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**SOURCES, EMISSION AND EXPOSURE FOR  
TRICHLOROETHYLENE (TCE)  
AND RELATED CHEMICALS**

National Center for Environmental Assessment–Washington Office  
Office of Research and Development  
U.S. Environmental Protection Agency  
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## TABLE OF CONTENTS

LIST OF TABLES .....	x
LIST OF FIGURES .....	xi
PREFACE .....	xii
AUTHORS, CONTRIBUTORS, AND REVIEWERS .....	xiii
SECTION A. SUMMARY AND INTRODUCTION .....	1
SUMMARY .....	1
INTRODUCTION .....	10
SECTION B. PARENT COMPOUNDS .....	13
1.0 TRICHLOROETHYLENE .....	13
1.1 CHEMICAL AND PHYSICAL PROPERTIES .....	13
1.1.1 Nomenclature .....	13
1.1.2 Formula and Molecular Weight .....	13
1.1.3 Chemical and Physical Properties .....	13
1.1.4 Technical Products and Impurities .....	14
1.2 PRODUCTION AND USE .....	14
1.2.1 Production .....	14
1.2.2 Uses .....	14
1.2.3 Disposal .....	15
1.3 POTENTIAL FOR HUMAN EXPOSURE .....	15
1.3.1 Natural Occurrence .....	15
1.3.2 Occupational Exposure .....	15
1.3.3 Environmental .....	15
1.4 HUMAN EXPOSURE AND POPULATION ESTIMATES .....	23
1.4.1 General U.S. Population .....	23
1.4.2 Occupational Exposure .....	26
1.4.3 Consumer Exposure .....	27
1.5 CHAPTER SUMMARY .....	27
2.0 TETRACHLOROETHYLENE (PERCHLOROETHYLENE) .....	30
2.1 CHEMICAL AND PHYSICAL PROPERTIES .....	30
2.1.1 Nomenclature .....	30
2.1.2 Formula and Molecular Weight .....	30
2.1.3 Chemical and Physical Properties .....	30
2.1.4 Technical Products and Impurities .....	31
2.2 PRODUCTION AND USE .....	31

## TABLE OF CONTENTS (continued)

2.2.1	Production	31
2.2.2	Uses	32
2.2.3	Disposal	32
2.3	POTENTIAL FOR HUMAN EXPOSURE	32
2.3.1	Natural Occurrence	32
2.3.2	Occupational	32
2.3.3	Environmental	33
2.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	40
2.4.1	General U.S. Population	40
2.4.2	Occupational Exposure	41
2.4.3	Consumer Exposure	41
2.5	CHAPTER SUMMARY	41
3.0	1,1,1-TRICHLOROETHANE (METHYL CHLOROFORM)	44
3.1	CHEMICAL AND PHYSICAL PROPERTIES	44
3.1.1	Nomenclature	44
3.1.2	Formula and Molecular Weight	44
3.1.3	Chemical and Physical Properties	44
3.1.4	Technical Products and Impurities	45
3.2	PRODUCTION AND USE	45
3.2.1	Production	45
3.2.2	Uses	46
3.2.3	Disposal	46
3.3	POTENTIAL FOR HUMAN EXPOSURE	46
3.3.1	Natural Occurrence	46
3.3.2	Occupational	46
3.3.3	Environmental	47
3.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	52
3.4.1	General U.S. Population	52
3.4.2	Occupational Exposure	52
3.4.3	Consumer Exposure	54
3.5	CHAPTER SUMMARY	54
4.0	1,2-DICHLOROETHYLENE	56
4.1	CHEMICAL AND PHYSICAL PROPERTIES	56
4.1.1	Nomenclature	56
4.1.2	Formula and Molecular Weight	56
4.1.3	Chemical and Physical Properties	56
4.1.4	Technical Products and Impurities	57
4.2	PRODUCTION AND USE	57
4.2.1	Production	57
4.2.2	Uses	57
4.2.3	Disposal	58
4.3	POTENTIAL FOR HUMAN EXPOSURE	58

## TABLE OF CONTENTS (continued)

4.3.1	Natural Occurrence	58
4.3.2	Occupational	58
4.3.3	Environmental	58
4.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	62
4.4.1	General U.S. Population	62
4.4.2	Occupational Exposure	62
4.4.3	Consumer Exposure	64
4.5	CHAPTER SUMMARY	64
5.0	CIS-1,2-DICHLOROETHYLENE	65
5.1	CHEMICAL AND PHYSICAL PROPERTIES	65
5.1.1	Nomenclature	65
5.1.2	Formula and Molecular Weight	65
5.1.3	Chemical and Physical Properties	65
5.1.4	Technical Products and Impurities	66
5.2	PRODUCTION AND USE	66
5.2.1	Production	66
5.2.2	Uses	66
5.2.3	Disposal	67
5.3	POTENTIAL FOR HUMAN EXPOSURE	67
5.3.1	Natural Occurrence	67
5.3.2	Occupational	67
5.3.3	Environmental	67
5.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	70
5.4.1	General U.S. Population	70
5.4.2	Occupational Exposure	70
5.4.3	Consumer Exposure	70
6.0	TRANS-1,2-DICHLOROETHYLENE	71
6.1	CHEMICAL AND PHYSICAL PROPERTIES	71
6.1.1	Nomenclature	71
6.1.2	Formula and Molecular Weight	71
6.1.3	Chemical and Physical Properties	71
6.1.4	Technical Products and Impurities	72
6.2	PRODUCTION AND USE	72
6.2.1	Production	72
6.2.2	Uses	72
6.2.3	Disposal	73
6.3	POTENTIAL FOR HUMAN EXPOSURE	73
6.3.1	Natural Occurrence	73
6.3.2	Occupational	73
6.3.3	Environmental	73
6.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	76
6.4.1	General U.S. Population	76

## TABLE OF CONTENTS (continued)

	6.4.2	Occupational Exposure	76
	6.4.3	Consumer Exposure	76
7.0		1,1,1,2-TETRACHLOROETHANE	77
	7.1	CHEMICAL AND PHYSICAL PROPERTIES	77
		7.1.1 Nomenclature	77
		7.1.2 Formula and Molecular Weight	77
		7.1.3 Chemical and Physical Properties	77
		7.1.4 Technical Products and Impurities	78
	7.2	PRODUCTION AND USE	78
		7.2.1 Production	78
		7.2.2 Uses	78
		7.2.3 Disposal	79
	7.3	POTENTIAL FOR HUMAN EXPOSURE	79
		7.3.1 Natural Occurrence	79
		7.3.2 Occupational	79
		7.3.3 Environmental	79
	7.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	81
		7.4.1 General U.S. Population	81
		7.4.2 Occupational Exposure	82
		7.4.3 Consumer Exposure	82
	7.5	CHAPTER SUMMARY	82
8.0		1,1-DICHLOROETHANE	83
	8.1	CHEMICAL AND PHYSICAL PROPERTIES	83
		8.1.1 Nomenclature	83
		8.1.2 Formula and Molecular Weight	83
		8.1.3 Chemical and Physical Properties	83
		8.1.4 Technical Products and Impurities	84
	8.2	PRODUCTION AND USE	84
		8.2.1 Production	84
		8.2.2 Uses	84
		8.2.3 Disposal	84
	8.3	POTENTIAL FOR HUMAN EXPOSURE	85
		8.3.1 Natural Occurrence	85
		8.3.2 Occupational	85
		8.3.3 Environmental	85
	8.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	88
		8.4.1 General U.S. Population	88
		8.4.2 Occupational Exposure	88
		8.4.3 Consumer Exposure	88
	8.5	CHAPTER SUMMARY	90
		SECTION C. METABOLITES OF TRICHLOROETHYLENE AND PARENT COMPOUNDS	91

## TABLE OF CONTENTS (continued)

9.0	CHLORAL	91
9.1	CHEMICAL AND PHYSICAL PROPERTIES	91
9.1.1	Nomenclature	91
9.1.2	Formula and Molecular Weight	91
9.1.3	Chemical and Physical Properties	91
9.1.4	Technical Products and Impurities	92
9.2	PRODUCTION AND USE	92
9.2.1	Production	92
9.2.2	Uses	93
9.2.3	Disposal	93
9.3	POTENTIAL FOR HUMAN EXPOSURE	93
9.3.1	Natural Occurrence	93
9.3.2	Occupational	93
9.3.3	Environmental	94
9.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	96
9.4.1	General U.S. Population	96
9.4.2	Occupational Exposure	96
9.4.3	Consumer Exposure	96
9.5	CHAPTER SUMMARY	96
10.0	CHLORAL HYDRATE	98
10.1	CHEMICAL AND PHYSICAL PROPERTIES	98
10.1.1	Nomenclature	98
10.1.2	Formula and Molecular Weight	98
10.1.3	Chemical and Physical Properties	98
10.1.4	Technical Products and Impurities	99
10.2	PRODUCTION AND USE	99
10.2.1	Production	99
10.2.2	Uses	100
10.2.3	Disposal	100
10.3	POTENTIAL FOR HUMAN EXPOSURE	100
10.3.1	Natural Occurrence	100
10.3.2	Occupational	100
10.3.3	Environmental	100
10.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	102
10.5	CHAPTER SUMMARY	102
11.0	MONOCHLOROACETIC ACID	103
11.1	CHEMICAL AND PHYSICAL PROPERTIES	103
11.1.1	Nomenclature	103
11.1.2	Formula and Molecular Weight	103
11.1.3	Chemical and Physical Properties	103
11.1.4	Technical Products and Impurities	104
11.2	PRODUCTION AND USE	104

## TABLE OF CONTENTS (continued)

11.2.1	Production	104
11.2.2	Uses	104
11.2.3	Disposal	104
11.3	POTENTIAL FOR HUMAN EXPOSURE	105
11.3.1	Natural Occurrence	105
11.3.2	Occupational	105
11.3.3	Environmental	105
11.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	107
11.5	CHAPTER SUMMARY	107
12.0	DICHLOROACETIC ACID	109
12.1	CHEMICAL AND PHYSICAL PROPERTIES	109
12.1.1	Nomenclature	109
12.1.2	Formula and Molecular Weight	109
12.1.3	Chemical and Physical Properties	109
12.1.4	Technical Products and Impurities	110
12.2	PRODUCTION AND USE	110
12.2.1	Production	110
12.2.2	Uses	110
12.2.3	Disposal	110
12.3	POTENTIAL FOR HUMAN EXPOSURE	110
12.3.1	Natural Occurrence	110
12.3.2	Occupational	110
12.3.3	Environmental	111
12.4	HUMAN EXPOSURE AND POPULATION ESTIMATES	112
12.4.1	General U.S. Population	112
12.4.2	Occupational Exposure	112
12.4.3	Consumer Exposure	112
12.5	CHAPTER SUMMARY	112
13.0	TRICHLOROACETIC ACID	113
13.1	CHEMICAL AND PHYSICAL PROPERTIES	113
13.1.1	Nomenclature	113
13.1.2	Formula and Molecular Weight	113
13.1.3	Chemical and Physical Properties	113
13.1.4	Technical Products and Impurities	114
13.2	PRODUCTION AND USE	114
13.2.1	Production	114
13.2.2	Uses	114
13.2.3	Disposal	115
13.3	POTENTIAL FOR HUMAN EXPOSURE	115
13.3.1	Natural Occurrence	115
13.3.2	Occupational	115
13.3.3	Environmental	115

**TABLE OF CONTENTS (continued)**

13.4	HUMAN EXPOSURE AND POPULATION ESTIMATES .....	118
13.4.1	General U.S. Population .....	118
13.4.2	Occupational Exposure .....	118
13.4.3	Consumer Exposure .....	118
13.5	CHAPTER SUMMARY .....	118
14.0	DICHLORO-VINYL CYSTEINE .....	119
	REFERENCES .....	120

## LIST OF TABLES

Table A-1.	Summary of Potential Exposure Pathways and Potentially Exposed Populations . . . . .	5
Table A-2.	Preliminary Dose Estimates of TCE and Related Chemicals . . . . .	8
Table A-3.	Summary of U.S. Production Data . . . . .	9
Table 1-1.	Annual Releases of Trichloroethylene in the U.S. (lbs) . . . . .	16
Table 1-2.	Concentrations of Trichloroethylene in Ambient Air . . . . .	17
Table 1-3.	Mean TCE Air Levels Across Monitors by Year . . . . .	18
Table 1-4.	Mean TCE Air Levels Across Monitors by Land Setting and Use (1985 to 1998) . . . . .	18
Table 1-5.	Modeled TCE Air Concentrations in Continental U.S. for 1990 . . . . .	18
Table 1-6.	Concentrations of Trichloroethylene in Water . . . . .	21
Table 1-7.	TCE Levels in Whole Blood by Population Percentile . . . . .	22
Table 1-8.	Modeled Exposure Estimates for TCE . . . . .	25
Table 1-9.	Comparison of Measured and Modeled TCE Concentrations . . . . .	25
Table 1-10.	Trichloroethylene Summary . . . . .	29
Table 2-1.	Releases of Tetrachloroethylene (lbs) . . . . .	33
Table 2-2.	Concentrations of Tetrachloroethylene in Ambient Air . . . . .	34
Table 2-3.	Concentrations of Tetrachloroethylene in Water . . . . .	35
Table 2-4.	Tetrachloroethylene Levels in Whole Blood by Population Percentile . . . . .	37
Table 2-5.	Modeled Exposure Estimates for Tetrachloroethylene . . . . .	38
Table 2-6.	Comparison of Measured and Modeled Perchloroethylene Concentrations . . . . .	38
Table 2-7.	Tetrachloroethylene (Perchloroethylene) Summary . . . . .	43
Table 3-1.	Releases of 1,1,1-Trichloroethane (lbs) . . . . .	47
Table 3-2.	Level of 1,1,1-Trichloroethane in Food . . . . .	49
Table 3-3.	1,1,1-Trichloroethane in Common Household Products . . . . .	54
Table 3-4.	1,1,1-Trichloroethane (Methyl Chloroform) Summary . . . . .	55
Table 4-1.	1,2-Dichloroethylene Summary . . . . .	64
Table 7-1.	1,1,1,2-Tetrachloroethane Summary . . . . .	82
Table 8-1.	1,1-Dichloroethane Summary . . . . .	90
Table 9-1.	Concentrations of Chloral (As Chloral Hydrate) in Drinking Water in the United States . . . . .	94
Table 9-2.	Chloral Summary . . . . .	97
Table 10-1.	Chloral Hydrate Summary . . . . .	102
Table 11-1.	Release of Chloroacetic Acid (lbs/yr) . . . . .	105
Table 11-2.	Monochloroacetic Acid Summary . . . . .	108
Table 12-1.	Concentrations of Dichloroacetic Acid in Water . . . . .	111
Table 12-2.	Dichloroacetic Acid Summary . . . . .	112
Table 13-1.	Concentrations of Trichloroacetic Acid in Water . . . . .	116
Table 13-2.	Trichloroacetic Acid Summary . . . . .	118

## LIST OF FIGURES

Figure A-1.	Trichloroethylene, Related Parent Compounds, and Their Metabolites .....	11
Figure 1-1.	Modeled TCE Levels in Air from Cumulative Exposure Project by Census Tract, New Jersey .....	19
Figure 1-2.	Frequency of NPL Sites with Trichloroethylene Contamination .....	28
Figure 2-1.	Concentration of Tetrachloroethylene in Blood at Selected Population Percentiles .....	36
Figure 2-2.	Frequency of NPL Sites with Tetrachloroethylene Contamination .....	42
Figure 3-1.	Concentration of 1,1,1-Trichloromethane in Blood at Selected Population Percentiles .....	50
Figure 3-2.	Frequency of NPL Sites with 1,1,1-Trichloromethane Contamination .....	53
Figure 4-1.	Frequency of NPL Sites with 1,2-Dichloroethene (Unspecified) Contamination .....	63
Figure 8-1.	Frequency of NPL Sites with 1,1-Dichloroethane Contamination .....	89

## **PREFACE**

This document was based mostly on the report, "Sources, Emission and Exposure for Trichloroethylene (TCE)" which was prepared in August 1997 by the Versar, Inc. of Springfield, Virginia under U.S. Environmental Protection Agency (EPA) Contract No. 68-D5-0051. Additional information was later added/updated, especially for the Trichloroethylene chapter.

This document is published as a state-of-the-science report on the exposure assessment of TCE, its metabolites and other related chemicals known to produce similar metabolites. A summary of much of the information contained in this report was also published in Environmental Health Perspectives, Supplements, May 2000 and underwent the peer review process required by the journal.

The scientific literature search for this assessment is generally current through January 1997, although a number of more recent publications on key topics have been included.

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## SECTION A. SUMMARY AND INTRODUCTION

### SUMMARY

This report is an exposure assessment of Trichloroethylene (TCE), its metabolites, and other chemical compounds known to produce identical metabolites. In addition to TCE, other parent compounds considered here are 1,1,1-trichloroethane (methyl chloroform), tetrachloroethylene (PCE or PERC), 1,2-dichloroethylene (cis-, trans-, and mixed isomers), 1,1,1,2-tetrachloroethane, and 1,1-dichloroethane. The metabolites are chloral, chloral hydrate, monochloroacetic acid, dichloroacetic acid, trichloroacetic acid, and dichloro-vinyl cysteine (DCVC). Although listed here, no information was found for the metabolite, DCVC.

