPA 1995 Region 3 Risk based concentration (RBC) for fish tissue to protect human health:

120 mg/Kg [903].

The EPA oral RfD for this substance has been withdrawn pending further review by the RfD/RfC Work Group [893].

Acceptable Daily Intake [366]:

9.4 mg/l based upon a low dose of 375 mg/kg [USEPA; Drinking Water Criteria Document for 1,1,1-Trichloroethane (Draft) p.VIII-12 (Jan 85)].

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

Body Burdens [366]:

Body fat of 8 subjects - 1.6-24 ng/g, various organs - <5.1 ng/g(1). Sample residents of Old Love Canal, breath - 290 ng/cu m median, 2800 ng/cu m maximum, blood - 0.85 ng/ml median, 2.0 ng/ml maximum, urine - 80 ng/l median, 180 ng/l maximum(2). Detected in all eight samples of mother's milk from four urban areas(3). 59% of individuals (39 subjects, 23-54 years of age) from Dusseldorf, West Germany who were not occupationally exposed to 1,1,1-trichloroethane-whole had blood levels of the chemical ranging from <0.1-3.4, ppb median 0.2 ppb(4). Whole blood samples of those occupationally exposed contained 1,1,1-trichloroethane ranging from <0.1-0.2 ppb for motor vehicle mechanics, <0.1 for painters, 0.1-15.5 ppb for precision tool makers, 389.0-2497.9 ppb for dry cleaners using tetrachloroethylene as dry-cleaning agent, and 17.6-48.2 ppb for dry cleaners using trichlorofluoromethane as a dry-cleaning agent(4). Blood samples were drawn during the work day after 4 to 7 hr exposure. In another study, 1,1,1-trichloroethane in the whole blood of 250 patients who suffered from a variety of symptoms that may have been related to exposure to environmental pollutants ranged from not detectable to 26 ppb, 1.0 ppb mean(5). As part of EPA's Total Exposure Assessment Methodology (TEAM) study, the concentration of various toxic substances in breath sample populations was measured(6). The weighted median results for 1,1,1-trichloroethane in Bayonne and Elizabeth, New Jersey, an industrial/chemical manufacturing area, was 6.6, 5.2, and 2.3 ug/cu m in the fall 1981, summer 1982, and winter 1983, respectively(6). For comparison, breath samples of residents of a small, rural, and agricultural town in North Dakota contained 9.3 ug/cu m of 1,1,1-trichloroethane(6). Human tissue sample collected in Turku, Finland in 1987 contained the following levels of 1,1,1-trichloroethane: kidney, 0.1 ug/kg; lungs, 0.1 ug/kg; muscle, 0.4 ug/kg(7). [(1) McConnell G et al; Endeavour 34: 13-8 (1975) (2) Barkley J et al; Biomed Mass Spectrom 7: 139-47 (1980) (3) Pellizzari ED et al; Environ Sci Technol 16: 78-5 (1982) (4) Hajimiragha H et al; Int Arch Occup Environ Health 58: 141-50 (1986) (5) Antoine SR et al; Bull Environ Contam Toxicol 36: 364-71 (1986) (6) Wallace LA et al; Environ Res 43: 290-307 (1987) (7) Kronfeld R, Reunanen M; Bull Environ Contam Toxciol 42: 873-7 (1989).

Detected in all eight samples of mother's milk from four urban areas(1). Pasteurized milk samples collected from suburban areas in Finland contained a mean 1,1,1-trichloroethane conc of 0.008 ug/L(2). [(1) Pellizzari ED et al; Environ Sci Technol 16: 781-5 (1982) (2) Kronfeld R, Reunanen M; Bull Environ Contam Toxicol 44: 917-23 (1990).

The fate of methyl chloroform (MC) was evaluated in six healthy male Caucasian volunteers (26 to 54 years old) receiving a single six hour exposures to the test material at 350 and 35ppm in a dynamic air flow chamber. The concentration of MC in blood and expired air were proportional to the exposure concentration and indicated about 25% of the inhaled MC was absorbed. Elimination of MC was tri-exponential with half-lives estimated as 44 minutes, 5.7 hours and 53 hours for the initial, intermediated and terminal phases. Over 91% of the absorbed MC was eliminated as the parent chemical via the lungs, 5-6% was eliminated as the metabolites trichloroethanol and trichloroacetic acid, and less than 1% remained in the body after 9 days. It was concluded that elimination of MC was first order. [Dow Toxicology Research Laboratory; Kinetics and Metabolism of Inhaled Methyl Chloroform in Human Volunteers, (1983), EPA Document No. 878213685, Fiche No. OTS0206356].

Tis.Misc. (Other Tissue Information):

No information found.

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

Bioconcentration [366]:

The BCF in bluegill sunfish in a 28 day test was 8.9(2). This indicates that 1,1,1-trichloroethane has little tendency to bioconcentrate in fish. Although the amount of experimental data for 1,1,1-trichloroethane is limited, confidence in this result is increased because values of BCFs in related compounds are similar(1). [(1) Barrows ME et al; Dyn Exp Hazard Assess Toxic Chem Ann Arbor Mi: Ann Arbor Sci p. 379-92 (1980) (2) Davies RP, Dobbs AJ; Ater Res 18: 1253-62 (1984)].

Biological Half-Life [366]:

8.7 + or - 1.8 hr (in human urine). [Seki Y; Int Arch Arbeitsmed 34: 39-49 (1975) as cited in NIOSH; Criteria Document: 1,1,1-Trichloroethane p.34 (1979) DHEW Pub. NIOSH 76-184].

Human half-life of elimination was calculated for the following compartments: Vessel-rich tissues (0.8 hr); Muscle and skin (7 hr); Adipose tissue (35 hr) following exposure of subjects to 72 and 215 ppm methyl chloroform. [Humbert BE, Fernandez JG; Arch Mal Prof 38: 415-25 (1977) as cited in USEPA; Health Assessment Document: 1,1,1-Trichloroethane p.4-16 (1982) EPA-600/8-82-003].

Interactions:

Information from HSDB [366]:

A 24 HR inhalation of methyl chloroform by male mice decr sodium hexobarbital (80 mg/kg) induced hypnosis, but had no effect on sodium barbital or chloral hydrate induced hypnosis. [Lal H, Shah HC; Toxicol Appl Pharmacol 17 (3): 625-33 (1970)].

Acute behavioral & lethal effects of oral ethanol & inhaled 1,1,1-trichloroethane (TCE) (sic) alone & in combination were determined in mice. For lethality, ethanol shifted TCE (sic) concn-effect curve to left in parallel manner, with magnitude of shift directly related to dose of ethanol. Combinations of low doses of ethanol with TCE (sic) were usually supraadditive, while higher doses of ethanol were additive or infraadditive with TCE (sic). Shifts to left of TCE (sic) concn-effect curves for behavioral testing similarly depended on dose of ethanol, but were nonparallel. Probably, in many combinations, significant acute toxicity may occur with joint admin. Health hazards to workers who ingest ethanol prior to on-the-job exposure to TCE (sic) are discussed. [Woolverton WL, Balster RL; Toxicol Appl Pharmacol 59 (1): 1-7 (1981)].

Isopropanol & acetone enhanced hepatotoxicity with 1,1,1-trichloroethane. [Doull, J., C.D.Klassen, and M.D. Amdur (eds.). Casarett and Doull's Toxicology. 3rd ed., New York: Macmillan Co., Inc., 1986. 304].