The parent compounds are used in many diverse manufacturing industries such as food processing, textiles, wood products, furniture and fixtures, paper, printing and publishing, chemicals, petroleum, rubber, leather, stone and clay, primary metals, fabricated metals, industrial machinery, electronics, and transportation equipment. They are primarily used as solvents, carriers, or extractants; in dry cleaning of textiles; in metal cleaning and degreasing; in textile manufacturing; as insulating fluids/coolants; and as chemical intermediates. The metabolites have more restricted uses in industry as chemical intermediates, herbicides, and pharmaceuticals.

The major routes of exposure for these chemicals are inhalation, ingestion, and dermal absorption. The following paragraphs summarize available information concerning the general population, occupational, and consumer exposure to these chemicals. A summary of the potential exposure pathways and potential exposed populations for each chemical is presented in Table A-1. Although inhalation seems to be the dominant route of exposure for most of the chemicals, exposure can also occur through the ingestion of contaminated foods and drinking water and through dermal contact (spills). Using media levels of the chemicals considered here, one may predict the range of estimated exposures and the estimated range of daily doses. These values are presented in Table A-2.

More research is needed to assess the exposure of these chemicals for the non-occupational population (IARC, 1995; ATSDR, 1990, 1995, 1996a,b, 1997a,b). Most of the monitoring data for humans are from occupational studies of specific workers exposed to the chemical. Current data are needed for all chemicals for production, use in consumer products, releases, and the efficiency of current disposal practices. Additionally, more data are needed on the degradation of these chemicals in groundwater (specifically TCE, PCE, 1,1,1-trichloroethane, and 1,2-dichloroethylene) and their rates of transformation in the soil. Current data to characterize the levels of these chemicals in air, water, soil, and food also are needed. Current monitoring data for these media will aid in the assessment of exposure for the general population, especially persons living near waste sites. Biological monitoring data are also needed for humans. Because TCE and PCE have been detected in breast milk samples (NHANES III, 1997) of the general population, children ages 12 months and less who ingest breast milk may potentially be exposed. Unspecified levels of TCE have been found in breast milk, however, levels of PCE detected have ranged up to 43 µg/l in the general population. According to NAS

(1991), in 1989, the initiation of breast-fed newborn infants in the hospital was reported to 52.2 percent and by age 5-6 months, only 19.6 percent of the infants were breast-fed. Since some of these chemicals (e.g., TCE and PCE) are present in soil, children may be exposed through activities such as playing in or ingesting soil. Table A-3 presents the production data (production, import, and export). As shown in this table, however, most of the production data are old or non-existent.

### **Trichloroethylene**

The general U.S. population is exposed via inhalation, ingestion, or dermal pathways. The most important pathways appear to be inhalation of contaminated ambient air and ingestion of contaminated drinking water. Because of pervasiveness of TCE in the environment, most people are exposed to low levels of TCE. Occupational exposure results primarily from its use as a degreasing or metal cleaning agent. Workers in the vapor degreasing industry are exposed to the highest levels through inhalation. Consumers are exposed through their use of wood stains, varnishes, finishes, lubricants, adhesives, typewriter correction fluid, paint removers, and cleaners that contain TCE. Levels of TCE in consumer products appear to be declining. Elevated exposure may occur to people living near waste facilities, those being exposed through occupational activities, and residents of some urban and industrial areas where TCE-contaminated media occur. Since TCE has been detected in breast milk, nursing infants may be exposed via this pathway.

### **Tetrachloroethylene (Perchloroethylene; PCE)**

The general U.S. population is exposed to PCE via inhalation and ingestion. The most important pathways appear to be inhalation of contaminated ambient air (including indoor air) and ingestion of contaminated drinking water. Dermal exposure does not appear to be important. The greatest chance of exposure is occupational, primarily through inhalation, especially in the dry cleaning industry. Consumers may be exposed through the use of adhesives, water repellents, fabric finishes, spot removers, and wood cleaners. Since PCE has been detected in breast milk, nursing infants may be exposed via this pathway.

### **1,1,1-Trichloroethane (methyl chloroform)**

The general U.S. population is exposed to this chemical via inhalation of ambient air (including indoor air). Exposure can also occur through ingestion of contaminated foods and drinking water and through dermal contact. Exposure from commercial products may be more significant than exposure resulting from industrial releases. Occupational exposure results from degreasing, electric component manufacture, mixing and application of commercial resins, spray painting and gluing. Occupational exposure is primarily through inhalation pathway. Consumers are exposed via use of a wide variety of household products such as fingernail polish, paint thinner, caulking compounds, paint removers, and antifreeze.

### **1,2-Dichloroethylene (cis-, trans-, and mixed isomers)**

The general U.S. population is exposed to this chemical via the inhalation of contaminated ambient air and from ingestion of water from contaminated groundwater sources. Potentially high exposures are possible to those living near production/processing facilities, municipal wastewater sites, hazardous waste sites, and municipal landfills. The National Institute for Occupational Safety and Health (NIOSH) estimates that a small number of workers (about 275) are potentially exposed occupationally via an inhalation or dermal pathway to one or both of the isomers. No data are available for consumer exposure.

### **1,1,1,2-Tetrachloroethane**

The general U.S. population is exposed to this compound through the inhalation of ambient air. No data are available for occupational exposures. Consumers are possibly exposed through their use of paints and varnishes, but confirmatory data are not available.

### **1,1-Dichloroethane**

The general U.S. population is exposed to this chemical via the inhalation of ambient air and the ingestion of contaminated drinking water. Higher exposures may exist for persons living near industrial and hazardous waste sites. Occupational exposure occurs primarily via inhalation during manufacturing processes using 1,1,-dichloroethane as a chemical intermediate, solvent, and component of fumigant formulations. No data are available for consumer exposure.

### **Chloral**

The general U.S. population may be exposed to chloral from drinking chlorinated water and from pharmaceutical use. Some occupational exposure may result from chloral's production and manufacture. No data are available for consumer exposure.

### **Chloral hydrate**

The general U.S. population may be exposed to chloral hydrate from drinking chlorinated water and from pharmaceutical use. No data are available for consumer exposure.

### **Monochloroacetic acid**

No data are available for general U.S. population, occupational, and consumer exposure.

### **Dichloroacetic acid**

The general U.S. population is exposed to this chemical via ingestion of chlorinated drinking water and chlorinated water in swimming pools. No data are available for occupational and consumer exposure.

**Trichloroacetic acid**

The general U.S. population is exposed to this chemical via the ingestion of contaminated drinking water and foods. Occupational exposure may occur during the production and use of trichloroacetic acid as a pesticide. No data are available for consumer exposure.

**Dichloro-Vinyl Cysteine**

There are no data for this chemical.

**Table A-1. Summary of Potential Exposure Pathways and Potentially Exposed Populations**

Chemical	Potential Exposure Pathway			Potentially Exposed Population			Populations with Potentially High Exposure	Remarks
	Inhalation	Ingestion	Dermal	General	Occupational	Consumer		
TCE	a				b ~401,000 U.S. employees (1981-83 survey)	Likely from use of consumer products that contain TCE.	People living near waste sites, in urban and industrial areas with populations living near military bases, and with occupational populations who are continuously exposed to elevated levels. Exposure to the consumer population is possible from use of consumer products. Products that generally contain TCE include (paint removers, adhesives, etc.). Short-term exposure to high levels include people using consumer products containing TCE with inadequate ventilation. TCE has been detected in breast milk, so exposure to nursing infants may occur.	Work is being conducted at Rutgers University to develop a model for describing exposure from TCE contaminated groundwater living near Superfund sites because of its persistence in groundwater.
PCE	a				b ~450,000 workers in the dry-cleaning industry; 688,110 other employees (1981-83 survey)	Many consumer products such as spot removers, inks, fabric finishes have been found to contain PCE.	Persons working in dry cleaning industries and metal degreasing most heavily exposed; people living with workers in the dry cleaning industries; other populations who may have elevated exposures include people living near hazardous waste facilities and people using products containing PCE in areas with inadequate ventilation. PCE has been detected in breast milk, so exposure to nursing infants may occur.	Research addressing waste treatment technology is underway at Cornell University. Studies at New York Department of Health.
1,1,1-Trichloroethane	a				~2.5 x 10 <sup>6</sup> workers (1981-83 survey). Subcategories include nurses, maids, janitors, electricians, electronics workers, and apparel industry.	Consumer products such as paints, paint thinners, caulking compounds, fingernail polish, paint removers, and food packaging adhesives have been reported to contain 1,1,1-trichloroethane	elevated exposures may occur to populations in occupational categories such as degreasing operations.	Exposure may also occur through inhalation from visiting dry cleaners; working in chemistry labs; using household cleaners, pesticides, and paints. Exposure to general population from use of commercial products may be more significant than from industrial releases.
1,2-Dichloroethylene (cis-, trans-, and mixed isomers)	a				Occupational exposure to ~275 people (mixed isomers and cis isomer only; data not available for trans isomer)	Reported uses are in the manufacture of pharmaceuticals, artificial pearls, and in the extraction of oil and fats from fish and meat. However, these data are old (1985) and consumer exposure data were not available.	People living near waste sites and production/processing facilities and persons with occupational exposure.	Difficult to distinguish between the isomers using standard method analyses.

**Table A-1. Summary of Potential Exposure Pathways and Potentially Exposed Populations (continued)**

Chemical	Potential Exposure Pathway			Potentially Exposed Population			Populations with Potentially High Exposure	Remarks
	Inhalation	Ingestion	Dermal	General	Occupational	Consumer		
1,1,2,2-Tetrachloroethane	a	-- <sup>c</sup>	--		Probably exposed through inhalation of contaminated ambient air	Reported use is primarily a feed stock in the production of solvent. It is not known if this is a closed production process.	Reported uses are in the manufacture of paints and varnishes. It is not known if this use is current or if the products are consumer or industrial products.	
1,1-Dichloroethane			--		Estimated at 715-1,957 workers in early 1980s. Exposure primarily from use of chemical as intermediate and solvent in manufacturing processes	NA	Persons living near industrial and hazardous waste sites.	General population exposed via inhalation of ambient air and ingestion of contaminated water.
Chloral and Chloral Hydrate	--		--		Approximately 2,757 employees (1981-83 survey - chloral only)	NA	NA	General population may be potentially exposed from drinking chlorinated water and pharmaceutical use. Chloral hydrate is used in pharmaceuticals.
Monochloroacetic Acid	NA	<sup>c</sup>	NA	NA	NA	NA	NA	
Dichloroacetic Acid					Approximately 1,592 employees (1981-83 survey)	NA	NA	General population potentially exposed through the ingestion of chlorinated drinking water, water in swimming pools, and contaminated surface water.
Trichloroacetic Acid	--				Estimated employees exposed is 35,124 (1981-83 survey)	NA	NA	General population exposed through ingestion of chlorinated drinking water and contact with chlorinated surface water and ingestion of foods contaminated with this chemical.
Dichloro-vinyl Cysteine	NA	NA	NA	NA	NA	NA	NA	NA

**Table A-1. Summary of Potential Exposure Pathways and Potentially Exposed Populations (continued)**

NA = Information not available.

= Possible exposure pathway.

a Believed to be most prominent route of exposure, according to available data.

b Population with the greatest chance of elevated exposure (for longer periods of time).

c Probable exposure pathway, but not confirmed.

**Table A-2. Preliminary Dose Estimates of TCE and Related Chemicals**

Chemical	Population	Media	Range of Estimated Adult Exposures (ug/day)	Range of Adult Doses (mg/kg/day)	Data Sources
Trichloroethylene	General	Air	11 -- 33	1.57E-04 -- 4.71E-04	ATSDR (1997a)
	General	Water	2 -- 20	2.86E-05 -- 2.86E-04	ATSDR (1997a)
	Occupational	Air	2,232 -- 9,489	3.19E-02 -- 1.36E-01	ATSDR (1997a)
Tetrachloroethylene (PERC)	General	Air	80 -- 200	1.14E-03 -- 2.86E-03	ATSDR (1997b)
	General	Water	0.1 -- 0.2	1.43E-06 -- 2.86E-06	ATSDR (1997b)
	Occupational	Air	5,897 -- 219,685	8.43E-02 -- 3.14	ATSDR (1997b)
1,1,1-Trichloroethane	General	Air	10.8 -- 108	1.54E-04 -- 1.54E-03	ATSDR (1995)
	General	Water	0.38 -- 4.2	5.5E-06 -- 6.00E-05	ATSDR (1995)
1,2-Dichloroethylene	General	Air	1 -- 6	1.43E-05 -- 8.57E-05	ATSDR (1996a)
	General	Water	2.2	3.14E -05	ATSDR (1996a)
Cis-1,2-Dichloroethylene	General	Air	5.4	7.71E -05	HSDB (1996)
	General	Water	0.5 -- 5.4	7.14E-06 -- 7.71E-05	HSDB (1996)
1,1,1,2-Tetrachloroethane	General	Air	142	2.03E -03	HSDB (1996)
1,1-Dichloroethane	General	Air	4	5.71E -05	ATSDR (1990)
	General	Water	2.47 -- 469.38	3.53E-05 -- 6.71E-03	ATSDR (1990)
Chloral	General	Water	0.02 -- 36.4	2.86E-07 -- 5.20E-04	HSDB (1996)
Monochloroacetic Acid	General	Water	2 -- 2.4	2.86E-05 -- 3.43E-05	USEPA (1994)
Dichloroacetic Acid	General	Water	10 -- 266	1.43E-04 -- 3.80E-03	IARC (1995)
Trichloroacetic Acid	General	Water	8.56 -- 322	1.22E-03 -- 4.60E-03	IARC (1995)

**Table A-3. Summary of U.S. Production Data**

Chemical	U.S. Production Data (kilograms)		
	Production (yr)	Import (yr)	Export (yr)
TCE	1.17 x 10 <sup>5</sup> (1981) 7.72 x 10 <sup>7</sup> (1985) 1.45 x 10 <sup>8</sup> (1991)	1.98 x 10 <sup>7</sup> (1985)	1.06 x 10 <sup>7</sup> (1985)
PCE	3.08 x 10 <sup>8</sup> (1985) 1.84 x 10 <sup>8</sup> (1986) 2.14 x 10 <sup>8</sup> (1989) 1.60 x 10 <sup>8</sup> (1990) 1.08 x 10 <sup>8</sup> (1991) 1.12 x 10 <sup>8</sup> (1992) 1.23 x 10 <sup>8</sup> (1993)	1.70 x 10 <sup>7</sup> (1982) 6.36 x 10 <sup>7</sup> (1985) 8.3 x 10 <sup>4</sup> (1986)	2.47 x 10 <sup>7</sup> (1983) 9.84 x 10 <sup>6</sup> (1985)
1,1,1-Trichloroethane	3.64 x 10 <sup>8</sup> (1990) 3.13 x 10 <sup>8</sup> (1992)	4.54 x 10 <sup>4</sup> (1981) 5.99 x 10 <sup>6</sup> (1992) 9.08 x 10 <sup>4</sup> (1993)	5.20 x 10 <sup>7</sup> (1990) 7.39 x 10 <sup>7</sup> (1991) 6.34 x 10 <sup>7</sup> (1992) 3.44 x 10 <sup>7</sup> (1993)
1,2-Dichloroethylene	NA	NA	NA
Cis-1,2-Dichloroethylene	5.0 x 10 <sup>5</sup> (1977 - captive production)	NA	NA
Trans-1,2-Dichloroethylene	NA	NA	NA
1,1,1,2-Tetrachloroethane	NA	NA	NA
1,1-Dichloroethane	NA	NA	NA
Chloral	2.83 x 10 <sup>7</sup> (1969) 2.27 x 10 <sup>7</sup> (1975)	1.02 x 10 <sup>5</sup> (1984)	Negligible (1972; 1975)
Chloral Hydrate	1.14 x 10 <sup>7</sup> (1972 - anhydrous) 5.9 x 10 <sup>5</sup> (1975)	2.83 x 10 <sup>4</sup> (1972) 4.8 x 10 <sup>4</sup> (1975) 5.41 x 10 <sup>3</sup> (1984)	NA
Monochloroacetic Acid	3.5 x 10 <sup>7</sup> (1978) >6.81 x 10 <sup>3</sup> (1982)	1.25 x 10 <sup>7</sup> (1978) 1.35 x 10 <sup>7</sup> (1982)	Negligible (1993)
Dichloroacetic Acid	NA	NA	NA
Trichloroacetic Acid	>3.6 x 10 <sup>3</sup> (1975) >2.27 x 10 <sup>3</sup> (1976)	3.67 x 10 <sup>6</sup> (1984)	8.6 x 10 <sup>6</sup> (1984)
Dichloro-vinyl Cysteine	NA	NA	NA

NA = Not available.

Sources: HSDB, 1996; IARC, 1995.

## INTRODUCTION

This report summarizes currently available exposure related information about TCE, its metabolites, and other parent compounds that produce these same metabolites. Thus, this assessment is a departure from typical exposure assessment of a chemical in that it considers exposure to metabolites as well as parent compounds. Exposure information is summarized for the following 14 compounds:

- C Trichloroethylene;
- C The primary metabolites of trichloroethylene: dichloro-vinyl cysteine, chloral, chloral hydrate, trichloroacetic acid, dichloroacetic acid, monochloroacetic acid; and
- C The primary parent compounds which produce the same metabolites as trichloroethylene: tetrachloroethylene, methyl chloroform, 1,1,1,2-tetrachloroethane, cis-1,2-dichloroethylene, trans-1,2-dichloroethylene, 1,2-dichloroethylene, and 1,1-dichloroethane.

Not all possible metabolites of trichloroethylene and related parent compounds were included in the scope of this document. The metabolites were limited to human metabolites that are produced in the largest quantities and are most important in producing toxic effects. The parent compounds were limited to those to which humans are most commonly exposed. The two parent compounds of most importance were trichloroethylene and tetrachloroethylene, and the two metabolites of most importance were trichloroacetic acid and dichloroacetic acid. These four compounds were given the highest priority in terms of the level of effort spent in developing this document.

Figure A-1 shows the parent-metabolite relationships between the compounds covered in this document. The actual pathways of metabolism are much more complicated than shown here and it should be understood that this diagram is intended only to give the reader a general understanding of which parent compounds lead to which metabolites. The key limitations of this diagram are summarized below:

- C The diagram does not include all metabolites of trichloroethylene.
- C The diagram does not include all potential parent compounds which could lead to the listed metabolites. For example, acetic acids are common metabolites of many compounds.
- C The diagram does not show the intricacies of the metabolic pathways. For example, interconversion can occur between some metabolites, many reactions include intermediate steps and the reactions can be affected by enterohepatic circulation and renal reabsorption.

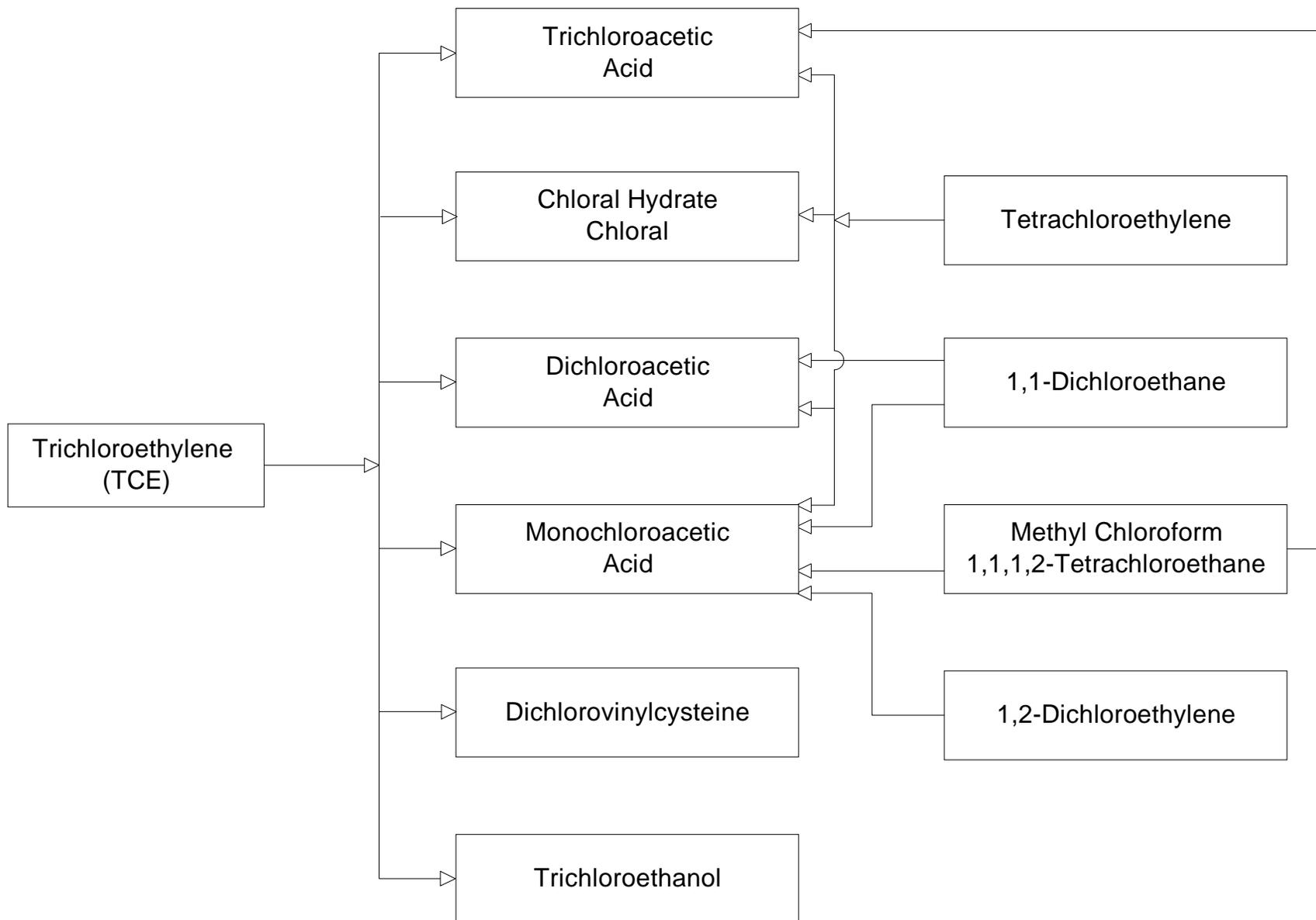


Figure A-1. Trichloroethylene, Related Parent Compounds, and Their Metabolites

- C The diagram does not represent quantitative relationships (i.e., some metabolites are produced in much higher quantities than others and concepts such as half-life and reaction kinetics are not represented).

This report has drawn heavily on information presented in the 1995 International Agency for Research on Cancer publication (IARC 1995) and profiles on several chemicals from the Agency for Toxic Substances and Disease Registry (ATSDR 1990, 1995, 1996a, 1997a,b). Additional informational sources include electronic literature searches, on-line searches of the Hazardous Substances Data Base, and data retrievals from the U.S. EPA Toxic Release Inventory (TRI).

This report is organized in three sections. Section A includes this introduction and summary of the results. Section B summarizes readily available information on the physical-chemical properties, production and use, potential for human exposure, and exposure and population estimates for TCE and the other parent compounds. The final section, Section C, summarizes the same exposure-related information for the TCE metabolites.

There are a number of limitations and uncertainties in this report that result primarily from the lack of information and that much of the data are not current, although found in current publications. It should be noted that monitored chemical levels presented in this report are primarily for the United States. Information on most metabolites is relatively sparse and is completely lacking for one chemical.

Research is needed to gather data, especially to confirm current production, use, release, and disposal practices and study fate of the chemicals in certain media (especially groundwater and soils). Reliable, current monitoring data for levels in environmental media are needed to assess human exposures. Most of the monitoring data reported are old and based on occupational studies data. Additionally, the monitoring data for humans are basically for levels in blood and urine only. Research is needed to address monitored levels of these chemicals in other human tissues for the general population and populations around hazardous waste sites as well.

## SECTION B. PARENT COMPOUNDS

### 1.0 TRICHLOROETHYLENE

#### 1.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

##### 1.1.1 Nomenclature

CAS No.:	79-01-6
Synonyms:	1-chloro-2,2-dichloroethylene; ethene, trichloro-; acetylene trichloride, TCE.
Trade Names:	Chlorylea, Chlorylen, CirCosolv, Crawhaspol, Dow-Tri, Dukeron, Per-A-Chlor, Triad, Trial, TRI-Plus M, Vitran, Perm-A-Chlor (and others).

##### 1.1.2 Formula and Molecular Weight

Molecular Formula:	$C_2HCl_3$
Molecular Weight:	131.40

##### 1.1.3 Chemical and Physical Properties

Description:	Clear, colorless, or blue mobile liquid (Remington's Pharm. Sci., 16th Ed., 1980); chloroform-like odor (Weast, 1986-87).
Boiling Point:	87° C (Weast, 1987-1988).
Melting Point:	-73° C (Weast, 1987-1988).
Density:	1.4649 @ 20° C/4° C (Merck Index, 11th Ed., 1989).
Spectroscopy Data:	Sadtler Ref. Number: 185 (IR, Prism); Max. Absorption: less than 200 nm (vapor) (Weast, 1979); Index of refraction: 1.4773 @ 20° C/D (Weast, 1986-87); IR: 62 (Weast, 1979).
Solubility:	1,100 mg/l water at 25° C (Verschueren, 1983).
Volatility:	Vapor Pressure: 19.9 mm Hg @ 0° C; 57.8 mm Hg @ 20° C (NRC, 1981).

Vapor Density: 4.53 (air = 1) (Merck Index, 1989).

Stability: Relatively stable in air (Browning, Tox Metab Indus Solv, 1965); Unstable in light and moisture (Osal, 1980).

Reactivity: Incompatible with strong caustics and alkalis; chemically-active metals such as barium, lithium, sodium, magnesium, titanium, and beryllium (NIOSH Pocket Guide Chemical Hazards, 1994).

Octanol/Water

Partition Coefficient:  $\log K_{ow} = 2.29$  (Hansch, 1979).

#### 1.1.4 Technical Products and Impurities

Trichloroethylene is available in the USA in high-purity, electronic USP, technical, metal degreasing, and extraction grades (IARC Monographs, 1972-present, V20, 1979). Commonly used stabilizers found in commercial trichloroethylene products include: pentanol-2 triethanolamine, 2,2,4-trimethylpentene-1, and iso-butanol. Tetrachloroethane is a contaminant in commercial trichloroethylene (ARENA, 1986). Impurities found in commercial trichloroethylene products include: carbon tetrachloride, chloroform, 1,1,1,2-trichloroethane, and benzene (WHO, 1985).

### 1.2 PRODUCTION AND USE

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996) and IARC (1995).

#### 1.2.1 Production

U.S. Production: (1981)  $1.17 \times 10^8$  g (USITC, 1981); (1985)  $7.72 \times 10^{10}$  g estimated (USITC, 1985); (1991)  $1.45 \times 10^{11}$  g (SRI. Directory Chem. Producers-USA, 1992).

Import Volume: (1985)  $1.98 \times 10^{10}$  g (Bureau of the Census, U.S. Imports, 1985).

Export Volume (1985)  $1.06 \times 10^{10}$  g (Bureau of the Census, U.S. Exports, 1985).

#### 1.2.2 Uses

The major use of trichloroethylene is degreasing (IARC, 1995). About 85 percent of the TCE produced is used in metal cleaning. Other uses include the manufacture of organic chemicals; as a solvent in adhesives and paint-stripping formulations, paints, lacquers, varnishes; heat transfer medium-EG; in case hardening of metals; a solvent base for metal phosphatizing systems; and solvent in characterization test for asphalt (SRI). It was also used earlier as an extractant for spice oleoresins, natural fats and oils, hops and decaffeination of coffee (IARC,

1995), and a carrier solvent for the active ingredients of insecticides and fungicides, and for spotting fluids (WHO; Environ. Health Criteria, 1985). TCE has been replaced in the dry cleaning industry with tetrachloroethylene (ATSDR, 1997a). Its use as a fumigant and as an extractant for decaffeinating coffee has been discontinued in the U.S. (ATSDR, 1997a). Its use in cosmetics and drug products was also discontinued (IARC, 1995).

### **1.2.3 Disposal**

Generators of waste (equal to or greater than 100 kg/month) containing this contaminant (EPA hazardous waste numbers U228, D040, and F002) must conform with U.S. EPA regulations in storage, transportation, treatment, and disposal of waste (40 CFR 240-280, 7/1/91). Incineration is a method of disposal, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids produced. An alternative to disposal for trichloroethylene is recovery and recycling (Sittig, 1985. Handbook Toxic Hazardous Chemicals and Carcinogens). This compound should be susceptible to removal from wastewater by air stripping (U.S. EPA, 1980).

## **1.3 POTENTIAL FOR HUMAN EXPOSURE**

### **1.3.1 Natural Occurrence**

The natural occurrence of trichloroethylene has been reported in one red microalga and in temperate, subtropical and tropical algae (IARC, 1995).

### **1.3.2 Occupational Exposure**

Occupational exposure to TCE of workers in industries using TCE may result from inhalation of vapors or through dermal contact with TCE from spills.

### **1.3.3 Environmental**

#### **1.3.3.1 *Environmental Releases***

Total Toxic Release Inventory (EPA, 1996) releases for years 1987 to 1994 are shown in Table 1-1. The receiving media are air, water, land, and for underground injection, POTW (Public Owned Treatment Works) transfer and other transfers. These releases are reported from manufacturing and processing facilities. Only certain facilities are required to report.

**Table 1-1. Annual Releases of Trichloroethylene in the United States (lbs)**

Year	Number of reporting facilities	Fugitive air releases	Stack air releases	Surface water releases	Underground injection	Land disposal	POTW transfer	Other transfers	Total
1987	959	25,978,879	29,436,952	30,104	18,720	56,733	130,178	11,689,590	67,341,156
1988	951	26,168,126	29,759,510	13,801	390	21,186	85,652	6,509,867	62,558,532
1989	899	22,629,351	27,054,328	15,849	390	8,686	31,519	4,962,054	54,702,177
1990	807	19,030,377	20,900,640	14,285	805	12,554	11,949	3,879,599	43,850,209
1991	724	17,078,485	18,860,997	12,784	800	62,991	73,195	10,625,967	46,715,219
1992	681	15,585,757	14,866,100	8,606	466	20,726	70,149	9,807,719	40,359,523
1993	790	14,524,316	15,939,964	5,220	460	8,212	42,987	10,143,591	40,664,750
1994	783	14,788,788	15,083,085	1,671	288	4,417	50,325	12,307,585	42,236,159

Source: TRI 1996

**Air:** Most of the TCE used in the U.S. is released to the atmosphere primarily from vapor degreasing operations by evaporation (ATSDR, 1997a). Releases to air also occur at treatment and disposal facilities, water treatment facilities, and landfills (ATSDR, 1997a). TCE has also been detected in stack emissions from the municipal and hazardous waste incineration (ATSDR, 1997a). TCE has been detected in the air throughout the United States. Industrial releases to the environment in the U.S. ranged from 55.6 million pounds in 1987 down to 29.9 million pounds in 1994 (TRI, 1996).

**Water:** TCE has been reported in rainwater, surface waters, groundwater, drinking water, and seawater (IARC, 1995). TCE is released to the aquatic systems from industrial discharges of wastewater streams (ATSDR, 1997a). It has been reported that TCE in landfill leachate can contaminate groundwater; TCE has been reported to be one of the most frequent contaminants of groundwater (ATSDR, 1997a).

**Other Media:** TCE has been reported in marine sediments, marine invertebrates, marine mammals, foods, mother's milk, and human urine and blood (IARC, 1995) (HSDB, 1996).

### 1.3.3.2. Monitored Environmental Media Levels

**Air:** TCE has been detected in the air throughout the United States. According to ATSDR (1997a), atmospheric levels are highest in areas concentrated with industry and population, and lower in remote and rural regions. Air levels of TCE are highly variable (fluctuate widely over relatively short periods of time), depending on strength of emission sources, variation of wind direction and velocity and other meteorological factors, rain scavenging, and photodecomposition. Levels of TCE measured in the ambient air at a variety of locations in the U.S. are shown in Table 1-2. These data were derived from studies conducted in the late 1970's and early 1980's.

**Table 1-2. Concentrations of Trichloroethylene in Ambient Air**

Area	Year	Concentration ( $\mu\text{g}/\text{m}^3$ )*	
		Mean	Range
<b><i>Rural</i></b>			
Whiteface Mountain, NY	1974	0.5	<0.3-1.9
Badger Pass, CA	1977	0.06	0.005-0.09
Reese River, NV	1977	0.06	0.005-0.09
Jetmar, KS	1978	0.07	0.04-0.11
<b><i>Urban and Suburban</i></b>			
New Jersey	1973-79	9.1	ND-97
New York City, NY	1974	3.8	0.6-5.9
Los Angeles, CA	1976	1.7	0.14-9.5
Lake Charles, LA	1976-78	8.6	0.4-11.3
Phoenix, AZ	1979	2.6	0.06-16.7
Denver, CO	1980	1.07	0.15-2.2
St. Louis, MO	1980	0.6	0.1-1.3
Portland, OR	1984	1.5	0.6-3.9
Philadelphia, PA	1983-84	1.9	1.6-2.1

Source: IARC, 1995.

\*  $1 \mu\text{g}/\text{m}^3 = 0.17 \text{ ppb}$ 

Other ambient air measurement data for TCE were obtained from the Aerometric Information Retrieval System (AIRS) using the AIRS Website: <http://www.epa.gov/airsdata/>. (U.S. EPA, 1999a). These data were collected from a variety of sources including State and local environmental agencies and cover the years 1985 to 1998. They represent about 1,200 measurements from 25 states. The most recent data (1998) come from 115 monitors located in 14 states. The 1998 air levels in  $\text{g}/\text{m}^3$  across all 115 monitors can be summarized as follows: range = 0.01 to 3.9; mean = 0.88, 50th percentile = 0.32 and 90th percentile = 1.76. Table 1-3 summarizes the data by year, showing the average and number of samples. Relatively few samples were collected in 1985 and 1986, but each year after 1986 is represented by at least 50 samples. The data suggest a general downward trend from about  $1.5 \text{ g}/\text{m}^3$  in the late 1980s to  $0.8 \text{ g}/\text{m}^3$  in the late 1990s. Table 1-4 shows the monitoring data organized by land setting (rural, suburban, or urban) and land use (agricultural, commercial, forest, industrial, mobile, and residential). Urban air levels are about three times higher than rural areas. Among the land use categories, TCE levels are highest in commercial/industrial areas and lowest in forest areas.