The potentiation of haloalkane hepatotoxicity occurs with a number of different ketonic solvents (methyl n-butyl ketone, methyl ethyl ketone, 2,5-hexanedione). ... /Haloalkanes/ [Doull, J., C.D.Klassen, and M.D. Amdur (eds.). Casarett and Doull's Toxicology. 3rd ed., New York: Macmillan Co., Inc., 1986. 304].

Uses/Sources:

Trichloroethane is a component in commercially available adhesive tape removers such as: Uni-Solve(R), Clinipad(R), and Whisk(R) [363]. It has been used as a propellant and as a solvent in pesticides [498].

Major Uses [366]:

Solvent for natural & synthetic resins, oils, waxes, tar & alkaloids [Browning, E. Toxicity and Metabolism of Industrial Solvents. New York: American Elsevier, 1965. 254].
Dry cleaning agent [Hamilton, A., and H. L. Hardy. Industrial Toxicology. 3rd ed. Acton, Mass.: Publishing Sciences Group, Inc., 1974. 285].

In cold type metal cleaning of plastic molds [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989. 1516].
Formerly used with ethylene gas for degreening citrus fruits & postharvest fumigation of strawberries [Farm Chemicals

Handbook 1984. Willoughby, Ohio: Meister Publishing Co., 1984.,p. C-231].

Solvent for various insecticides /Former use/ [Farm Chemicals Handbook 1984. Willoughby, Ohio: Meister Publishing Co., 1984.,p. C-231].

Spotting fluid in textile processing; ... Chem int for org chems (eg, vinylidene chloride); solvent for adhesives & coatings; coolant & lubricant in metal cutting oils; extraction solvent; component of inks & drain cleaners; solvent for photoresist polymers; solvent in textile dyeing. [SRI].

In aerosols, in which it acts both as a vapor pressure depressant and as a solvent and carrier for many of the active ingredients used in aerosols. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V20 518 (1979)].

Vapor degreasing [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. V5 731 (1979)].

Solvent for cleaning precision instruments; metal degreasing, pesticide, textile processing. [Sax, N.I. and R.J. Lewis, Sr. (eds.). Hawley's Condensed Chemical Dictionary. 11th ed. New York: Van Nostrand Reinhold Co., 1987. 1176].

Natural Occurring Sources [366]:

1,1,1-Trichloroethane is not known to occur as a natural product(1). [IARC; Monograph Some Halogenated Hydrocarbons 19: 515-31 (1979)].

Artificial Sources [366]:

Wastewater and stack and fugitive emissions from production; Volatilization losses from its use in the cold cleaning of metals, vapor degreasing and as a solvent and aerosol, etc(1). Mean emissions rate of 1,1,1-trichloroethane that would contribute to its presence in indoor air are (source - rate (ng/min-sq m): cleaning agents and pesticides - 37,000; painted sheetrock - 31; glued wallpaper - 84; glued carpet 260(2). 1,1,1-Trichloroethane can be released to the environment in leachates from municipal and industrial landfills(3,4,5); it can also be released in volatile emissions from landfills(6). [(1) USEPA; Source Assessment: Chlorinated Hydrocarbon Manufacture USEPA-600/2-79-019G (1979) (2) Wallace LA et al; Atmos Environ 21: 385-93 (1987) (3) Battista JR, Connelly JP; VOC Contamination at Selected Wisconsin Landfills - Sampling Results and Policy Implication.

Wisconsin Dept of Nat Res, Madison, Wisc. Publ-SW-094 89 (1989) (4) Baker JF; Water Pollut Res J Can 22: 33-48 (1987) (5) Foerst C et al; Vom Wasser 72: 295-305 (1989) (6) Koenig HP et al; J Aerosol Sci 18: 837-40 (1987)].

Of the 1026 brand samples of household products representing 67 products categories (cleaners, polishes, lubricants, and paint removers), 14.1% of samples and 47.8% of product categories contained 1,1,1-trichloroethane ranging from 3.3 to 100%(1). [(1) Frankenberry M et al; Household products containing methylene chloride and other chlorinated solvents: A shelf survey. Rockville, MD: Westat Inc (1987)]].

Forms/Preparations/Formulations:

Information from HSDB [366]:

1,1,1-Trichloroethane is available commercially in the USA in technical & solvent grades, which differ only in amt of stabilizer added to prevent corrosion of metal parts. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work).,p. V20 516 (1979)].

Chlorothene SM, industrial grade [Kuney, J.H. and J.N. Nullican (eds.) Chemcyclopedia. Washington, DC: American Chemical Society, 1988. 120].

Aerothene TT, aerosol grade [Kuney, J.H. and J.N. Nullican (eds.) Chemcyclopedia. Washington, DC: American Chemical Society, 1988. 120].

Industrial grade; aerosol grade; general solvent grade, 99.999% grade [Kuney, J.H. and J.N. Nullican (eds.) Chemcyclopedia. Washington, DC: American Chemical Society, 1988. 120].

Chlorothene VG solvent is a specially inhibited grade of 1,1,1-trichloroethane. Chlorothene SM & Aerothene MM solvents are special grades of 1,1,1-trichloroethane & methylene chloride. [Flick, E.W. Industrial Solvents Handbook. 3rd ed. Park Ridge, NJ: Noyes Publications, 1985. 139].

Stabilized grades contain 3-8% stabilizers such as nitromethane, N-methylpyrrole ... butylene oxide, 1,3-dioxolane, and secondary butyl alcohols. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V20 516 (1979)].

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

Solubilities [366]:

Sol in acetone, benzene, methanol, carbon tetrachloride [The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 1377].

> 10% in ethanol [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985.,p. V1 607].

4,400 mg/l in water at 20 deg C [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 606].

Sol in carbon disulfide [International Labour Office. Encyclopedia of Occupational Health and Safety. Vols. I&II. Geneva, Switzerland: International Labour Office, 1983. 2213].

> 10% in ethyl ether [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985.,p. V1 607].

> 10% in chloroform [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985.,p. V1 607].

Vapor Pressure [366]:

127 MM HG AT 25 DEG C [Sunshine, I. (ed.). CRC Handbook of Analytical Toxicology. Cleveland: The Chemical Rubber Co., 1969. 663].

Octanol/Water Partition Coefficient [366]:

log Kow= 2.49 [Hansch, C. and A. Leo. The Log P Database. Claremont, CA: Pomona College, June 1984].

Henry's Law Constant [366]:

1,1,1-Trichloroethane has a high Henry's Law constant (8X10-3 atm-cu m/mole) [Lyman WJ et al; pp. 15-1 to 15-43 in Handbook of Chem Property Estimation Methods NY: McGraw-Hill (1982)].

Molecular Weight [366]:

133.42 [The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 1377].

Density/Specific Gravity [366]:

1.3376 AT 20 DEG C/4 DEG C [The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 1377].

Boiling Point [366]:

74.1 DEG C AT 760 MM HG [Weast, R.C. (ed.) Handbook of Chemistry and Physics, 68th ed. Boca Raton, Florida: CRC Press Inc., 1987-1988.,p. C-266].

Melting Point [366]:

-30.4 DEG C [Weast, R.C. (ed.) Handbook of Chemistry and Physics, 68th ed. Boca Raton, Florida: CRC Press Inc., 1987-1988.,p. C-266].

Corrosivity [366]:

Readily corrodes aluminum and aluminum alloys [ITII. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1982. 536].