TCE ambient air concentrations in 1990 were modeled for all census tracts of the continental United States as part of the U.S. EPA Cumulative Exposure Project (CEP, see [www.epa.gov/cumulativeexposure/air/air.htm](http://www.epa.gov/cumulativeexposure/air/air.htm)). (U.S. EPA, 1999b). A variety of sources were used to obtain emissions data and the air modeling was done using a Gaussian dispersion model. Table 1-5 shows the distribution of modeled TCE ambient air concentrations across the continental United States. The modeling suggests that 97% of the census tracts have TCE concentrations ranging from 0 to  $1.5 \text{ g}/\text{m}^3$ . The average level was estimated as  $0.37 \text{ g}/\text{m}^3$  and the maximum as  $32 \text{ g}/\text{m}^3$ . The averages and percentiles are better interpreted as population-weighted values than spatial averages because all census tracts have roughly equal populations, but are more variable in geographic area. Figure 1-1 is a map of the CEP-modeled TCE air concentrations in New Jersey. The average across all population tracts in the state is  $0.5 \text{ g}/\text{m}^3$ . The map indicates, however, that the vast majority of the state, on an area basis, has levels under

**Table 1-3. Mean TCE Air Levels Across Monitors by Year\***

	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998
Mean Concentration (: g/m <sup>3</sup> )	1.4	1.39	1.68	4.87	1.69	1.84	2.86	1.37	1.12	0.95	0.78	0.65	0.74	0.88
n	11	21	53	57	96	59	70	76	84	89	146	150	129	115

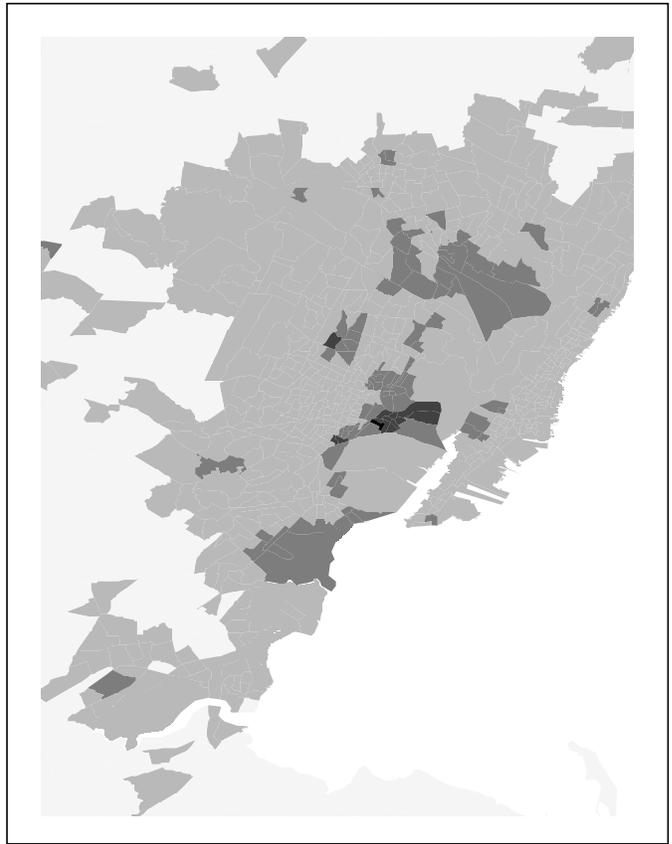
**Table 1-4. Mean TCE Air Levels Across Monitors by Land Setting and Use (1985 to 1998)\***

	Rural	Suburban	Urban	Agricultural	Commercial	Forest	Industrial	Mobile	Residential
Mean Concentration (: g/m <sup>3</sup> )	0.42	1.26	1.61	1.08	1.84	0.1	1.54	1.5	0.89
n	93	500	558	31	430	17	186	39	450

**Table 1-5. Modeled TCE Air Concentrations in Continental U.S. for 1990\***

	25 <sup>th</sup> Percentile	50 <sup>th</sup> Percentile	75 <sup>th</sup> Percentile	95 <sup>th</sup> Percentile	Maximum	Overall Mean	Urban Mean
Concentration (: g/m <sup>3</sup> )	0.13	0.24	0.45	1.1	32	0.37	0.5

\*1 ppb = 5.36 : g/m<sup>3</sup>.



Inset

Figure 1-1. Modeled TCE Levels in Air from Cumulative Exposure Project by Census Tract, New Jersey (:  $\text{g}/\text{m}^3$ )

0.5 : g/m<sup>3</sup>. Relatively high levels (generally 1 to 12 : g/m<sup>3</sup>) were estimated for the densely populated areas around Camden and Newark - Paterson. The highest levels (up to 30 : g/m<sup>3</sup>) were estimated for a few (presumably industrial) sectors within these areas. The CEP data suggest that this pattern (i.e., generally low TCE levels in rural areas, moderate levels in urban areas, and highest levels in small commercial/industrial sectors) is common across most states. The monitoring data, as discussed earlier, also suggest that this is the general pattern across the country.

These modeled values should be interpreted with caution. Clearly they are not as reliable as measured values for specific locations. As discussed earlier, the AIRS data shows an average for 1990 across 59 monitoring stations of 1.84 : g/m<sup>3</sup>. This is much higher than the national average from CEP of 0.37 : g/m<sup>3</sup>. An important difference, though, is that the CEP estimate represents all areas of the continental United States, whereas the 1990 AIRS data for TCE represent only 59 monitors located in 8 states. CEP compared modeled estimates with measured values in the same locations and found that for most chemicals, agreement was usually within a factor of three, with underestimates being more common than overestimates. More variability, however, was found in the model-monitor comparisons for TCE than for other HAPs (hazardous air pollutants). In addition, the tendency for underestimation in the model observed for other HAPs was not seen for TCE. The TCE model-monitor comparisons can be summarized as follows: model-monitor comparisons were made at 57 monitoring sites, the median of the model-monitor ratios was 0.76, arithmetic mean ratio = 2.33, geometric mean ratio = 1.02, 53% of ratios were less than 1.0, 51% were within a factor of 3 (i.e. within the range of 0.33 to 3.0), 19% were less than 0.33 and 30% were greater than 3.0.

**Water:** According to IARC (1995), the reported median concentrations of TCE in 1983-84 were 0.5 µg/l in industrial effluents and 0.1 µg/l in ambient water. ATSDR (1997a) has reported that TCE is the most frequently reported organic contaminant in groundwater and the one present in the highest concentration in a summary of ground water analyses reported in 1982. It has been estimated that between 9 percent and 34 percent of the drinking water supply sources tested in the U.S. may have some trichloroethylene contamination. This estimate is based on available Federal and State surveys (ATSDR, 1997a). Results from an analysis of the EPA STORET Data Base (1980-1982) showed that TCE was detected in 28 percent of 9,295 surface water reporting stations nationwide (ATSDR, 1997a). Levels of TCE found in rainwater, groundwater, and drinking water are shown in Table 1-6.

More recently, the U.S. EPA Office of Ground Water and Drinking Water reported that most water supplies are in compliance with the maximum contaminant level [maximum contaminant level (MCL), 5 : g/L] and that only 407 samples out of many thousands taken from community and other water supplies throughout the country over the past 11 years (1987-1997) have exceeded the MCL limit for TCE (U.S. EPA, 1998).

TCE concentrations in ground water have been measured extensively in California. The data were derived from a survey of large water utilities (i.e., utilities with more than 200 service connections). The survey was conducted by the California Department of Health Services (DHS, 1986). From January 1984 through December 1985, wells in 819 water systems were sampled for organic chemical contamination. The water systems use a total of 5,550 wells, 2,947 of which were sampled. TCE was found in 187 wells at concentrations up to 440 : g/L, with a median

**Table 1-6. Concentrations of Trichloroethylene in Water**

Water Type	Location	Year	Mean	Median	Range	Number of Samples	Ref.
Industrial Effluent	U.S.	83		0.5		NR	IARC, 1995
Surface Waters	U.S.	83		0.1		NR	IARC, 1995
Rainwater	Portland, OR	84	0.006		0.002-0.02	NR	Ligoeki, et.al , 1985
Groundwater	MN	83			0.2-144	NR	Sabel, et.al, 1984
	NJ	76			≤1530	NR	Burmaster, et. al. '82
	NY	80			≤3800	NR	Burmaster, et. al. '82
	PA	80			≤27300	NR	Burmaster, et. al. '82
	MA	76			≤900	NR	Burmaster, et. al. '82
	AZ				8.9-29	NR	IARC, 1995
Drinking water	U.S.	76			0.2 - 49		IARC, 1995
	U.S	77			0 - 53		IARC, 1995
	U.S.	78			0.5 - 210		IARC, 1995
	MA	84			max. 267		IARC, 1995
	NJ	84-	23.4		max. 67	1130	Cohn, et.al., 1994
	CA	85			8-12	486	EPA, 1987
	CA	84	66			486	EPA, 1987
	NC	84	5			48	EPA, 1987
	ND	84	5			48	EPA, 1987

NR - Not Reported

concentration of 3.0 : g/L. Generally, the most contaminated wells and the wells with the highest concentrations were found in the heavily urbanized areas of the state. Los Angeles County registered the greatest number of contaminated wells (149).

**Other Media:** Levels of TCE were found in the sediment and marine animal tissue collected in 1980-81 near the discharge zone of a Los Angeles County waste treatment plant. Concentrations were 17 µg/l in the effluent, <0.5 µg/kg in dry weight in sediment, and 0.3-7 µg/kg wet weight in various marine animal tissue (IARC, 1995). TCE has also been found in foods in the U.S. and the United Kingdom. The average concentrations of TCE in food in the U.S. were the following (IARC, 1995):

- C 0.9 µg/kg in grain-based foods;
- C 1.8 µg/kg in table-ready foods;
- C 73.6 µg/kg in butter and margarine;
- C 0.5 µg/kg in peanut butter;
- C 3.0 µg/kg in ready-to-eat cereals;
- C 1.3 µg/kg in highly processed foods; and
- C 3.8 µg/kg in cheese products.

**Biological Monitoring:** Biological monitoring studies have detected TCE in human blood and urine in the U.S. and other countries such as Croatia, China, Switzerland, and Germany (IARC, 1995). Concentrations of TCE in persons exposed through occupational degreasing operations were most likely to have detectable levels (IARC, 1995). In 1982, eight of

eight human breastmilk samples from four U.S. urban areas had detectable levels of TCE. The levels of TCE detected, however, were not specified (HSDB, 1996; ATSDR, 1997a).

The Third National Health and Nutrition Examination Survey (NHANES III) examined TCE concentrations in blood in 677 non-occupationally exposed individuals drawn from the general U.S. population who were selected on the basis of age, race, gender and region of residence (IARC, 1995 and Ashley et al., 1994). The samples were collected during 1988 to 1994. TCE levels in whole blood were below the detection limit of 0.01 : g/l for about 90% of the people sampled (Table 1-7). Assuming that nondetects equal half of the detection limit, the mean concentration was about 0.017 µg/l.

### 1.3.3.3 Environmental Fate and Transport

#### 1.3.3.3.1 Summary

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of trichloroethylene released to surface soils is volatilization. Because of its moderate to high mobility in soils, trichloroethylene introduced into soil (e.g., landfills) has the potential to migrate through the soil into groundwater. The relatively frequent detection of trichloroethylene in groundwater confirms the mobility of trichloroethylene. Biodegradation in soil and groundwater may occur at a relatively slow rate (half-lives on the order of months to years) (Howard et al., 1991).

**Fate in the Atmosphere:** In the atmosphere, trichloroethylene is expected to be present primarily in the vapor phase rather than sorbed to particulates because of its high vapor pressure. Some removal by scavenging during wet precipitation is expected because of the moderate solubility of trichloroethylene in water (1.1 g/L). The major degradation process affecting vapor phase trichloroethylene is photo-oxidation by hydroxyl radicals (half-life on the order of 1 to 11 days) (HSDB, 1996).

**Fate in Aquatic Environments:** The dominant fate of trichloroethylene released to surface waters is volatilization (predicted half-life of minutes to hours). Bioconcentration, biodegradation, and sorption to sediments and suspended solids are not thought to be significant (HSDB, 1996).

**Table 1-7. TCE Levels in Whole Blood by Population Percentile\***

Percentiles	10	20	30	40	50	60	70	80	90
Concentration (: g/l)	0.005	0.005	0.005	0.005	0.005	0.005	0.005	0.005	0.012

\* Nondetects assumed equal to half the detection limit (0.01 : g/L).

Data from IARC (IARC, 1995) and Ashley (Ashley, 1994)

### **1.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:**  $K_{oc}$ s ranging from 30 to 150 have reported in studies with various soil types indicate that trichloroethylene should exhibit moderate to high mobility in soil. The mobility of trichloroethylene in soil has been confirmed in soil column studies and river bank infiltration studies (HSDB, 1996).

**Volatilization:** The dominant removal mechanism for trichloroethylene in surface waters is volatilization. The half-life will depend on wind and mixing conditions and is estimated to range from several minutes to hours in rivers, lakes, and ponds based on laboratory experiments and field studies. Because of its high vapor pressure (73 torr at 25 degrees C) and relatively low soil adsorption coefficient (30 to 150), trichloroethylene is expected to volatilize from soil surfaces and also from suspended particulate matter in the atmosphere (HSDB, 1996).

**Bioconcentration:** Bioconcentration factors of 17 to 39 have been reported in bluegill sunfish and rainbow trout. Marine monitoring data suggest BCFs of 2 to 25. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996).

### **1.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** Based on limited acclimated soil screening test data, trichloroethylene undergoes aerobic biodegradation at a very slow rate with a half-life estimated at 6 months to a year. Slow degradation under anaerobic conditions is expected (half-life of months to years) based on the results of limited anaerobic sediment studies (Howard et al., 1991).

**Photodegradation:** Photolysis in the atmosphere or in aquatic environments is expected to proceed very slowly, if at all. Trichloroethylene does not absorb UV light at wavelengths of less than 290 nm and thus will not directly photolyze. Based on measured rate data for the vapor phase photo-oxidation reaction with hydroxyl radicals, the estimated half-life of trichloroethylene in the atmosphere is on the order of 1 to 11 days with production of phosgene, dichloroacetyl chloride, and formyl chloride. Under smog conditions, degradation is more rapid (half-life on the order of hours) (HSDB, 1996; Howard et al., 1991).

**Hydrolysis:** Trichloroethylene is not hydrolyzed under normal environmental conditions. However, slow photo-oxidation in water (half-life of 10.7 months) has been reported (HSDB, 1996; Howard et al., 1991)

## **1.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **1.4.1 General U.S. Population**

Because of the pervasiveness of TCE in the environment, most people are exposed to it through ingestion of drinking water, inhalation of ambient air, or ingestion of food (ATSDR, 1995a). Contamination of drinking water with TCE varies according to location and with the drinking water source (whether source is surface water or groundwater). TCE readily volatilizes from water and inhalation of indoor air may be a major route of exposure in homes with

contaminated water supply (ATSDR, 1997a). Available data indicate that for most people, dermal exposure is not an important route of exposure (ATSDR, 1997a).

The 1998 AIRS monitoring data indicate a mean outdoor air level of  $0.88 : \text{g/m}^3$ . Using this value and an inhalation rate of  $20 \text{ m}^3 \text{ air/day}$  yields an exposure estimate of  $18 : \text{g/day}$ . This is consistent with ATSDR (ATSDR, 1997a), which reported an average daily air intake for the general population of  $11 \text{ to } 33 : \text{g/day}$ . The California survey of large water utilities in 1984 found a median concentration of  $3.0 : \text{g/L}$  (DHS, 1986). Using this value and a  $2 \text{ L/day}$  water consumption rate yields an estimate of  $6 : \text{g/day}$ . This is consistent with ATSDR (ATSDR, 1997a) which reported an average daily water intake for the general population of  $2 \text{ to } 20 : \text{g/day}$ .

The use of ambient air data to estimate inhalation exposure does not account for possible differences between contaminant levels in indoor vs. outdoor air. TCE readily volatilizes from water and indoor inhalation exposure may be comparable or greater than ingestion exposures in homes where the water supply contains TCE (ATSDR, 1997a, Andelman, et.al., 1985, Giardino, et.al., 1992, Andelman, et.al., 1986a, Andelman, et.al., 1986b). For example, in two homes using well water with TCE levels averaging  $22 \text{ to } 128 : \text{g/L}$ , the TCE levels in bathroom air ranged from  $<0.5 \text{ to } 40 \text{ mg/m}^3$  when the shower was run less than 30 minutes (Andelman et al., 1985). In one study, the transfer of TCE from shower water to air had a mean efficiency of 61% (independent of water temperature); it was concluded that a 10-minute shower in TCE-contaminated water could result in a daily inhalation exposure comparable to that expected from drinking TCE-contaminated tap water (ATSDR, 1997a). Indoor use of TCE containing products can also contribute to exposures. Wallace et al. (Wallace, et.al., 1985) concluded that indoor air contributes more to overall TCE exposure than outdoor air. This was based on monitoring of expired breath of 190 people in New Jersey. This is also indicated in the TEAM (Total Exposure Assessment Methodology) Study (U.S. EPA, 1987), which shows, for example, that the ratio of the indoor to outdoor TCE concentration for Greensboro, NC was about 5:1. Accordingly, ambient air-based exposure estimates probably under represent total inhalation exposures.

TCE in bathing water can also cause dermal exposure. A modeling study has suggested that a significant fraction of the total dose associated with exposure to volatile organics in drinking water results from dermal absorption (Brown, et.al., 1984).

Pharmacokinetic modeling can be used to gain further understanding of general population exposure. Clewell et al. (Clewell, et.al., 1995) developed a physiologically based pharmacokinetic model for TCE that can be used to estimate the long-term average inhaled air concentration that would result in a measured blood concentration, assuming no other TCE exposure. The model can also estimate the long-term average ingested dose that would result in a measured blood concentration, assuming no other TCE exposure. This dose can be converted to a TCE water concentration assuming an ingestion rate such as  $2 \text{ L/day}$ . For each of these exposure scenarios, the model also provides the corresponding concentrations of trichloroacetic acid (TCA) and dichloroacetic acid (DCA) in blood and the amount of TCE metabolized per day. This model was applied to the range of TCE levels in blood as measured in NHANES III. Table 1-8 shows the resulting exposure estimates corresponding to the range of TCE blood levels. The TCE environmental concentrations modeled from blood levels exceeded the range of measured values for air and water: modeled mean concentration in drinking water was  $59.5 : \text{g/L}$  (measured range was trace to  $50 : \text{g/L}$ ) and the modeled mean air concentration was  $4.2 : \text{g/m}^3$

(measured range was for 0.01 to 3.9 : g/m<sup>3</sup>) . This implies that neither inhalation nor water ingestion dominate exposure; rather both contribute to the total exposure. Exposure estimates derived from blood cannot distinguish among exposure routes and sources. It is generally believed that TCE exposure occurs primarily via water consumption and air inhalation, but it is impossible to use the blood data to directly estimate how much of the total exposure is attributable to each. A wide range of combinations of exposures from air and water could have produced the measured blood levels. As noted earlier, most water supplies have TCE levels under the MCL of 5 : g/L. The modeling suggests that exposure at the MCL would correspond to a very low blood level. This implies that the TCE exposure via the air and other nonwater pathways may generally be more important than water ingestion. Table 1-8 provides the modeled exposure estimates corresponding to a range of blood levels, and Table 1-9 shows a comparison of measured and modeled TCE concentrations in air and drinking water.

#### 1.4.1.1 Extent of General Population Exposure

Because of the pervasiveness of TCE in the environment, most people are likely to have some exposure via one or more of the following pathways: ingestion of drinking water, inhalation of ambient air, or ingestion of food (ATSDR, 1995a). As noted earlier, the NHANES survey suggests that about 10% of the population has detectable levels of TCE in blood. The exposures in these individuals may be higher than those in others in the general population as a result of a number of factors. As discussed below, some occupations and the use of certain consumer products can cause increased TCE exposure via inhalation. In addition, some members of the general population may have increased TCE exposure via their drinking water. The extent of TCE exposure via drinking water is difficult to estimate, but the following discussion provide some perspective on this issue.

**Table 1-8. Modeled Exposure Estimates for TCE**

	Air concentration (: g/m <sup>3</sup> )	Ingested dose (: g/kg-day)	Water concentration (: g/L)
10th percentile blood level (0.005 : g/L)	1.25	0.5	17.5
90th percentile blood level (0.012 : g/L)	3.0	1.2	42.0
Mean blood level (0.017 : g/L)	4.3	1.7	59.5

**Table 1-9. Comparison of Measured and Modeled TCE Concentrations**

	Measured Range	Modeled Mean
Air	0.0005 to 16 ug/m <sup>3</sup>	4.58 : g/m <sup>3</sup>
Drinking Water	trace to 50 : g/L	59.5 : g/l

TCE is the most frequently reported organic contaminant in ground water (ATSDR, 1997a), 93% of the public water systems in the United States obtain water from groundwater (U.S. EPA, 1995) and between 9% and 34% of the drinking water supply sources tested in the United States may have some TCE contamination (ATSDR, 1997a). Although commonly detected in water supplies, the levels are generally low since, as discussed earlier, MCL violations for TCE in public water supplies are relatively rare for any extended period (U.S. EPA, 1998). Private wells, however, are often not closely monitored and if located near TCE disposal/contamination sites where leaching occurs, may have undetected contamination levels. About 10% of Americans (27 million people) obtain water from sources other than public water systems, primarily private wells (U.S. EPA, 1995). TCE is a common contaminant at Superfund sites. It has been identified in at least 861 sites of the 1,428 hazardous waste sites proposed for inclusion on the EPA National Priorities List (NPL) (See Figure 1-2. ATSDR, 1997a). Studies have shown that many people live near these sites: 41 million people live less than 4 miles from one or more of the nation's NPL sites, and on average 3,325 people live within 1 mile of any given NPL site (ATSDR, 1996b). Thus, although exact estimates cannot be made, many people are probably exposed to TCE via drinking water from private wells. It is not known how often such exposures would be above the MCL.

Some members of the general population may have elevated TCE exposures. ATSDR (ATSDR, 1997a) has reported that TCE exposures may be elevated for people living near waste facilities where TCE may be released, residents of some urban or industrialized areas, people exposed at work (discussed further below) and individuals using certain products (also discussed further below). Because TCE has been detected in breast milk samples of the general population, infants who ingest breast milk may be exposed. Also, since TCE can be present in soil, children may be exposed through activities such as playing in or ingesting soil.

### **1.4.2 Occupational Exposure**

Occupational exposure to TCE in the U.S. has been identified in various degreasing operations, silk screening, taxidermy, and electronic cleaning (IARC, 1995). The major use of trichloroethylene is for metal cleaning or degreasing (IARC, 1995). Degreasing is used to remove oils, greases, waxes, tars, and moisture before galvanizing, electroplating, painting, anodizing, and coating. The five primary industrial groups are: furniture and fixtures; electronic and electric equipment; transport equipment; fabricated metal products; and miscellaneous manufacturing industries (IARC, 1995). Additionally, TCE is used in the manufacture of plastics, appliances, jewelry, plumbing fixtures, automobile, textiles, paper, and glass (IARC, 1995). NIOSH conducted a survey of various industries from 1981 to 1983 and estimated that approximately 401,000 U.S. employees in 23,225 plants in the U.S. are potentially exposed to TCE (IARC, 1995; ATSDR, 1997a). The majority of published worker exposure data are for degreasing operations; time weighted average (TWA) concentrations from personal monitoring ranged from 6,535-27,775  $\mu\text{g}/\text{m}^3$  (1.2 to 5.1 ppm) at individual industrial sites where TCE was used (ATSDR, 1997a).

According to ATSDR (1997a), workers, especially in the vapor degreasing industry, are exposed to the highest levels of TCE through inhalation. These workers may be exposed to

levels ranging from approximately 5,446-544,600  $\mu\text{g}/\text{m}^3$  (1 to 100 ppm), based on monitoring survey (ATSDR, 1997a).

### **1.4.3 Consumer Exposure**

Consumer products reported to contain TCE include wood stains, varnishes, and finishes; lubricants; adhesives; typewriter correction fluids; paint removers; and cleaners (ATSDR, 1997a). Use of TCE has been discontinued in some consumer products (i.e., as an inhalation anesthetic, fumigant, and an extractant for decaffeinating coffee) (ATSDR, 1997a).

## **1.5 CHAPTER SUMMARY**

Table 1-10 summarizes the findings of TCE.

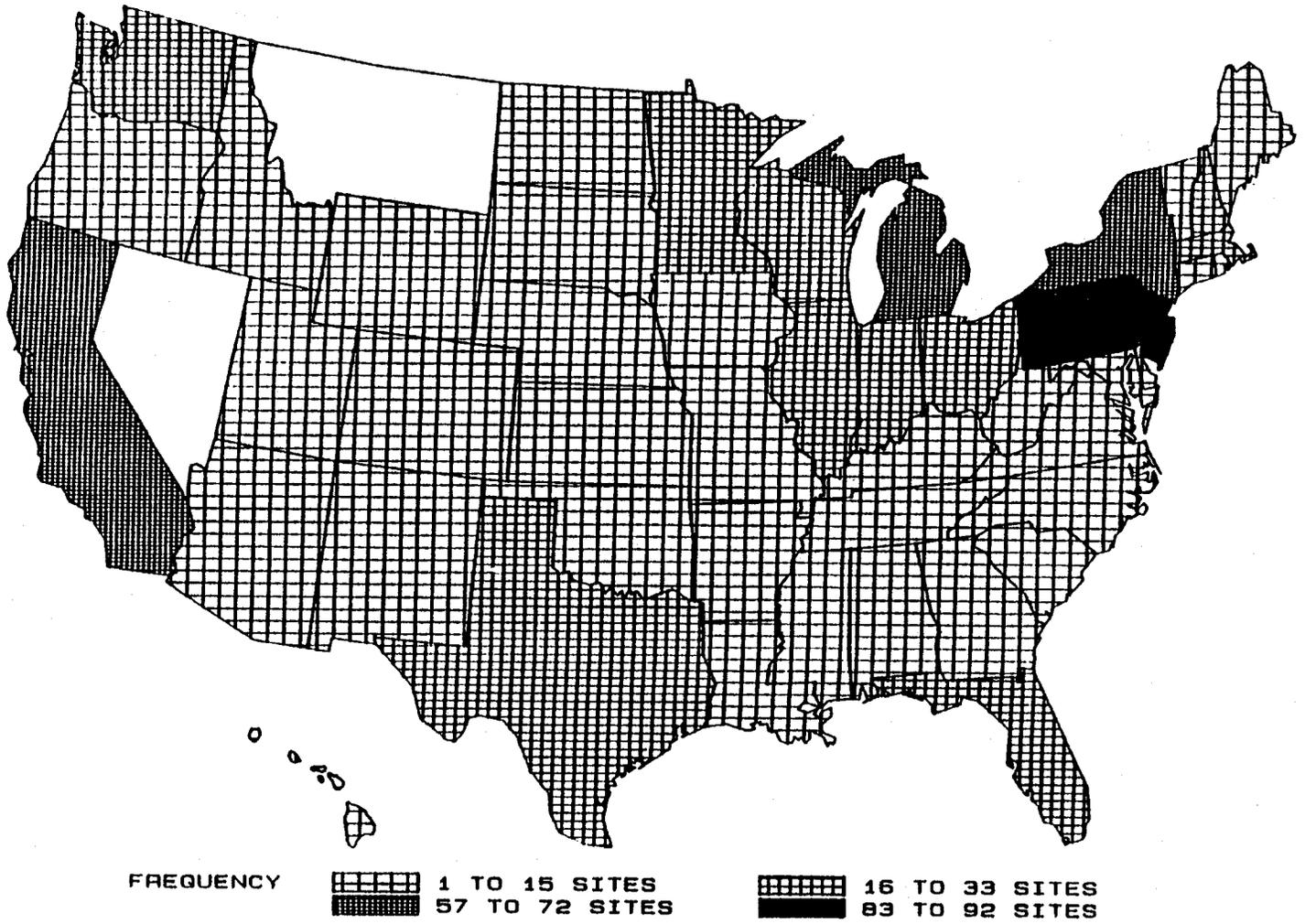


Figure 1-2. Frequency of NPL Sites with Trichloroethylene Contamination (Source: ATSDR, 1997a)

**Table 1-10. Trichloroethylene Summary**

	<b>Estimates</b>	<b>Support</b>
<b>Uses</b>	Metal cleaning and degreasing; many other solvent applications	Well documented in numerous studies, recent information
<b>Production</b>	1.45 x 10 <sup>8</sup> kg/yr	1991 data
<b>Releases</b>	All media - 42 million lb/yr (mostly to ai) in 1994	TRI (U.S. EPA, 1996) is primary source, so current but uncertain due to self reporting and exemptions
<b>Properties/Fate</b>	Volatile, water soluble, stable in air, no significant bio-degradation or bio-concentration	Well documented in numerous studies, recent information
<b>Media Levels</b>	<ul style="list-style-type: none"> <li>- Air: mean = 0.88 : g/m<sup>3</sup></li> <li>- Drinking water: 2-7 : g/L</li> <li>- Groundwater: median = 3 : g/L</li> <li>- Human blood: mean = 0.017 : g/L</li> <li>- Some data on food, human milk, and other tissues</li> </ul>	<ul style="list-style-type: none"> <li>- Air data is from 1998 survey of 115 monitors in 14 states</li> <li>- Based on extensive data from public water systems which routinely monitor for TCE, private systems generally do not monitor for TCE and levels not well established</li> <li>- Groundwater estimate from 1985 survey of 819 water systems in CA</li> <li>- Blood data collected from 1988 to 1994 from 677 individuals</li> <li>- n's and dates for other data unclear, but appear very limited</li> </ul>
<b>General Population Exposure</b>	<ul style="list-style-type: none"> <li>- Inhalation: 11-33 : g/d (urban)</li> <li>- Water ingestion: 2-20 : g/d</li> <li>- Food exposure possible but probably low</li> </ul>	<ul style="list-style-type: none"> <li>- Inhalation and ingestion estimates based on very limited monitoring data (see above)</li> <li>- Insufficient food data for reliable estimates of exposure</li> </ul>
<b>Special Population Exposures</b>	<ul style="list-style-type: none"> <li>- Nursing infants</li> <li>- Workers in production plants or degreasing operations: 1-100 ppm</li> </ul>	<ul style="list-style-type: none"> <li>- Human milk data insufficient for estimating exposure</li> <li>- Worker data based on several recent surveys</li> </ul>

## 2.0 TETRACHLOROETHYLENE (PERCHLOROETHYLENE)

### 2.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 2.1.1 Nomenclature

CAS No.: 127-18-4

Synonyms: 1,1,2,2-tetrachloroethylene; ethene, tetrachloro-, perchloroethylene; tetrachloroethene; PCE.

Trade Names: ENT 1; 860; Perclene; Persec; Antisal 1; Dow-Per; Perchlor; Perklone.

#### 2.1.2 Formula and Molecular Weight

Molecular Formula:  $C_2Cl_4$

Molecular Weight: 165.83

#### 2.1.3 Chemical and Physical Properties

Description: Colorless liquid, ether-like or chloroform-like odor (Merck Index, 10th Ed., 1983).

Boiling Point: 121° C @ 760 mm Hg (Weast. Hdbk. Chem. & Phys., 68th Ed., 1987-88).

Melting Point: -19° C (Weast. Hdbk. Chem. & Phys., 68th Ed., 1987-88).

Density: 1.6227 at 20° C/4° C (Weast. Hdbk. Chem. & Phys., 68th Ed., 1987-88).

#### Spectroscopy

Data: Sadtler Ref. Number: 237 (IR, prism); 79 (IR, grating) (Weast. Hdbk. Chem. & Phys., 60th Ed., 1979). Index of refraction: 1.5053 @ 20° C/D (Weast. Hdbk. Chem. & Phys., 68th Ed., 1987-88). IR: 4786 (Coblentz Society Spectral Collection), Mass: 1053 (Atlas of Mass Spectral Collection)

Solubility: Soluble in water, 0.15 g/100 ml @ 25°C (IARC Monographs) (1972-present) 1979. Miscible with alcohol, ether, chloroform, benzene (Merck Index, 10th Ed., 1983).

Volatility: Vapor Pressure - 18.47 mm Hg at 25°C (Riddick, J.A., et al. (1986) Organic Solvents: Physical Properties and Methods of Purification).

Vapor Density - 5.7 (air = 1) (Browning Tox. & Metab. Indus. Solv., 1965).

Stability:	Rapidly deteriorates in warm climates (Goodman, 1975); tetrachloroethylene is stable up to 500°C in the absence of catalysts, moisture, and oxygen (WHO, Environ. Health Criteria, 1984).
Reactivity:	Reacts with metals to form explosive mixtures; sodium hydroxide, possible explosion (ITII. Tox. & Hazard Indus. Chem. Safety Manual, 1982). Incompatible with chemically active metals, such as barium, lithium, and beryllium (NIOSH Pocket Guide, 1985).
Octanol/Water Partition Coefficient:	log Kow = 3.40 (Hansch C., Leo A.J., 1985, Medchem Project Issue No. 26)

#### 2.1.4 Technical Products and Impurities

Tetrachloroethylene is available in the USA in the following grades: purified, technical, USP, spectrophotometric, and dry-cleaning. The technical and dry-cleaning grades both meet specifications for technical grade and differ only in the amount of stabilizer added to prevent decomposition. Stabilizers include amines or mixtures of epoxides and esters. Typical analysis of the commercial grade is nonvolatile residue, 0.0003%; free chlorine, none; moisture, no cloud at -5°C. USP grade contains not less than 99.0% and no more than 99.5% tetrachloroethylene, the remainder consisting of ethanol (IARC Monographs, 1972-Present V20 492, 1979). PCE is also available in the United States in veterinary preparation (Nema Worm Capsules) (AMA Drug Eval., 1986).