Dry, uninhibited 1,1,1-trichloroethane is not very corrosive with iron or zinc; corrosion rate with iron is < 2.54 um/yr (< 0.1 mpy) & with zinc < 25.4 um/yr (< 1.0 mpy). Addition of 7% water incr corrosion rates to 254 um/yr (< 10.0 mpy) for iron & > 254 um/yr (> 10.0 mpy) for zinc. The presence of both water & ethanol incr iron or tin attack at reflux. [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. V5 728 (1979)].

Color/Form [366]:

Colorless liquid [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. 3503].

Odor [366]:

Chloroform-like odor; sweetish [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5].

Critical Temperature and Pressure [366]:

1. 311.5 deg C; 4.48 MPa [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. V5 729 (1979)].

Heat of Combustion [366]:

1. 4700 BTU/LB= 2600 CAL/G= 110X10+5 J/KG [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5].

Heat of Vaporization [366]:

1. 8012.7 gcal/gmole [Weast, R.C. (ed.) Handbook of Chemistry and Physics, 68th ed. Boca Raton, Florida: CRC Press Inc., 1987-1988.,p. C-671].

Surface Tension [366]:

1. 25.4 DYNES/CM [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5].

Vapor Density [366]:

1. 4.63, relative (Air= 1) [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 1129].

Relative Evaporation Rate [366]:

1. 12.8 (Butyl acetate= 1) [Mackison, F. W., R. S. Stricoff, and L. J. Partridge, Jr. (eds.). NIOSH/OSHA - Occupational Health Guidelines for Chemical Hazards. DHHS(NIOSH) PublicationNo. 81-123 (3 VOLS). Washington, DC: U.S. Government Printing Office, Jan. 1981].

Viscosity [366]:

1. 0.858 cP @ 20 deg C [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. V5 729 (1979)].

Other Chemical/Physical Properties [366]:

1. Percent in saturated air: 16.7 AT 25 DEG C. [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. 3503].

2. Latent heat of vaporization: 100 BTU [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5].

3. Liquid-water interfacial tension: 45 dynes/cm (est) [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5].

4. Ratio of specific heats of vapor (gas): 1.104 [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5].

5. Sat concentrations(s) in air 726 g/cu m @ 20 deg C, 1,088 g/cu m @ 30 deg C [Verschueren, K. Handbook of Environmental

Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 606].

6. Partition coefficients at 37 deg C for 1,1,1-trichloroethane into blood= 3.3; into oil= 356. [Sato A, Nakajima T; Scand J Work Environ Health 13: 81-93 (1987)].

7. Dielectric constant: 7.53 @ 20 deg C (liq) /from table/ [Dean, J.A. Handbook of Organic Chemistry. New York, NY: McGraw-Hill Book Co., 1987.,p. 4-77].

8. Specific heat @ 20 deg C: 1.004 J/g (liq); 0.782 J/g [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. V5 729 (1979)].

9. Dipole moment: 1.78 Debyes [Weast, R.C. (ed.) Handbook of Chemistry and Physics, 68th ed. Boca Raton, Florida: CRC Press Inc., 1987-1988.,p. E-59].

10. Heat of capacity @ 25 deg C: 34.4 cal/gmole @ 1 atm (liq); 22.4 cal/gmole @ 1 atm (gas) [Weast, R.C. (ed.) Handbook of Chemistry and Physics, 68th ed. Boca Raton, Florida: CRC Press Inc., 1987-1988.,p. D-173].

11. Chlorothene VG Solvent: Freezing Point -36.9 deg C; Boiling range @ 760 mm Hg 72-88 deg C; Density 1.232 g/ml @ 20 deg C; Specific gravity 1.327 @ 20 deg C/20 deg C, 1.333 @ 60 deg C/60 deg C, 1.320 @ 25 deg C/25 deg C; Heat of vaporization 7.8 kcal/mol @ 20 deg C, 7.5 kcal/mol @ 50 deg C, 7.1 kcal/mol @ 80 deg C (calculated); Dielectric constant @ 24 deg C 10.0 @ 10+3 cps, 7.0 @ 10+5 cps [Flick, E.W. Industrial Solvents Handbook. 3rd ed. Park Ridge, NJ: Noyes Publications, 1985. 139].

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

Information from HSDB [366]:

TERRESTRIAL FATE: 1,1,1-Trichloroethane evaporates fairly rapidly into the atmosphere because of its high vapor pressure. Because 1,1,1-trichloroethane does not adsorb strongly to soil, it should leach extensively. (SRC).

AQUATIC FATE: Primary loss will be by evaporation into the atmosphere. Half-life will range from hours to a few weeks depending on wind and mixing conditions. Half-lives in a mesocosm simulating the conditions in Narragansett Bay were 24, 12, and 11 days under spring, summer and winter conditions, respectively(1). Biodegradation and adsorption onto particulate matter will be insignificant relative to volatilization (1). Turbulance in microcosm tanks are substantially less than in the bay or the open ocean so volatilization may be significantly (up to an order of magnitude) faster in the bay or open water than measured in the mesocosms. (SRC) [(1) Wakeham SG et al; Environ Sci Technol 17:611-7 (1983)].

ATMOSPHERIC FATE: 1,1,1-trichloroethane is fairly stable in the atmosphere and is transported long distances, being found even at the South Pole (1,2,3). It is transported to Barrows, Alaska from the mid-latitudes(1). It is slowly degraded principally by reaction with hydroxyl radicals and has a half-life of 6 months to 25 years (2,4). The global lifetime average has been estimated to be 6.0-6.9 years(7). The rate of degradation is increased by the presence of chlorine radicals and nitrogen oxides. 15% of the 1,1,1-trichloroethane drifts into the stratosphere where it is rapidly degraded by photodissociation (2,4). Due to the large input of 1,1,1-trichloroethane into the atmosphere and its slow degradation, the amount of 1,1,1-trichloroethane in the atmosphere is increasing by 4.8-17% a year (6,4,7). Some of the 1,1,1-trichloroethane returns to earth in rain as is evidenced by its presence in rainwater and a 40% reduction in air concentrations on rainy days(5). [(1) Khalil MAK, Rasmussen RA; Environ Sci Technol 17:57-64 (1983) (2) Battelle Columbus Labs; Multimedia Levels: Methylchloroform page 3-1 to 3-6 USEPA-560/6-77-030 (1977) (3) Rasmussen RA et al; Science 211:285-7 (1981) (4) Callahan MA et al; Water-related Environmental Fate of 129 Priority Pollutants Vol II p 45-1 to 45-12 USEPA-440/4-79-029B (1979) (5) Ohta T et al; Atmos Environ 11:985-7 (1977) (6) Khalil MAK, Rasmussen RA; J Air Pollut Control Assoc 31:1274-5 (1981) (7) Prinn R et al; Sci 238: 945-50 (1987)].