## 2.2 PRODUCTION AND USE

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

### 2.2.1 Production

- U.S. Production: (1985)  $3.08 \times 10^{11}$  g; (1986)  $1.84 \times 10^{11}$  g; (1989)  $2.14 \times 10^{11}$  g; (1990)  $1.6 \times 10^{11}$  g; (1991)  $1.08 \times 10^{11}$  g; (1992)  $1.12 \times 10^{11}$  g; (1993)  $1.23 \times 10^{11}$  g (ATSDR, 1995b; HSDB, 1996).
- Import volumes: (1982)  $1.70 \times 10^{10}$  g; (1985)  $6.36 \times 10^{10}$  g; (1986)  $8.3 \times 10^7$  g (Bureau of the Census, U.S. Imports for Consumption and General Imports, 1985; 1986).
- Export volumes: (1983)  $2.47 \times 10^{10}$  g (SRI); (1985)  $9.84 \times 10^9$  g (Bureau of the Census, U.S. Exports, 1985).

## **2.2.2 Uses**

The three major uses of tetrachloroethylene in the U.S. are textile dry-cleaning; processing and finishing in both cold cleaning and vapor degreasing of metals; and as a chemical intermediate in the synthesis of fluorocarbon 113, 114, 115, and 116. However, because of an international agreement to protect against ozone layer depletion, this latter use is being phased out (IARC, 1995). Additionally, PCE is used as a heat-exchange fluid; a scouring, sizing, and desizing agent; a carrier solvent for fabric dyes and finishes; a water repellent in textile manufacture; a component of aerosol laundry-treatment products; a solvent for silicones; insulating fluid and cooling gas in electric transformers (SRI); and a solvent in typewriter correction fluids (IARC, 1995). Other reported uses are extractant in the pharmaceutical industry; a pesticide; and a solvent for adhesive formulations, printing inks, leather treatments; and paper coatings. It has also been reported to be used as an anthelmintic in the treatment of hookworm and some trematode infestations (IARC, 1995) although it has been replaced now with other less toxic and easier-to-administer compounds.

The current end-use pattern for PCE is estimated to be 55% for chemical intermediates, 25% for metal cleaning and vapor degreasing, 15% for dry cleaning and textile processing, and 5% for other unspecified uses (ATSDR, 1997b).

## **2.2.3 Disposal**

Incineration at a temperature greater than 450°C is a method of disposal, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids that are produced (ATSDR, 1997b). PCE may be disposed of in landfills by adsorbing it in vermiculite, dry sand, earth, or a similar material and disposing in a secured sanitary landfill (ATSDR, 1997b). According to HSDB (1996), an environmental regulatory agency should be consulted prior to implementing land disposal of waste containing PCE. The HSDB database presents numerous disposal practice precautions for carcinogens from the IARC 1979 Scientific Publication No. 33.

## **2.3 POTENTIAL FOR HUMAN EXPOSURE**

### **2.3.1 Natural Occurrence**

The natural production of PCE in temperate, subtropical, and tropical algae, and in one red microalga has been reported (IARC, 1995).

### **2.3.2 Occupational**

There is considerable potential for exposure to PCE (dermal and inhalation) during its use in degreasing and dry cleaning operations (IARC, 1995). Other occupational areas where exposures may occur are urethane foam, automotive brake, and rubber molding manufacture; motion picture film processing; taxidermy; electroplating; and graphic arts.

### 2.3.3 Environmental

PCE is released to the environment through industrial emissions, from building products and consumer products. Releases are primarily to the atmosphere, but there are additional releases to surface water and land in sewage sludges, other liquids, and solid wastes. Because of the high vapor pressure, PCE is volatilized to the atmosphere from these sources (ATSDR, 1997b). The Toxic Release Inventory (TRI) industrial release data for PCE releases to air, water, land, and other media from manufacturing facilities are presented in Table 2-1. The number of reporting facilities and the total releases per year are also shown in Table 2-1.

#### 2.3.3.1 Environmental Releases

**Air:** Levels of PCE in air have been reported in numerous studies, both in the U.S. and worldwide. PCE has been found in ambient air, especially in the near vicinity of dry cleaning operations. The TRI emission estimate for total PCE industrial emissions to the atmosphere was 32.9 million pounds in 1987; 17 million pounds in 1991; and 5.2 million pounds in 1994 (TRI, 1996).

**Water:** PCE has been detected in rainwater, surface water, drinking water, and seawater. According to TRI, releases to surface water totaled 161,000 pounds in 1987; 7,448 pounds in 1991; and down to 3,872 pounds in 1994 (TRI, 1996).

**Other Media:** Levels of PCE have been reported in foods, marine invertebrates, fish, waterbirds, marine mammals, marine sediments, and human blood, urine, breast milk, and tissue (IARC, 1995; ATSDR, 1997b; HSDB 1996). TRI estimates of releases for land disposal were 618,026 pounds in 1993 down to 4,349 pounds in 1994 (TRI, 1996).

**Table 2-1. Releases of Tetrachloroethylene (lbs)**

Year	Number of Reporting Facilities	Fugitive Air Releases	Stack Air Releases	Surface Water Release	Underground Injection	Land Disposal	POTW Transfer	Other Transfers	Total
1987	715	15,628,341	17,273,459	160,921	354,000	5,220	468,295	9,155,484	43,046,435
1988	746	16,336,282	19,786,265	33,314	72,250	82,144	558,691	5,582,693	42,452,385
1989	732	12,187,707	15,753,023	53,940	50,000	10,791	467,181	4,356,193	32,879,567
1990	666	9,351,150	13,597,042	21,510	11,012	1,260	450,922	4,548,481	27,982,043
1991	577	6,669,093	10,339,157	7,448	14,000	23,309	234,642	16,290,418	33,578,644
1992	518	5,305,402	7,389,816	10,317	12,780	9,354	111,517	11,011,874	23,851,578
1993	490	4,538,411	6,634,275	10,152	15,041	618,026	111,002	9,564,687	21,492,084
1994	459	4,671,751	5,530,378	3,872	4,051	4,349	62,053	10,411,056	20,687,969

Source: TRI, 1996.

### 2.3.3.2 Monitored Environmental Media Levels

**Air:** Measured levels of PCE in air in rural, urban, and suburban locations in the U.S. are shown in Table 2-2.

**Water:** Measurements of PCE in surface waters, groundwater, and drinking water in U.S. locations are shown in Table 2-3.

**Other Media:** PCE was reported as a contaminant of cosmetic products (0.3-400 µg/l) and cough mixtures (0.2-97.1 µg/l) (IARC, 1995). PCE has been detected in blood and urine of occupationally exposed persons. It has also been reported in 7 of 42 breast milk samples from the general population in 4 urban areas of the U.S. (IARC, 1995; HSDB, 1996). PCE was detected at 1.4 - 5.7 ppt in rain/snow in California (HSDB, 1996). Levels found in food included (ATSDR, 1997b; HSDB, 1996):

- C Crab apple jelly - 2.5 µg/kg
- C Grape jelly - 1.6 µg/kg
- C Dairy products - 0.3 - 13 µg/kg
- C Oils and fats - 0.01 - 7 µg/kg
- C Beverages (canned fruit drinks, instant coffee, tea) - 2 - 3 µg/kg
- C Fruits and vegetables (potatoes, apples, pears, tomatoes) - 0.7 - 2 µg/kg
- C Grain-based products (wheat, corn, oats, corn grits, corn meal) - 1.8 - 2.5 µg/kg

**Table 2-2. Concentrations of Tetrachloroethylene in Ambient Air**

Area	Concentration (ng/m <sup>3</sup> )*	
	Mean	Range
<b><i>Rural</i></b>		
Southern Washington, USA	136	200-300
Rural California, USA	210	
Central Michigan, USA		
USA, 577 sites	1,085	
<b><i>Urban and Suburban</i></b>		
New York City, NY, USA	9,017	1,085-71,936
Houston, TX, USA	2,644	<678-30,510
Detroit, MI, USA	3,119	678-14,916
Los Angeles, CA, USA	10,034	1,180-14,001
Phoenix, AZ, USA	6,739	875-25,066
Oakland, CA, USA	2,054	359-9,831
San Diego, CA, USA	1,831	
San Francisco, CA, USA	1,559	
Sacramento, CA, USA	475	

Source: IARC, 1995. \* 1 ng/m<sup>3</sup>=0.00014 ppb

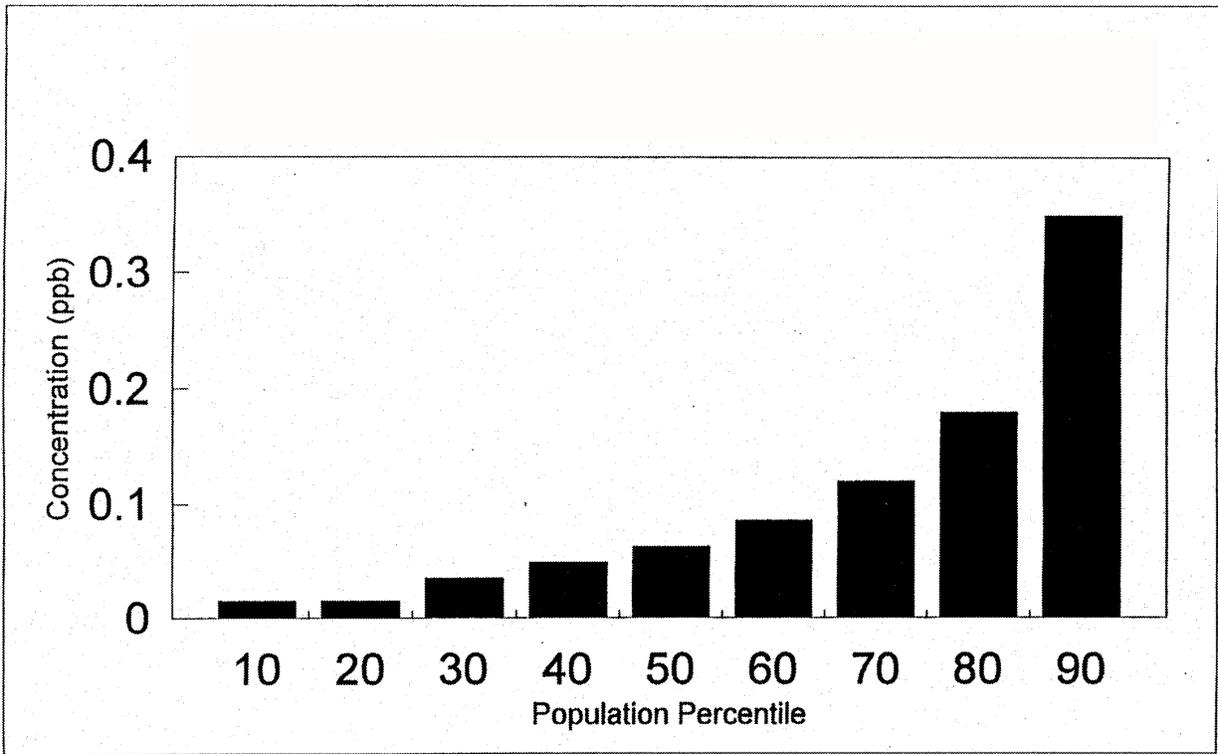
**Table 2-3. Concentrations of Tetrachloroethylene in Water**

Area	Concentration (µg/L)	
	Mean	Range
<b>Surface Waters:</b>		
<u>Seawater</u>		
Eastern Pacific		0.0001-0.0021
North Atlantic		0.00012-0.0008
<u>Rainwater</u>		
Los Angeles, CA, 1982	0.021	
La Jolla, CA	0.006	
Portland, OR		0.0008-0.009
Germany	0.08	
<u>Rivers</u>		
USA, five states, surface water (14% of samples positive)		max. 21
<u>Drinking Water</u>		
New Jersey, USA, 1981-83	0.4	
New Jersey, USA	7.7	
Woburn, MA, USA		max. 14 66-212
<b>Groundwater:</b>		
USA, CA, 945 Water supplies		max. 0.58-69
USA, five sites, 28% of samples positive		max. 1500

Source: IARC, 1995.

Levels of PCE detected in margarine from several supermarkets in the Washington, D.C., area were \$50 ppm in 10.7 percent of the products sampled. The highest levels, ranging from 500 to 5,000 ppb, were found in samples from a store located near a dry cleaning operation (ATSDR, 1995b). The concentrations were highest on the ends of the margarine stick and decreased towards the middle, suggesting that contamination occurred after manufacturing rather than during the manufacturing process (ATSDR, 1997b).

**Biological Monitoring:** The Third National Health and Nutrition Examination Survey (NHANES III) examined perchloroethylene concentrations in blood in 590 non-occupationally exposed individuals (IARC, 1995 and Ashley et al., 1994). This study involved persons in the general U.S. population who were selected on the basis of age, race, gender and region of residence. The samples were collected during 1988 to 1994. As shown in Table 2-4 below, the tetrachloroethylene levels in whole blood span over a wide range with a mean concentration of 0.19 µg/l. This result is also shown on Figure 2-1.



Source: NHANES III (Ashley, D., 1997, CDC). N=590

Figure 2-1. Concentration of Tetrachloroethylene in Blood at Selected Population Percentiles

**Table 2-4. Tetrachloroethylene Levels in Whole Blood by Population Percentile\***

Percentiles	10	20	30	40	50	60	70	80	90
Concentration (: g/l)	0.015	0.015	0.035	0.049	0.063	0.086	0.120	0.180	0.35

\* detection limit = 0.03 : g/L

Source: Personal communication from David Ashley, Center for Disease Control.

Clewell (personal communication to J. Schaum, 1997) applied the NHANES III blood data for tetrachloroethylene to a physiologically based pharmacokinetic model (described in Gearhart et al., 1993) to estimate the following quantities:

- C The long term average inhaled air concentration which would result in the measured blood concentration, assuming no other perchloroethylene exposure.
- C The long term average ingested dose which would result in the measured blood concentration, assuming no other perchloroethylene exposure. This dose was converted to a perchloroethylene water concentration assuming an ingestion rate of 2 l/day.
- C For each of these exposure scenarios, the model also provides the corresponding concentrations of TCA and DCA in blood and the amount of perchloroethylene metabolized per day.

This model (Gearhart et al., 1993) includes 30 to 40 parameters in its structure. Typically only 25 to 30 percent of these parameters have a significant enough impact on the model prediction to be considered. Significant parameters in this model include parameters such as blood/air and tissue/blood partition coefficients, organ volumes, body weight, ventilation rates, and *in vivo* metabolic rates.

Table 2-5 below provides the modeled exposure estimates corresponding to a range of blood levels.

As shown in Table 2-6 below, the modeled mean perchloroethylene concentrations fall within the range of measured values for both air and water.

Further interpretations of this analysis are discussed below:

- C The monitoring data are much older than the blood data (collection dates: air 1975-1981, water 1973-1994 and blood 1988 - 1994). Thus, the exposure estimates derived from blood should better reflect current conditions.
- C Environmental monitoring data (especially for air) may not be very representative of actual exposures. For example, ambient air monitors are fixed units typically located on top of buildings and do not sample the air that a person actually

**Table 2-5. Modeled Exposure Estimates for Tetrachloroethylene**

Blood Level	Air Concentration (: g/m <sup>3</sup> )	Ingested Dose (: g/kg-day)	Water Concentration (: g/l)
10th percentile (0.015 : g/l)	1.34	0.24	8.4
90th percentile (0.35 : g/l)	31.2	5.5	192.5
Mean (0.19 : g/l)	17.0	3	105

**Table 2-6. Comparison of Measured and Modeled Perchloroethylene Concentrations**

	Measured Range	Modeled Mean
Air	0.2 to 30 : g/m <sup>3</sup>	18.5 : g/m <sup>3</sup>
Water	0.0001 to 210 : g/l	105 : g/l

breathes throughout a day. Also, indoor air (which is not measured by ambient air monitors) may be a more important contributor to perchloroethylene exposure than outdoor air. In contrast, blood measurements reflect the actual exposure that an individual experiences. Thus, the exposure estimates derived from blood should more accurately reflect total exposure.

- C Exposure estimates derived from blood cannot distinguish between exposure routes and sources. It is generally believed that perchloroethylene exposure occurs primarily via water consumption and air inhalation, but it is impossible to use the blood data to estimate how much of the total exposure is attributable to each. A wide range of combinations of exposures from air and water could have produced the measured blood levels.

### **2.3.3.3 Environmental Fate and Transport**

#### **2.3.3.3.1 Summary**

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of tetrachloroethylene released to surface soils is volatilization. Because of its low to moderate mobility in soils, tetrachloroethylene introduced into soil (e.g., landfills) has the potential to migrate through the soil into groundwater. Biodegradation under anaerobic conditions in soil and groundwater may occur at a relatively slow rate (half-lives on the order of months or longer (HSDB, 1996).

**Fate in the Atmosphere:** In the atmosphere, tetrachloroethylene is expected to be present primarily in the vapor phase rather than sorbed to particulates because of its high vapor pressure. Removal by scavenging during wet precipitation is expected because of the moderate solubility of tetrachloroethylene in water (150 mg/L). The major degradation process affecting vapor phase tetrachloroethylene is photo-oxidation by hydroxyl radicals and the chlorine radicals formed by the hydroxyl radical reaction (half-life on the order of weeks to months).

**Fate in Aquatic Environments:** The dominant fate of tetrachloroethylene released into surface waters is volatilization (predicted half-life of hours to days (HSDB, 1996)). Bioconcentration and sorption to sediments and suspended solids are not expected to be significant transport/partitioning processes. Although biodegradation is not expected to be a significant degradation process, any tetrachloroethylene that reaches the sediment will undergo slow anaerobic biodegradation.

#### **2.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:** A  $K_{oc}$  of 1,685 is predicted for tetrachloroethylene based on its measured log octanol/water partition coefficient of 3.40. Actual  $K_{oc}$ s calculated from studies with various soils and sediments are less than 250 (HSDB, 1996). Based on the reported and measured  $K_{oc}$ s, tetrachloroethylene is expected to exhibit low to medium mobility in soil. Therefore, tetrachloroethylene may leach slowly to the groundwater particularly in soils with low organic content (HSDB, 1996).

**Volatilization:** The dominant removal mechanism for tetrachloroethylene in surface waters is volatilization. The half-life will depend on wind and mixing conditions and is estimated to range from 3 hours to 14 days in rivers, lakes, and ponds based on laboratory and mesocosm experiments. Because of its high vapor pressure and relatively low soil adsorption coefficient, tetrachloroethylene is expected to volatilize from soil surfaces and also from suspended particulate matter in the atmosphere (HSDB, 1996).

**Bioconcentration:** A bioconcentration factor of 226 is predicted for tetrachloroethylene based on its measured log octanol/water partition coefficient of 3.40. Actual BCFs measured in fish studies are less than 50. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996).

#### **2.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** Under aerobic conditions, tetrachloroethylene undergoes biodegradation at a very slow rate with a half-life estimated at 6 months to a year. Little or no degradation has been observed in several aerobic tests with acclimated or unacclimated inocula nor in river die-away and mesocosm tests. Slow degradation under anaerobic conditions (half-lives of weeks to months) has been demonstrated in laboratory screening tests. Trichloroethylene is the major intermediate observed with traces of vinyl chloride and dichloroethylene isomers also formed (HSDB, 1996; Howard et al., 1991).

**Photodegradation:** Photolysis in the atmosphere or in aquatic environments is expected to proceed very slowly if at all. Tetrachloroethylene does not absorb UV light at wavelengths greater than 260 nm and thus will not directly photolyze. Based on measured rate data for the vapor phase photo-oxidation reaction with hydroxyl radicals and with the chlorine radicals formed during this reaction, the estimated half-life of tetrachloroethylene in the atmosphere is on the order of weeks to months, although one study has reported complete degradation in one hour. The main reaction products are phosgene, carbon tetrachloride, dichloroacetyl chloride, and trichloroacetyl chloride (HSDB, 1996; Howard et al., 1991).

**Hydrolysis:** Tetrachloroethylene has no hydrolyzable groups. The rate constants at pH 3, 7, and 11 have been measured to be zero in one study. Another study reported a half-life of 9 months in purified, deionized water (HSDB, 1996; Howard et al., 1991)

## **2.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **2.4.1 General U.S. Population**

The most important routes of exposure to PCE for the general population are inhalation of PCE in ambient air and ingestion of contaminated drinking water from contaminated aquifers and drinking water distributed in pipelines with vinyl liners (HSDB, 1996). Available data indicates that dermal exposure to PCE is not an important route of exposure for most people (ATSDR, 1997b). Exposure from inhalation of ambient air varies according to location. In rural and remote areas, background levels are generally in the low ppt range, and both low ppb and high ppt are found in urban and industrial areas, and areas near point sources of emissions (ATSDR, 1997b).

Results of several studies have indicated that indoor air is a more significant source of exposure to PCE than outdoor air; reported concentrations in the air of four homes in North Carolina were consistently higher than the outdoor concentrations (ATSDR, 1997b). The detection of PCE in breast milk (see Section 2.3.3.2) indicates that infants may be exposed to PCE through breast feeding (ATSDR, 1997b). For the general population, the estimated amount of PCE that a person might breathe per day ranges from 0.08-0.2 mg/day and the most PCE people might drink in water is 0.0001-0.002 mg/day (ATSDR, 1997b).

The EPA estimated that in 1985, 11,430,000 individuals (5.3 percent of the U.S. population using municipal water supplies) in the U.S. were exposed to PCE at concentrations  $\leq 0.5$   $\mu\text{g/l}$ . Assuming a 70 kg person drinks 2 L/day of water containing 0.5 ppb PCE, the daily intake of PCE was 1  $\mu\text{g}$  or 0.014  $\mu\text{g/kg/day}$  (ATSDR, 1997b). Additionally, 874,000 individuals were estimated to be exposed to levels  $>5$   $\mu\text{g/l}$  (IARC, 1995). General population exposure from ingestion of contaminated foods has been approximated by EPA assuming individual average daily intakes of 0.753 kg dairy products; 0.262 kg meat, fish, and poultry; 0.073 kg fats and oils; and 0.128 kg beverages (ATSDR, 1997b). The average daily intake of PCE was determined to be between 0-4  $\mu\text{g}$  from dairy products; 0-1  $\mu\text{g}$  from meat, fish, and poultry; 0-9.5  $\mu\text{g}$  from fats and oils; and 0-0.06  $\mu\text{g}$  from beverages (ATSDR, 1997b).

Showering or bathing with contaminated water is also a mechanism for PCE exposure. Using results from a study and a model, it was estimated that the shower air would contain an average of 1 ppm and the air above a bath tub would contain an average of 0.725 ppm if the water contained 1 mg/L of PCE (ATSDR, 1997b). The model assumed that the shower or bath used 100 liters of water, the air volume in the shower stall or above the bath tub was 3 m<sup>3</sup>, and the shower flow rate was 6.667 L/minute (ATSDR, 1997b).

#### **2.4.2 Occupational Exposure**

Persons with the greatest chance of elevated exposure are those engaged in occupational activities using PCE. In a survey conducted between 1981 and 1983 by NIOSH, it was estimated that approximately 688,110 employees in 49,025 plants in the U.S. were potentially exposed to PCE (ATSDR, 1997b). Further, in 1994 an independent industry estimate indicated that approximately 450,000 workers in dry cleaning operations in the U.S. may be exposed (IARC, 1995). A NIOSH survey in 44 dry cleaning facilities showed PCE TWA exposures to machine operators ranged from 4.0 to 149 ppm with a geometric mean of 22 ppm. Mean exposures to pressers, seamstresses, and front counter workers were 3.3, 3.0, and 3.1 ppm, respectively (ATSDR, 1997b).

Tetrachloroethylene has been identified in at least 771 of 1,430 hazardous waste sites that have been proposed for inclusion in the EPA National Priorities List (NPL) (ATSDR, 1997b). The number of sites evaluated is not known; the frequency of the sites are shown in Figure 2-2.

#### **2.4.3 Consumer Exposure**

In a study to determine potential sources of indoor air pollution, approximately 63 of 1,159 common household products were found to contain PCE (IARC, 1995). Products that may contain PCE include adhesives; water repellents; fabric finishers; stain, spot, and rust removers; and wood cleaners (ATSDR, 1997b). Other consumer products that have been found to contain PCE are inks, polishes, rug and upholstery cleaners, sealants, and silicones.

### **2.5 CHAPTER SUMMARY**

Table 2-7 summarizes the findings of TCE.



**Table 2-7. Tetrachloroethylene (Perchloroethylene) Summary**

	Estimates	Support
Uses	Dry cleaning and metal degreasing	Well documented in numerous studies, recent information
Production	1.2 x 10 <sup>8</sup> kg/yr	1993 data
Releases	Air: 5.2 million lb/yr Water: 3,900 lb/yr Land: 4,300 lb/yr	TRI (U.S. EPA, 1996) is primary source, so current but uncertain due to self reporting and exemptions
Properties/Fate	Volatile, water soluble, photo-oxidizes slowly in air, no significant biodegradation or bioconcentration	Well documented in numerous studies, recent information
Media Levels	- Urban air: low ppb - Rural air: low ppt - Drinking water: 0.5-5 ug/L - Food: 0.3-3 ug/kg - Human blood: 0.19 ug/L - Human milk: 6.2 ug/L	- Air data represents only 4 rural and 9 urban locations, dates unclear - Blood data from NHANES III (n=590) - n's and dates unclear for water, food, and human milk data
General Population Exposure	- Inhalation: 0.08-0.2 mg/d (urban) - Water ingestion: 0.1-2 ug/d - Dairy: 0-4 ug/d - Meat: 0-1 ug/d - Fats/oils: 0-9 ug/d	- All estimates based on limited or unclear monitoring data (see above)
Special Population Exposures	- Nursing infants: ~4 ug/d - Workers in production plants, degreasing operations, dry cleaners (3-150) ppm	- Representativeness of human milk data unknown - Worker data based on several recent surveys

### 3.0 1,1,1-TRICHLOROETHANE (METHYL CHLOROFORM)

#### 3.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

##### 3.1.1 Nomenclature

CAS No.:	71-55-6
Synonyms:	Chloroethene; chloroform; methyl-, chlorotene; ethane, 1,1,1-trichloro-; methyl chloroform; trichloroethane
Trade Names:	alpha-t; algylen; baltana; gemalgene; inhibisol; solvent 111

##### 3.1.2 Formula and Molecular Weight

Molecular Formula:	$C_2H_3Cl_3$
Molecular Weight:	133.43

##### 3.1.3 Chemical and Physical Properties

Description:	Colorless liquid (Patty, 1981-82); chloroform-like odor, sweetish (Hazard Chem. Data Vol. II, 1984-85).
Boiling Point:	74.0°C @ 760 mm Hg (CRC Handbook Chem. & Physics, 1994-95).
Melting Point:	-30.4°C (CRC Handbook Chem. & Physics, 1994-95).
Density:	1.3376 @ 20°C/4°C (Merck Index, 11th Ed., 1989).
Spectroscopy Data:	Index of refraction: 1.43838 @ 20°C/D (Merck Index, 10th Ed., 1983); IR: 19461, NMR: 9171; Mass; 618 (Sadler Research Laboratories Prism Collection) (Weast, 1985).
Solubility:	Soluble in acetone, benzene, methanol, carbon tetrachloride (Merck Index, 11th Ed., 1989); 4,400 mg/l in water @ 20°C (Verschuere, 1983).
Volatility:	Vapor Pressure: 16.5 kPa @ 25°C (CRC Handbook, 1994-95) Vapor Density: 4.63, relative (air = 1) (Verschuere, 1983).
Stability:	No data.

Reactivity: Although apparently stable on contact, mixtures with potassium (or its alloys) with a wide range of halocarbons (including 1,1,2-trichloroethane) are shock-sensitive and may explode with great violence on light impact. Violent decomposition with evolution of hydrogen chloride may occur when it comes into contact with aluminum or its alloys with magnesium (Handbook Reactive Chem. Hazards, 1985). Reacts with strong caustics; strong oxidizers; chemically-active metals such as zinc, magnesium powders; sodium and potassium; water (note: reacts slowly with water to form hydrochloric acid) (NIOSH Pocket Guide Chem. Haz, 1994).

Octanol/Water

Partition Coefficient:  $\log K_{ow} = 2.49$  (Hansch. Log P Database, 1984)

### 3.1.4 Technical Products and Impurities

1,1,1-Trichloroethane is available commercially in the USA in technical and solvent grades, which differ only in the amount of stabilizer added to prevent corrosion of metal parts (IARC Monographs, V20:516, 1979). It is available as chlorothene SM (industrial grade) and aerothene TT (aerosol grade) (Kuney. Chemcyclopedia, 1988).

Impurities include 1,2-dichloroethane, 1,1-dichloroethane, chloroform, carbon tetrachloride, trichloroethylene, 1,1,2-trichloroethane, and vinylidene chloride (Stewart, RD, et al., 1969).

Stabilized grades contain 3-8% stabilizers such as nitromethane, N-methylpyrrole, butylene oxide, 1,3-dioxolane, and secondary butyl alcohols (IARC Monographs, V20:516, 1979). 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, 1976).

## 3.2 PRODUCTION AND USE

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996) and from ATSDR (1995).

### 3.2.1 Production

- (1990)  $3.64 \times 10^{11}$  g (ATSDR, 1995); (1992)  $3.13 \times 10^{11}$  g (HSDB, 1996).
- Import Volume: (1991)  $4.54 \times 10^7$  g; (1992)  $5.99 \times 10^9$  g; (1993)  $9.08 \times 10^7$  g (ATSDR, 1995).

- Export Volume: (1990)  $5.2 \times 10^{10}$  g; (1991)  $7.37 \times 10^{10}$  g; (1992)  $6.34 \times 10^{10}$  g; (1993)  $3.44 \times 10^{10}$  g (ATSDR, 1995).

### **3.2.2 Uses**

1,1,1-Trichloroethane is used as a solvent for adhesives (including food packaging adhesives) in pesticides, metal degreasing, textile processing, aerosols, lubricants, cutting oil formulations, cutting fluids, shoe polishes, spot cleaners, stain repellents, drain cleaners, and printing inks (ATSDR, 1995; HSDB, 1994). Its primary use in industry is for cold, dip, and bucket cleaning and in vapor degreasing operations of electric and electronic instruments, fabrics, wigs, and photographic film (ATSDR, 1995). It is also used as a chemical intermediate and for on-site cleaning of printing presses, food packaging machinery, and molds (ATSDR, 1995; HSDB, 1996). 1,1,1-Trichloroethane is also used extensively in household products that contain solvents.

### **3.2.3 Disposal**

Generators of waste containing this contaminant (i.e., EPA hazardous waste numbers U226 and F002) must conform with USEPA regulations in storage, transportation, treatment, and disposal of waste [40 CFR 240-280, 300-306, 702-799]. 1,1,1-trichloroethane is a waste chemical stream constituent which may be subjected to ultimate disposal by controlled incineration, preferably after mixing with another combustible fuel. Complete combustion to prevent the formation of phosgene must be exercised (U.S. EPA, 1981 Engineering Handbook for Hazardous Waste Incineration). 1,1,1-Trichloroethane is a potential candidate for liquid injection incineration at a temperature range of 650 to 1,600°C and a residence time of 0.1 to 2 seconds; for rotary kiln incineration at a temperature range of 820 to 1,600°C and residence times of seconds for liquids and gases, and hours for solids; and for fluidized bed incineration at a temperature range of 450 to 980°C and residence times of seconds for liquids and gases, and longer for solids (HSDB, 1996). Chemical treatability study results indicates that the chemical may be extractable with solvents, air and stream strippable, and treatable using biological treatment (U.S. EPA, 1982, Management of Hazardous Waste). Other methods that have shown promise for destruction of 1,1,1-trichloroethane are a combination of ozonation and ultraviolet treatment for groundwater and homogeneous sonochemical treatment for aqueous waste (ATSDR, 1995).

## **3.3 POTENTIAL FOR HUMAN EXPOSURE**

### **3.3.1 Natural Occurrence**

1,1,1-Trichloroethane is not known to occur as a natural product.

### **3.3.2 Occupational**

Humans may be exposed to 1,1,1-trichloroethane dermally and by inhalation of contaminated air at the workplace (HSDB, 1996).

### 3.3.3 Environmental

1,1,1-Trichloroethane is likely to enter the environment from air emissions or in the wastewater from its production or use in vapor degreasing, metal cleaning, and other operations. It can also enter the environment in leachates and volatile emissions from landfills (HSDB, 1996). Process and fugitive emissions may result from the use of both consumer and industrial products (ATSDR, 1995). Because 1,1,1-trichloroethane is used as a solvent in many products and is very volatile, it is most frequently found in the atmosphere due to volatilization from production and use (ATSDR, 1995).

#### 3.3.3.1 Environmental Releases

**Air:** Trichloroethane has been found in the ambient air around chemical manufacturing areas, in remote and rural areas, and around suburban sites. Toxic Release Inventory (TRI) data are shown in Table 3-1.

The TRI data for 1,1,1-trichloroethane have been correlated with industrial source code (SIC Codes) and shows that emissions of this chemical are associated with 122 different industrial classifications (ATSDR, 1995). The TRI data shown in Table 3-1 indicate that 1,1,1-trichloroethane emissions to air ranged from 166.3 million pounds in 1987 down to 38.1 million pounds in 1994 (TRI, 1996).