Biodegradation [366]:

No or very slow degradation in soils. No degradation has been observed in subsurface soils in 27 weeks; However in loamy sand, slow degradation has been observed under acclimated conditions (1,2). Slow degradation may occur in water under anaerobic or aerated conditions; Degradation may take several weeks and acclimation is important (3,4). In seawater, a half-life of 9 months has been determined and vinylidene chloride is the degradation product(5). No degradation in river water has been found(6). No utilization of 1,1,1-trichloroethane occurred in a continuously-fed aerobic biofilm reactor that utilized acetate as its primary substrate(8). However, 98% removal was obtained in a similar anaerobic reactor with a 2 day retention time after 8 wk acclimation(8). 1,1,1-Trichloroethane degraded to vinylidene chloride as a first step in its biotransformation in microcosms containing aquifer water and sediment collected from uncontaminated sites in the Everglades(7). Considerable degradation occurred within two weeks(7). Field evidence of biodegradation in aquifers was obtained by following the concentration of 1,1,1-

trichloroethane in a confined aquifer after it was injected with reclaimed groundwater(8). The half-life of 1,1,1-trichloroethane was 231 days with biodegradation given as the probable cause of loss(8). [(1) Wilson JT et al; Devel Indust Microbiol 24:225-33 (1983) (2) Bouwer EJ et al; Water Res 15:151-9 (1981) (3) Bouwer EJ, McCarty PL; Appl Environ Microbiol 45:1286-94 (1983) (4) Tabak HH et al; J Water Pollut Control Fed 53:1503-18 (1981) (5) Pearson CR, McConnell G; Proc Roy Soc London B 189:305-32 (1975) (6) Mudder TI; Amer Chem Soc Div Environ Chem p 52-3, Kansas City, MO (1982) (7) Parsons F, Lage GB; J Am Water Works Assoc 77: 52-9 (1985) (8) McCarthy PL et al; Groundwater Pollut Microbiol pp. 89-115 (1984)].

1,1,1-Trichloroethane has been shown to undergo biotransformation under methanogenic conditions(1,2,7); the biotransformation proceeds by a reductive dechlorination to 1,1-dichloroethane and chloroethane(1). Laboratory reactors using mixed acclimated anaerobic microbial populations have demonstrated that 1,1,1-trichloroethane can be biodegraded under anaerobic simulations(3,4,5); it was suggested that in-situ anaerobic biodegradation may be a viable alternative for clean-up for various contaminated soil and groundwater sites(5). 1,1,1-Trichloroethane biodegraded in anoxic bioflim columns with an effluent removal that exceeded 99% (at 10 ppb influent) after 9-12 wks of acclimation(6). [(1) Vogel TM, McCarty PL; Environ Sci Technol 21: 1208-13 (1987) (2) Henson JM et al; J Indust Microb 4: 29-35 (1989) (3) Vargas C, Alhert RC; J Water Pollut Control Fed 59: 964-8 (1987) (4) Boyer JD et al; Haz Waste Haz Mater 4: 241-61 (1987) (5) Boyer JD et al; J Water Pollut Contr Fed 60: 1843-9 (1988) (6) Bouwer EJ, Wright JP; J Contam Hydrol 2: 155-69 (1988) (7) Strand SE et al; J Water Pollut Control Fed 62: 124-9 (1990)].

Abiotic Degradation [366]:

Hydrolysis is not a significant degradation process having a half-life of approximately 6 months (1,2). The product of hydrolysis is vinylidene chloride(11). Direct photolysis is not important in the troposphere since 1,1,1-trichloroethane does not absorb light above 290 nm. In the stratosphere, photolysis is important and leads to the chemical's rapid degradation(2,3). 1,1,1-Trichloroethane reacts slowly with hydroxyl radicals which are produced by sunlight in the atmosphere. Based upon a rate constant of 1.19X10-14 cu cm/molcule-sec of 25 deg C, the half-life for this reaction is 3.7 yr, assuming a diurnally averaged OH radical concentration of 5X10+5 radicals/cu cm(12). Estimates of half-life in the troposphere range from 0.5 to 2.2 years, much slower than unsaturated chloroalkanes, but much greater than completely chlorinated compounds such as carbon tetrachloride(1,4,5). Products of photooxidation include phosgene, Cl2, HCl, and CO2(6,7). Degradation is reported to be greatly increased by exposure to ozone and chlorine but no actual data could be found in regard to 1,1,1-trichloroethane's reactivity with ozone(7). On exposure to nitrogen oxide, less than 5% degradation occurs in 8 hours(8). There is some evidence that photodegradation is catalyzed by surfaces which results in complete degradation within 2 weeks(9). Indirect evidence of photodegradation comes from the fact that levels of 1,1,1-trichloroethane are lowest in the afternoon and 8% less on sunny days than cloudy ones(10). Photodegradation is not observed in water(2). The neutral aqueous hydrolysis rate constants of 1,1,1-trichloroethane at 25 deg C has been experimentally determined to be 1.24X10-6 /min; the hydrolytic half-life at pH 7 is 1.1 yr(13). The basic hydrolysis rate constant is essentially zero(13). The aqueous hydrolysis half-life of 1,1,1-trichloroethane in water containing subsurface sediment at 25 deg C was measured to be 450 days(14): this is not significantly different than in pure water(14). [(1) Callahan MA et al; Water-Related Environmental Fate of 129 Priority Pollutants Vol II page 45-1 to 45-12 USEPA-440/4-79-029B (1979) (2) Dilling WL et al; Environ Technol 9: 833-8 (1975) (3) Hubrich C, Stuhl F; J Photochem 12: 93-107 (1980) (4) Singh HB et al; Atmos Environ 15: 601-12 (1981) (5) Hampson RF; FAA-EE-80-17, US Dept of Transportation (1980) (6) Pearson CR, McConnell G; Proc Roy Soc London B 189: 305-32 (1975) (7) Spence JW, Hanst PL; J Air Pollut Control Fed 28: 250-3 (1978) (8) Dilling WL et al; Environ Sci Technol 10: 351-6 (1976) (9) Buchardt O, Manscher OH; CEC Proceedings, 2nd Meeting (1978) (10) Singh HB et al; Environ Sci Technol 16: 872-80 (1982) (11) Haag WR et al; Am Chem Soc Div Environ Chem Preprint 26: 248-53 (1986) (12) Atkinson R; Chem Rev 85: 69-201 (1985) (13) Jeffers PM et al; Environ Sci Technol 23: 965-9 (1989) (14) Haag WR, Mill T; Environ Sci Technol 22: 658-63 (1988)].

Soil Adsorption/Mobility [366]:

The adsorption of 1,1,1-trichloroethane to soil is proportional to the organic carbon content of the soil(4-6). The mineral content of the soil is not a contributing factor(5). The partition coefficient of 1,1,1-trichloroethane to 5 soils (organic carbon 0.1-4.9%) ranged from <0.05 to 0.5 1/g while that adsorbed to sand and clay was too small to determine the isotherms(6). The partition coefficient of 6 chlorinated alkanes including 1,1,1-trichloroethane between bentonite and spring water ranged from 27-76 and between Neckar River sediment and water, 2-108(7). 1,1,1-Trichloroethane is adsorbed strongly to peat moss, less strongly to clay, very slightly to dolomite limestone and not at all to sand(2). It has a low adsorption to silt loam (Koc = 183)(3). From the fact that it is not retained in the soil during bank infiltration, and that it is frequently found in groundwater in high concentrations, one can safely conclude that it is not adsorbed strongly by soils, especially subsurface soils(1). Based upon experimental measurement, the mean Koc range of 1,1,1-trichloroethane in a silty clay soil and sandy loam soil is 81-89(8,SRC). [(1) Schwarzenbach RP et al; Environ Sci Technol 17: 472-9 (1983) (2) Dilling WL et al; Environ Sci Technol 9: 833-8 (1975) (3) Chiou CT et al; Science 206: 831-2 (1979) (4) Friesel P et al; Fresenius Z Anal Chim 319: 160-4 (1984) (5) Richter RO; Am Chem Soc Div Environ Chem Preprints 23: 193-4 (1983) (6) Urano K, Murata C; Chemosphere 14: 293-9 (1985) (7) Hellmann H; Dtsch Gewaesserkd Mitt 29: 111-5 (1985) (8) Gan DR, Dupont RR; Hazard Waste Hazard Materials 6: 363-83 (1989)].

Volatilization from Water/Soil [366]:

1,1,1-Trichloroethane has a high Henry's Law constant (8X10-3 atm-cu m/mole(4)) and will volatilize rapidly from water and soil with diffusion through the liquid phase controlling volatilization from water(1,4). Half-life for evaporation from water obtained from laboratory systems range from a fraction of an hour to several hours(2). Using the Henry's Law constant, one would calculate a half-life of 3.7 hr from a model river 1 m deep with a 1 m/sec current and a 3 m/sec wind(4). Using the experimentally determined ratio of the volatilization rate constants of 1,1,1-trichloroethane relative to oxygen, 0.59(5), and the oxygen reaeration coefficients for various bodies of water, one calculates that the volatilization half-lives range from 5.1-10.6 days for ponds, 3-29 hr for rivers, and 3.8-12 days for lakes(4,SRC). Loss in a mesocosm is entirely due to evaporation and half-lives ranged from 24 days in spring to 11 days in winter(3). The cumulative evaporation loss of a mass of 1,1,1-trichloroethane situated 1.0 to 1.3 meters beneath a soil surface for one year has been estimated to be 61.8% in sandy soil and 4.9% in clay soil(6). [(1) Shen TT; J Air Pollut Control Assoc 32: 79-82 (1982) (2) Dilling WL et al; Environ Sci Technol 9: 833-8 (1975) (3) Wakeham SG et al; Environ Sci Technol 17: 611-7 (1983) (4) Lyman WJ et al; pp. 15-1 to 15-43 in Handbook of Chem Property Estimation Methods NY: McGraw-Hill (1982) (5) Okouchi S; Wat Sci Tech 18: 137-8 (1986) (6) Jury WA et al; Water Resources Res 26: 13-20 (1990)].

Absorption, Distribution and Excretion [366]:

1. Trichloroethane is rapidly absorbed through both the lungs and gastrointestinal tract, but cutaneous absorption probably is too slow to produce significant toxicity unless trapped against the skin by an impermeable barrier. /Trichloroethane/ [Ellenhorn, M.J. and D.G. Barceloux. Medical Toxicology - Diagnosis and Treatment of Human Poisoning. New York, NY: Elsevier Science Publishing Co., Inc. 1988. 988].

2. Wide variations in tissue trichloroethane concentrations occur with the largest amounts found in the lipid-rich brain tissue. /Trichloroethane/ [Ellenhorn, M.J. and D.G. Barceloux. Medical Toxicology - Diagnosis and Treatment of Human Poisoning. New York, NY: Elsevier Science Publishing Co., Inc.

1988. 988].

3. The lungs excrete most of an absorbed dose unchanged. Small amounts are metabolized to trichloroacetic acid and trichloroethanol, which are excreted by the kidney. Chronic accumulation probably does not occur, although repeated exposure induces hepatic p450 mixed-function oxidase enzymes. /Trichloroethane/ [Ellenhorn, M.J. and D.G. Barceloux. Medical Toxicology - Diagnosis and Treatment of Human Poisoning. New York, NY: Elsevier Science Publishing Co., Inc. 1988. 988].

4. The low partition coefficent of 1,1,1-trichloroethane in blood and the low rate of metabolism (3.5%) in humans combine to result in a rapid, but small uptake upon inhalation and a consequently rapid rate of excretion. [National Research Council. Drinking Water & Health. Volume 5. Washington, D.C.: National Academy Press, 1983. 74].

5. After inhalation in mice 1,1,1-trichloroethane was found in brain & kidney at approx equal concentrations & in liver at higher concentrations. In rats, more than 98% of absorbed dose was rapidly expired unchanged; 0.5% Was converted to CO2. Much of remainder was excreted as glucuronide of 2,2,2-trichloroethanol in urine. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V20 524 (1979)].

6. Marked difference found in the rate of penetration of an equal area of /human/ skin by different compounds: methylene chloride was fastest, tetrachlorethylene was slowest, & 1,1,1-trichlorethane ... Intermediate. ...It may be calculated ... That absorption of 1,1,1-trichloroethane during 30 min was about 62 ug/square cm/min. True rate ... /Probably/ greater ... [Hayes, W. J., Jr. Toxicology of Pesticides Baltimore: Williams & Wilkins, 1975. 142].

7. Twelve healthy subjects were exposed to approx 250 & 350 ppm of methyl chloroform in air during rest & physical exercise on a bicycle ergometer. The duration of exposure for each subtrial was 30 min. Pulmonary ventilation, cardiac output & methyl chloroform concentrations(s) in alveolar air, & arterial & venous blood were determined during & after exposure. The concentrations(s) in alveolar air & arterial blood was of the same magnitude at an exposure to 350 ppm at rest as at 250 ppm during light exercise. As exercise intensity incr a kind of levelling-off value was obtained. Incr ventilation was more important to the incr in alveolar air & arterial blood concentrations(s) than incr circulation. There was a high degree of correlation between alveolar air & arterial blood concn. [ASTRAND I ET AL; WORK-ENVIRON-HEALTH 10 (2): 69-81 (1973)].

8. Following intermittent inhalation exposure by adult male

rats for 5 days, for 6 hr daily, the adipose tissue served as a storage site. The fat-stored molecules were not totally mobilized during the intermissions in exposure. [SAVOLAINEN H; EUR J DRUG METAB PHARMACOKINET 6 (2): 85-90 (1981)].

9. In human males exposed to 1,1,1-trichloroethane (213 or 72 ppm) for 8 hr the absorption rate changed continuously with a retention rate between 26-32%. Pulmonary elimination over a period of 8 days was approx 90%. Urinary excretion of the metabolites (eg, trichloroacetic acid & trichloroethanol) was slow & lasted approx 12 days. The urinary metabolites may be used as a biological indicator of exposure to 1,1,1-trichloroethane. [HUMBERT BE, FERNANDEZ JG; ARCH MAL PROF MED TRAV SECUR SOC 38 (4-5): 415-25 (1977)].

10. Dogs inhaling 1,1,1-trichloroethane at 700, 1500, & 2000 ppm showed cumulative uptake after 1 hr of 27.3, 44.7, & 71.2 Mg/kg, respectively. Excretion after 1 hr was 66-77% at all 3 doses. During the exposure, a highly significant neg correlation was seen between the arterial/venous blood concentrations(s) ratio & expired/inspired air concentrations(s) ratio. In the post-exposure period, highly significant pos correlations were seen between expired air concentrations(s) & venous or arterial blood concn. The mean ratio of the total absorption value to the total inspired value was 14% at all 3 levels of exposure. [HOBARA T ET AL; SANGYO IGAKU 24 (6): 599-607 (1982)].

11. Following exposure of rats to 500 ppm in air 6 hr/day for 5 days, concentrations(s) of methyl chloroform in peritoneal fat was much greater than in other organs, but methyl chloroform also detected in cerebellum, liver, cerebrum and blood. [Savolainen H, et al; Arch Toxicol 38: 229-37 (1977) as cited in USEPA; Health Assessment Document: 1,1,1-Trichloroethane p.4-14 to 4-15 (1982) EPA-600/8-82-003].

Laboratory and/or Field Analyses:

In the past, many methods have been used to analyze for 1,1,1-trichloroethane [861,936,1010,1011]. EPA methods for NPDES permits are specified in 40 CFR Part 136 [1010]. EPA methods for drinking water are specified in 40 CFR Part 141 [1011].

EPA (RCRA Group) publishes requirements for solid waste methods in 40 CFR Part 261, Appendix III, with details in the following periodically updated publication [861,1013]:

> Environmental Protection Agency. 1995. Test methods for evaluating solid waste, physical/chemical methods, SW-846, EPA Office of Solid Waste and Emergency Response, EPA, Washington, D.C. [1013]. Available from NTIS.

The guidance in SW-846 must be used in some states, but is considered "guidance of acceptable but not required methods" in most federal applications. In the past, EPA has also published separate (separate from SW-846) guidance documents with suggestions on field sampling and data quality assurance related to sampling of sediments [1016] and soils [1017,1018,1019].

RCRA (SW-846) methods tend to include provisions for using the specified method or something better, whereas the CERCLA CLP methods tend to require things done exactly per contract specifications. RCRA SW-846 methods typically require instrument calibration before analyses, but some labs don't do it, and many labs actually use some kind of hybrid between RCRA, CERCLA, or other "standard protocols" (Roy Irwin, Park Service, Personal Communication, 1997, based on conversation with various EPA and lab staff).

EPA (CERCLA) publishes various Contract Laboratory Program (CLP) methods documents periodically, available from EPA and NTIS. These methods are for very polluted sites. A few past examples (this list is not complete) [861]:

User's Guide CLP CERCLA User's Guide to the Contract Laboratory Program. USEPA - Office of Emergency and Remedial Response. Dec 1988

9240_0-0XFS Multi-Media/Conc Superfund OSWER CERCLA Multi-Media, Multi-Concentration Organic/Inorganic Analytical Service for Superfund, Quick Reference Fact Sheets, 9240.0-08FS (organic) and 9240-0-09FS (inorganic), August 1991. The organic/inorganic analytical service provides a technical and contractual framework for laboratories to apply EPA/Contract Laboratory Program (CLP) analytical methods for the isolation, detection and quantitative measurement of 33 volatile, 64 semi-volatile, 28 pesticide/Aroclor, and 24 inorganic target analytes in water and soil/ sediment environmental samples.

Recommended Detection Limits: For optimum risk or hazard assessment work, volatile compound lab methods with very low detection limits may be necessary. In concert with need to compare values with low benchmark concentrations, the regulatory requirements of States such as Wisconsin and the capabilities of better labs, detection limits should be as low as possible to prevent false negatives. In all cases, they should be lower than comparison benchmarks or standards for various media of concern. Ideally, the detection limit should be at least 10 times higher than the comparison benchmark or criteria [676].

Water Detection Limits:

GC/Hall Detector can achieve 0.003 ppb detection limits for water [936]. For routine NPDES permit applications using EPA method 601 for purgeable halocarbons, EPA specifies a water detection limit of 0.03 ug/L for this compound (40 CFR, Part 136, Appendix A, Table 1) [1010]. USGS can achieve detection limits of 0.05 ug/L or less for this compound using advanced methods such as USGS 1996

Custom Method 9090. However, at very polluted superfund sites, the lowest detection limits are unecessary and CLP methods might do:

> Under EPA's Contract Laboratory Program, all contract laboratories are required to maintain certain levels of performance to meet specific quantitation levels [931]. For volatiles, the EPA Superfund/CERCLA Contract Required Quantitation Level (CRQL) for water is 1 ug/L (AOC/Contract Laboratory Program --CLP, Routine Analytical Services, Summary on EPA Home Page under Superfund Subdirectory, EPA Office of Remedial and Emergency Response, 1997, Internet).

Detection Limits for Solids:

GC/ECD (electron capture detector) methods can achieve 0.6 ppb for tissues [936]. GC/MS methods can achieve detection limits of 5 ppb for sediments and soil [936]. These detection limits should be used as default detection limits when potential impacts to living things are being considered. However, at polluted superfund sites, the CLP methods may suffice:

> Under EPA's Contract Laboratory Program, all contract laboratories are required to maintain certain levels of performance to meet specific quantitation levels [931]. For volatiles,the EPA Superfund/CERCLA Contract Required Quantitation Level (CRQL) for soil is 10 ug/kg (AOC/Contract Laboratory Program --CLP, Routine Analytical Services, Summary on EPA Home Page under Superfund Subdirectory, EPA Office of Remedial and Emergency Response, 1997, Internet).

The investigator should also specify the addition of any relevant compounds (such as breakdown products trichloroacetic acid, trichloroethanol, 1,1-dichloroethane, and chloroethane) suspected of being present but not typically found on the standard EPA scans.

Holding time: According to EPA, for this purgeable halocarbon, the maximum holding time for NPDES water samples is 14 days; samples should be kept iced or refrigerated (4 degrees C, with no headspace or bubbles in the container (40 CFR, Part 136,3, 1994) [1010]. Holding time in soil, sediments, and sludge is also 14 days [1013].

Containers: Both EPA and APHA (Standards Methods Book) recommend glass containers for the collection of organic compounds [141,1010]. EPA specifies the use of teflon lined caps and teflon lined cap septums in glass vial containers for volatiles (VOCs and purgeable halocarbons such as the common organic solvents) [1010,1013]. No headspace is allowed [1010]. Actually, vials are not the best choice for avoiding false negatives in soil samples through volatilization losses, since the use of brass liners for collection resulted in 19 fold higher VOCs than when 40 mL vials were used [798] (see Wisconsin protocol discussion below). Some states specify that volatiles can be stored in EnCoreTM samplers (no government endorsement implied) if analyzed within 48 hours after collection (Donalea Dinsmore, State of Wisconsin DNR, personal communication, 1997).

Guidance from other federal agencies (USGS, FWS, NOAA) also recommends glass containers for organics, and discourages the use of plastic containers for a variety of reasons (Roy Irwin, National Park Service, Personal Communication, 1997, based on a glance through recent internal guidance of several agencies). Some federal agency quality control procedures call for voiding or red-flagging the results of organic analyses if the lab receives the sample in plastic containers (Roy Irwin, National Park Service, Personal Communication, 1997). The APHA pointed out some the potential hazards of the use of certain plastic containers for storing organic samples [141]:

A) Potential contamination of the sample via leaching of compounds from the plastic, and/or

B) The plastic container walls can sometimes be attacked by certain organics and fail, and/or

C) The possibility that some of organic compound will dissolve into the walls of the plastic container, reducing the concentration of the compound in the container [141].

Field Collection Protocols:

Standard field collection method protocols are published by the Fish and Wildlife Service, the USGS, NOAA, DOE, and EPA. These recommendations change over time, with the newest recommendations sometimes being quite different than the old, thereby producing different results. The Fish and Wildlife Service methods are similar in many ways to NOAA field protocols [676]. Many recommended EPA field methods for organics are not very detailed, although the 3rd update of SW-846 for RCRA solid waste methods is becoming more detailed [1013].

The various EPA methods for organics are different from each other, with the selection of the appropriate method depending upon the specific application (RCRA vs. CERCLA vs. NPDES permits, vs. Drinking Water, etc.) [861,1010,1013]. The EPA-recommended field methods are scattered through various EPA and ASTM publications. EPA requires the proper cleaning of collection bottles and collecting gear for both volatile and semi-volatile

> organics [1010,1013]. Typical "standard method" protocols recommend proper cleaning of glass containers before use. Some collectors simply use pre-cleaned jars from I-Chem or Eagle Pitcher (no government endorsement implied) or equivalent suppliers. EPA [1010], USGS, and most other federal agencies recommend cleaning procedures for the glass containers, usually involving detergent rinsing, baking, and sometimes HCL rinses (Roy Irwin, National Park Service, Personal Communication, 1997).
>
> ASTM also publishes standard method guidance for numerous very specific applications, like sampling from pipes (D 3370-95a) and sampling for VOCs in soils (ASTM method D 4547] [1018].
>
> EPA recommends certain detailed collecting protocols for NPDES permit applications, including the use of grab samples rather than composites, and the proper cleaning for both volatile and semi-volatile organics [1010]. In other publications, EPA recommends caution in the use of composite soil samples whether organic or inorganic, citing statistical complications and stating that the compositing of samples cannot, in general, be justified unless for a stated specific purpose and unless a justification is provided [1017]. Mixing composite samples of volatile samples (and even samples of the lighter semi-volatiles such as naphthalene) is not advisable since some of the compounds can thereby be lost through volatization to the air during the mixing process (Roy Irwin, National Park Service, Personal Communication, 1997).

Regardless of what lab methods are used, the investigator must take special precautions to prevent the escape of volatiles during sample shipment, storage, extraction, and cleanup [798]. This is especially true for soil and sediment sampling. The results of analyses of volatiles can be dramatically effected by small details such as how the samples are collected, stored, held, and analyzed in the lab, since volatile compounds can readily volatilize from samples in both field and lab procedures.

The realization that better methods were needed began when the lab results of EPA methods 8020 and 8240 were negative even when contamination by volatiles was obvious in the field, in other words, when investigators began seeing clearly false negative results [798]. In one study, the use of brass liners for collection of soil samples resulted in 19 fold higher VOCs than when 40 mL vials were used [798].

National guidance for minimizing loss of volatiles in field sampling is found in EPA RCRA method 5035 as described in update 3 of SW-846 [1013,1017]. Several states (WI,MN,NJ, and MI) have developed their own detailed guidance, often including the use of methanol as a preservative.

After researching various papers which documented volatile losses of 9 to 99% during sampling and then finding 100% losses in samples held over 14 days in their own facilities, the Wisconsin DNR requires the following for soil sampling of volatiles [913]:

> 1) Concentrated (1:1 by weight of preservative vs soil) methanol preservation be used for all samples [913], and
>
> 2) samples stored in brass tubes must be preserved in methanol within 2 hours and samples stored in EnCoreTM samplers must be preserved in 48 hours [913].
>
> 3) Detection limits should be no higher than 25 ug/Kg (ppb) dry weight for VOCs or petroleum volatiles in soil samples [913].
>
>> Note: The use of methanol for soil sample preservation can make lower detection limits difficult, but the tradeoff can be worth it since otherwise high percentages of volatiles can be lost in very short periods of time, for example in 2 hours for benzene. In other words, low detection limits do not help much if you are losing all the volatiles from the soil sample before analysis. A possible alternative to using methanol for soil samples of volatiles would be to use the EnCoreTM sampler and to analyze as soon as possible (no later than 48 hours) after collection using the methods that give lower detection limits (Donalea Dinsmore, State of Wisconsin DNR, personal communication, 1997).

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, which are so easily lost to the air at various steps along the way. Contaminants data from different labs, different states, and different agencies, collected by different people, are often not very comparable (see disclaimer section at the top of this entry for more details).

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].

However, 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 inappropriate lab or field methods. The loss of volatliles through inappropriate sampling and storage methods is particularly common related to solvent VOCs such as this one.

The basics of quality assurance plans for chemical analyses should include the following quality control steps:

> 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. Typical lab quality control techniques should have included the following considerations (John Moore, Fish and Wildlife Service, Personal Communication, 1997):
>
> Procedural Blanks should be analyzed to assure that no contaminants are added during the processing of the samples. The standards for adequacy depend on the method and the media being measured.
>
> > Different federal agencies publish different acceptable limits. For one program, NOAA stated that at least 8% of samples should be blanks, reference or control materials [676].
> >
> > The basic idea is that neither samples nor blanks should be contaminated. Because the only way to measure the performance of the modified procedures is through the collection and analysis of uncontaminated blank samples in accordance with this guidance and the referenced methods, it is highly recommended that any modifications be thoroughly evaluated and demonstrated to be effective before field samples are collected [1003].
>
> Duplicate samples are analyzed to provide a measure of precision of the methods. The standards for adequacy depend on the method and the media being measured.
>
> > Different federal agencies publish different acceptable limits. There appears to be an inverse relationship between precision and sensitivity [676].
> >
> > Some EPA methods state that a field duplicate must be collected at each sampling site, or one field duplicate per every ten samples, whichever is more frequent [1003]. Some protocols call for the preparation of one Ongoing precision and recovery (OPR) standard for every ten or

> fewer field samples. Great care should be taken in preparing ongoing precision and recovery standards [1003].

Spiked samples are analyzed to provide a measure of the accuracy of the analysis methods. The standards for adequacy depend on the method and the media being measured.

> Different federal agencies publish different acceptable limits.

USGS 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.

For drinking water, in the past, EPA has recommended the following less rigorous methods for analyses of certain volatiles: Purge and trap capillary gas chromatography (EPA 502.2); gas chromatographic/mass spectrometry (EPA 524.2); purge and trap gas chromatography (EPA 503.1); gas chromatography/mass spectrometry (EPA 524.1); PQL= 0.005 mg/L [893]. This detection limit is no longer low enough. Other EPA 1996 IRIS Information on drinking water [893]:

> Analysis of 1,1,1-trichloroethane is by a purge-and-trap gas chromatographic procedure used for the determination of volatile organohalides in drinking water. Confirmatory analysis is by mass spectrometry.
>
> Analytical Methods
>
> > All systems to be monitored for four consecutive quarters; repeat monitoring dependent upon detection, vulnerability status and system size.
>
> Best Available Technology
>
> > Gas chromatography (EPA 502.1, 502.2, 503.1); gas chromatographic/mass spectrometry (EPA 524.1, 524.2).

Description of EPA standard methods 8240 and 8260 (8260 is replacing 8240) from EPA EMMI Database on Lab methods [861]:

> EPA Method 8240 for Volatile Organics [861]:
>
> > 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].

Note: Method 8260 is replacing 8240 in the third update of SW-846 [1013].

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].

EPA Method 8260 (for GC/MS Volatile Organics):

Note: Method 8260 is replacing 8240 in the third update of SW-846 [1013].

Older EPA description [861]:

OSW 8260 Volatile Organics - CGCMS 58 SW-846 CGCMS ug/L MDL Method 8260 "Volatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC/MS): Capillary 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]. Purged sample components are trapped in a tube containing suitable sorbent

> materials [861]. When purging is complete, the sorbent tube is heated and backflushed with helium to desorb trapped sample components [861]. The analytes are desorbed directly to a large bore capillary or cryofocussed on a capillary precolumn before being flash evaporated to a narrow bore capillary for analysis [861]. The column is temperature programmed to separate the analytes which are then detected with a mass spectrometer interfaced to the gas chromatograph [861]. Wide capillary columns require a jet separator, whereas narrow bore capillary columns can be directly interfaced to the ion source [861]. If the above sample introduction techniques are not applicable, a portion of the sample is dispersed in solvent to dissolve the volatile organic constituents [861]. A portion of the solution is combined with organic- free reagent water in the purge chamber [861]. It is then analyzed by purge and trap GC/MS following the normal water method [861]. Qualitative identifications are confirmed by analyzing standards under the same conditions used for samples and comparing resultant mass spectra and GC retention times [861]. Each identified component is quantified by relating the MS response for an appropriate selected ion produced by that compound to the MS response for another ion produced by an internal standard [861].

Other Misc. (mostly less rigorous) lab methods which have been used in the past in media such as drinking water for volatiles [893] (lab method description from EPA [861]):

> EMSLC 502.2 ELCD VOA's - P&T/CGCELCD/CGCPID 44 DRINKING_WATER CGCELD ug/L MDL "Volatile Organic Compounds in Water by Purge and Trap Capillary Column Gas Chromatography with Photoionization and Electrolytic Conductivity Detectors in Series" This method is used for the identification and measurement of purgeable volatile organic compounds in finished drinking water, raw source water, or drinking water in any treatment stage [861]. The method is applicable to a wide range of organic compounds, including the four trihalomethane disinfection by-products, that have sufficiently high volatility and low water solubility to be efficiently removed from water samples with purge and trap procedures [861]. An inert gas is bubbled through a 5 mL water sample [861]. The volatile compounds with low water solubility are purged from the sample and trapped

in a tube containing suitable sorbent materials [861]. When purging is complete, the tube is heated and backflushed with helium to desorb trapped sample components onto a capillary gas chromatography (GC) column [861]. The column is temperature programmed to separate the analytes which are then detected with photoionization detector (PID) and halogen specific detectors in series [861]. Analytes are identified by comparing retention times with authentic standards and by comparing relative responses from the two detectors [861]. A GC/MS may be used for further confirmation [861].

EMSLC 502.2 PID VOA's - P&T/CGCELCD/CGCPID 33 DRINKING_WATER CGCPID ug/L MDL "Volatile Organic Compounds in Water by Purge and Trap Capillary Column Gas Chromatography with Photoionization and Electrolytic Conductivity Detectors in Series" This method is used for the identification and measurement of purgeable volatile organic compounds in finished drinking water, raw source water, or drinking water in any treatment stage [861]. The method is applicable to a wide range of organic compounds, including the four trihalomethane disinfection by-products, that have sufficiently high volatility and low water solubility to be efficiently removed from water samples with purge and trap procedures [861]. An inert gas is bubbled through a 5 mL water sample [861]. The volatile compounds with low water solubility are purged from the sample and trapped in a tube containing suitable sorbent materials [861]. When purging is complete, the tube is heated and backflushed with helium to desorb trapped sample components onto a capillary gas chromatography (GC) column [861]. The column is temperature programmed to separate the analytes which are then detected with photoionization detector (PID) and halogen specific detectors in series [861]. Analytes are identified by comparing retention times with authentic standards and by comparing relative responses from the two detectors [861]. A GC/MS may be used for further confirmation [861].

EMSLC 503.1 Volatile Aromatics in Water 28 DRINKING_WATER GCPID ug/L MDL "Volatile Aromatic and Unsaturated Organic Compounds in Water by Purge and Trap Gas Chromatography" This method is applicable for the determination of various volatile aromatic and unsaturated compounds in finished drinking water, raw source water, or drinking water in any treatment stage [861].

Highly volatile organic compounds with low water solubility are extracted (purged) from a 5-ml sample by bubbling an inert gas through the aqueous sample [861]. Purged sample components are trapped in a tube containing a suitable sorbent material [861]. When purging is complete, the sorbent tube is heated and backflushed with an inert gas to desorb trapped sample components onto a gas chromatography (GC) column [861]. The gas chromatograph is temperature programmed to separate the method analytes which are then detected with a photoionization detector [861]. A second chromatographic column is described that can be used to help confirm GC identifications or resolve coeluting compounds [861]. Confirmation may be performed by gas chromatography/mass spectrometry (GC/MS) [861].

APHA 6230 D Volatile Halocarbons - CGCELCD STD_METHODS GCELCD "6230 Volatile Halocarbons" GCPID 6230 D [861]. Purge and Trap Capillary-Column Gas Chromatographic Method: This method is similar to Method 6230 C., except it uses a wide-bore capillary column, and requires a high-temperature photoionization detector in series with either an electrolytic conductivity or microcoulometric detector [861]. This method is equivalent to EPA method 502.2; see EMSLC\502.2 [861]. Detection limit data are not presented in this method, but the method is identical to 502.2; therefore, see EMSLC\502.2 for detection limit data [861]. Method 6230 B., 17th edition, corresponds to Method 514, 16th edition [861]. The other methods listed do not have a cross-reference in the 16th edition [861].

EMSLC 524.1 Purgeable Organics - GCMS 48 DRINKING_WATER GCMS ug/L MDL "Measurement of Purgeable Organic Compounds in Water by Packed Column Gas Chromatography/Mass Spectrometry" This is a general purpose method for the identification and simultaneous measurement of purgeable volatile organic compounds in finished drinking water, raw source water, or drinking water in any treatment stage [861]. Volatile organic compounds and surrogates with low water solubility are extracted (purged) from the sample matrix by bubbling an inert gas through the aqueous sample [861]. Purged sample components are trapped in a tube containing suitable sorbent materials [861]. When purging is complete, the trap is backflushed with helium to desorb the trapped sample components into a packed gas chromatography (GC) column interfaced to a mass spectrometer (MS) [861]. The column is temperature programmed to separate the method analytes which are then detected with the MS [861]. Compounds eluting from the GC column are identified by comparing their measured mass spectra and retention times to reference spectra and retention times in a data base [861]. Reference spectra and retention times for analytes are obtained by the measurement of calibration standards under the same conditions used for samples [861]. The concentration of each identified component is measured by relating the MS response of the quantitation ion produced by that compound to the MS response of the quantitation ion produced by a compound that is used as an internal standard [861]. Surrogate analytes, whose concentrations are known in every sample, are measured with the same internal standard calibration procedure [861].

EMSLC 524.2 Purgeable Organics - CGCMS 60
DRINKING_WATER CGCMS ug/L MDL "Measurement of Purgeable Organic Compounds in Water by Capillary Column Gas Chromatography/Mass Spectrometry" This is a general purpose method for the identification and simultaneous measurement of purgeable volatile organic compounds in finished drinking water, raw source water, or drinking water in any treatment stage [861]. Volatile organic compounds and surrogates with low water solubility are extracted (purged) from the sample matrix by bubbling an inert gas through the aqueous sample [861]. Purged sample components are trapped in a tube containing suitable sorbent materials [861]. When purging is complete, the sorbent tube is heated and backflushed with helium to desorb the trapped sample components into a capillary gas chromatography (GC) column interfaced to a mass spectrometer (MS) [861]. The column is temperature programmed to separate the method analytes which are then detected with the MS [861]. Compounds eluting from the GC column are identified by comparing their measured mass spectra and retention times to reference spectra and retention times in a data base [861]. Reference spectra and retention times for analytes are obtained by the measurement of calibration standards under the same conditions used for samples [861]. The concentration of each identified component is measured by relating the MS response of the quantitation ion produced by that compound to the MS response of the quantitation ion produced by a compound that is used as an internal standard [861]. Surrogate analytes, whose concentrations are known in every sample, are measured with the same internal standard calibration procedure [861].