**Table 3-1. Releases of 1,1,1-Trichloroethane (lbs)**

Year	Number of Reporting Facilities	Fugitive Air Releases	Stack Air Releases	Surface Water Release	Underground Injection	Land Disposal	POTW Transfer	Other Transfers	Total
1987	3494	90,428,647	75,825,060	37,181	28,325	199,191	412,010	32,141,143	199,071,557
1988	3915	92,995,587	87,654,575	95,624	1,000	204,923	305,358	19,389,542	200,646,609
1989	4201	94,100,022	86,086,417	27,564	2,318	70,547	312,515	16,815,840	197,415,223
1990	4210	85,672,408	83,099,485	16,984	1,586	62,446	173,444	13,099,706	182,126,059
1991	3732	72,670,441	71,770,764	22,308	2,805	174,730	253,812	39,451,571	184,346,431
1992	3210	57,760,109	59,857,572	13,707	561	76,131	119,263	32,080,182	149,907,525
1993	2111	33,199,831	31,568,263	11,146	2528	42,743	60,463	20,842,953	85,727,927
1994	1207	20,070,741	17,981,336	1,980	102	2,732	6,439	11,387,618	49,450,948

Source: TRI, 1996.

Other sources for small emissions of 1,1,1-trichloroethane to the atmosphere include coal fired plants, incineration of medical waste, incineration of industrial waste containing waste solvents and certain plastics, and municipal wastewater sludge (ATSDR, 1995). When contained in consumer products, 1,1,1-trichloroethane can be released to the atmosphere during application, drying, or curing of the consumer products.

**Water:** 1,1,1-Trichloroethane has been reported in groundwater, surface water, and drinking water in the United States. It has also been reported in seawater. TRI data on water releases are presented in Table 3-1.

**Other Media:** Levels of 1,1,1-trichloroethane has been reported in raw, processed, and prepared foods. Additionally, it has been detected in soils and sediments (ATSDR, 1995). TRI estimates of releases to land are presented in Table 3-1.

### 3.3.3.2 *Monitored Environmental Media Levels*

**Air:** Numerous studies have reported levels of 1,1,1-trichloroethane in air throughout the U.S. Monitoring data have been reported with sampling dates ranging primarily from years 1972 through 1986. However, there are several studies for years 1987 through 1990. Measured concentrations in urban air range from 0.1 to 1 ppb; for large urban areas or areas near hazardous waste sites, levels #1,000 ppb have been observed (ATSDR, 1995; HSDB, 1996). Level of this chemical in rural areas typically are <0.2 ppb. ATSDR (1995c) provides a summary of monitored levels in ambient air in the U.S. that includes sampling dates, number of samples, concentrations (range and mean), study location, and author. Level of 1,1,1-trichloroethane in indoor air seems to depend on parameters such as outdoor concentration, age of building, individual practices, and building air exchange characteristics (ATSDR, 1995).

**Water:** 1,1,1-Trichloroethane has been detected in surface water, groundwater, drinking water, rain, snow, effluent, and urban runoff (ATSDR, 1995). The levels detected in surface water and groundwater depends upon the sampling point location. For groundwater random samples, levels have ranged from 0 to 18 ppb; groundwater samples obtained near sources of release to soil have been as high as 11,000 ppb (ATSDR, 1995). Drinking water from reported surface or groundwater sources contained concentrations of 0.01 to 3.5 ppb (ATSDR, 1995).

Levels in raw surface water in 105 U.S. cities were 0.2 ppb (median) and 1.2 ppb (maximum) (HSDB, 1996). In studies of surface water near industrialized sites, the measured levels ranged up to 334 ppb (HSDB, 1996).

**Other Media:** 1,1,1-Trichloroethane has been detected in human adipose tissues (not detected - 830 ppb); milk; blood; and breath. It has been found in foods which include unprepared, uncooked foods; fruits; nuts; dairy products; etc. A range of the mean values for levels of 1,1,1-trichloroethane reported in ATSDR (1995) are shown in Table 3-2 for some of these foods. 1,1,1-Trichloroethane has been found in average concentrations in fish at 2.7 ppm; shrimp at <0.3 ppm; and clams and oysters ranging from 39 to 310 ppm.

**Table 3-2. Level of 1,1,1-Trichloroethane in Food**

Food Type	Concentration (ppb) (Range of Means)
Cereals	3-35
Vegetables (processed/cooked)	1-9
Baked goods (breads, cookies, cakes)	2-40
Dairy products	1-520
Nuts/nut products	10-228
Meats, meat dishes (cooked/processed)	2-76
Fruits (raw/dried)	2-32
Infant/toddler blend	6

Source: ATSDR, 1995.

The National Health and Nutrition Examination Survey (NHANES III) (1988-91) is a national survey of the U.S. civilian non-institutionalized population. It provides data to monitor changes in dietary, nutritional, and health status of the U.S. population. As part of this survey, data were analyzed for the level of selected VOCs in the blood. Figure 3-1 presents the level of 1,1,1-trichloroethane in blood at selected percentiles.

Levels of 1,1,1-trichloroethane in soils have been measured in grab samples from two former sludge lagoons of a solvent recovery operation, at a residence near a landfill, at a production facility, and at several NPL sites. The reported levels were 23,000 to 120,000 ppb at the lagoon, up to 230,000 ppb at the NPL sites, and 0.06 to 1.0 ppb at the production facility (ATSDR, 1995). Levels of 1,1,1-trichloroethane in sediment have been reported up to 2 ppb for non-NPL sites and ranged from 50 to 2,500 ppb at an NPL site (ATSDR, 1995). Monitoring data for the occurrence of 1,1,1-trichloroethane in soil is limited and may be due to its rapid volatilization from soil and/or its ability to leach through soil (ATSDR, 1995).

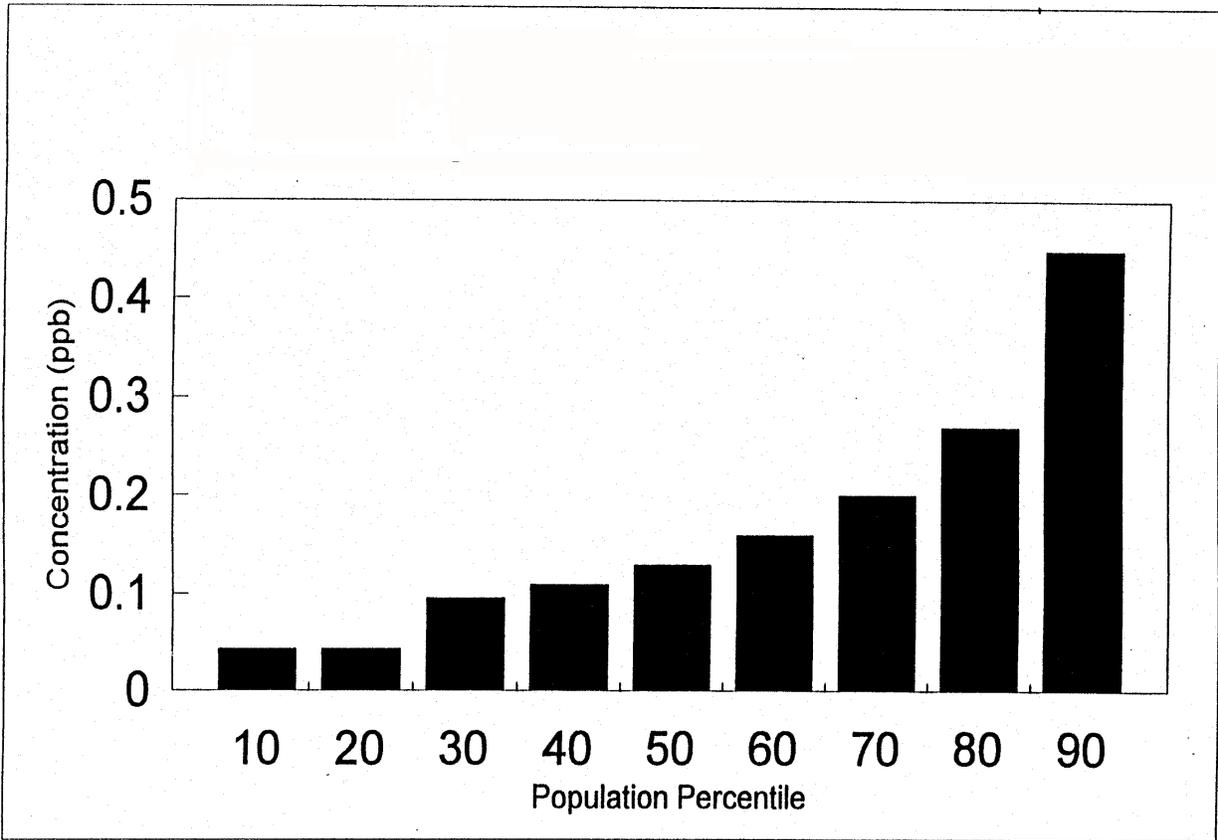
### **3.3.3.3 Environmental Fate and Transport**

#### **3.3.3.3.1 Summary**

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of 1,1,1-trichloroethane released to surface soils is volatilization. Because of its moderate mobility in soils, 1,1,1-trichloroethane introduced into soil (e.g., landfills) has the potential to migrate through the soil into groundwater.

**Fate in the Atmosphere:** In the atmosphere, 1,1,1-trichloroethane is expected to be present primarily in the vapor phase rather than sorbed to particulates because of its moderate vapor pressure. Removal by scavenging during wet precipitation is expected because of the moderate solubility of 1,1,1-trichloroethane in water; 40 percent reductions in air concentrations have been reported on rainy days. The major degradation process affecting vapor phase 1,1,1-trichloroethane is photo-oxidation by hydroxyl radicals (half-life on the order of years). Due to its persistence, 1,1,1-trichloroethane will disperse over long distances and slowly diffuse into the



Source: NHANES III (Ashley, D., 1997, CDC). N=574

Figure 3-1. Concentration of 1,1,1-Trichloromethane in Blood at Selected Population Percentiles

stratosphere where it would be rapidly degraded. The global atmospheric average half-life has been estimated to be 6 to 7 years (HSDB, 1996; ATSDR, 1995).

**Fate in Aquatic Environments:** The dominant fate of 1,1,1-trichloroethane released to surface waters is volatilization (predicted half-life of hours to weeks depending on wind and mixing conditions). Bioconcentration and sorption to sediments and suspended solids are not expected to be significant transport/partitioning processes relative to volatilization.

### **3.3.3.3.2 *Transport and Partitioning***

**Soil Adsorption/Mobility:** The mean  $K_{oc}$  range of 1,1,1-trichloroethane in a silty clay soil and sandy loam soil is 81 to 89. 1,1,1-Trichloroethane is sorbed strongly to peat moss but not at all to sand. From these measured  $K_{oc}$ s and the fact that 1,1,1-trichloroethane is frequently detected in groundwater, it can be concluded that 1,1,1-trichloroethane is not sorbed strongly by soils. It can be expected to leach to groundwater particularly in soils with low organic content (HSDB, 1996).

**Volatilization:** The dominant removal mechanism for 1,1,1-trichloroethane in surface waters is volatilization. The half-life will depend on wind and mixing conditions and is estimated to range from 3 to 29 hours in rivers, 4 to 12 days in lakes, and 5 to 11 days in ponds based on laboratory experiments. Because of its moderate vapor pressure and relatively low soil adsorption coefficient, 1,1,1-trichloroethane is expected to volatilize from soil and also from suspended particulate matter in the atmosphere. 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 percent in sandy soil and 4.9 percent in clay soil (HSDB, 1996).

**Bioconcentration:** A bioconcentration factor of 8.9 was measured in a 28-day test with bluegill sunfish. BCFs measured in fish studies are less than 10 for structurally similar halogenated aliphatic compounds. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996).

### **3.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** 1,1,1-Trichloroethane has been shown to undergo reductive dechlorination to 1,1-dichloroethane and chloroethane under anaerobic conditions in laboratory tests using acclimated microorganisms with half-lives on the order of weeks to months. Biodegradation under aerobic conditions has also been demonstrated to occur at a slow rate (weeks to months) with vinylidene chloride formed as a degradation product (HSDB, 1996; Howard et al., 1991).

**Photodegradation:** 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 1,1,1-trichloroethane will be rapidly degraded. Photolytic degradation has not been observed in aqueous media exposed to sunlight for one year. Based upon measured rate constants for the vapor phase photo-oxidation reaction with photochemically produced hydroxyl radicals, the half-life of 1,1,1-trichloroethane in the atmosphere is on the order of years. Products of

photodegradation include phosgene, chlorine radicals, and hydrochloric acid. Degradation is reported to be greatly increased by exposure to ozone and chlorine but no quantitative data are available (HSDB, 1996; Howard et al., 1991).

**Hydrolysis:** The hydrolysis half-life of 1,1,1-trichloroethane has been reported to range from 0.73 to 1.1 years. The half-life in water containing suspended sediment is 1.2 years. The product of hydrolysis is vinylidene chloride (HSDB, 1996; Howard et al., 1991).

### **3.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

#### **3.4.1 General U.S. Population**

The general population may be exposed to 1,1,1-trichloroethane through the inhalation of ambient air and inhalation of indoor air contaminated by use of household products containing this chemical. The general population may be potentially exposed to 1,1,1-trichloroethane through emissions from hazardous waste sites. 1,1,1-Trichloroethane has been identified at 696 of 1,408 NPL hazardous waste sites. The frequency of these sites in the U.S. is shown in Figure 3-2. Inhalation is expected to be the predominant exposure route; however, exposure can also occur through ingestion of contaminated foods and drinking water and through dermal contact. Therefore, available data suggest that because of its ubiquitous occurrence in the environment and its use in many consumer products, much of the general population is exposed to low levels of 1,1,1-trichloroethane (ATSDR, 1995).

Exposure of the general population from the commercial use of products may potentially be more significant than exposure resulting from industrial release. ATSDR reported maximum exposure levels to this chemical during a variety of personal activities: visiting the dry cleaners (185 ppb); working in chemistry lab (18.5 ppb) and as lab technician (12 ppb); using pesticides (20 ppb); and using paint (20 ppb) (ATSDR, 1995).

The average daily intake (ADI) for air is assumed in HSDB (1996) to be: in rural areas (0.110 ppb) - 12.2 µg; urban/suburban areas (0.420 ppb) - 46.5 µg; for residents in source dominated areas assume (1.2 ppb) - 133.0 µg. The ADI for water is assumed in HSDB (1996) to be: surface water source (0.4 ppb) - 0.8 µg; groundwater source (2.1 ppb) - 4.2 µg. ATSDR (1995) assumed an average urban air concentration of 1,1,1-trichloroethane of 1 ppb and the average rural concentration of 0.1 ppb and calculated daily nonoccupational intakes of 108 and 10.8 µg/day, respectively. The estimate is based on an average human air intake of 20 m<sup>3</sup>/day. ATSDR (1995) noted that Wallace et al. (1985) has determined the mean daily air exposures for 12 subjects at 2 urban areas at 37 mg and the mean daily intake from all sources (air, food, water) between 50 and 1,000 mg/day.

#### **3.4.2 Occupational Exposure**

NIOSH estimated in a 1981-1983 survey that approximately 2,528,300 workers were potentially exposed to 1,1,1-trichloroethane in the U.S. (ATSDR, 1995). Trichloroethane concentration in the air of various industries (degreasing, manufacture of electric components,



mixing and application of commercial resins, spray painting, and gluing) applications of 1,1,1-trichloroethane might result in elevated levels of exposure (ATSDR, 1995). Occupational exposures predominantly occur through inhalation pathways.

### 3.4.3 Consumer Exposure

In a shelf survey for household products containing methylene chloride, 14.1 percent of the samples and 47.8 percent of the product categories contained 1,1,1-trichloroethane (HSDB, 1996). Consumer products that may contain this chemical include typewriter correction fluid, fingernail polish, paint thinner, caulking compounds, lacquer, paint removers, and antifreeze. A list of common household products that contain 1,1,1-trichloroethane is presented in Table 3-3.

**Table 3-3. 1,1,1-Trichloroethane in Common Household Products**

Product	Concentration (% w/w)	Product	Concentration (% w/w)
Adhesive cleaners	0.1-95.0	Oven cleaners	97
Adhesives	0.2-121.1	Paint removers/strippers	0.1-25.7
Aerosol spray paint	0.2-1.0	Primers	1.2-61.8
Battery terminal protectors	37.1	Rust removers	0.7
Belt lubricants	11.4-72	Silicone lubricants	0.2-91.1
Brake cleaners	0.4-75.6	Specialized aerosol cleaners	0.2-83.8
Carburetor cleaners	0.2-0.3	Spot removers	10.5-110.8
Circuit board cleaners	NS	Spray shoe polish	11.4-62.3
Door spray lubricants	95.6	Stereo/record player cleaners	0.7
Drain cleaner (nonacid)	97.8	Suede protectors	4.8-118.5
Electric shaver cleaners	2.5-20.3	Tape recorder cleaners	0.2-101.5
Engine degreasers	0.2	Tire cleaners	0.1-90.3
Fabric finishes	77.9-85.1	Transmission cleaner/lubricant	113
Gasket removers/adhesives	0.2-1.0	TV/computer screen cleaners	0.3
General purpose spray degreasers	0.1-71.4	Typewriter correction fluid	6-110
General purpose liquid cleaners	72.7-126.7	VCR cleaners	97.8
Ignition wire driers	24.3-43.6	Video disk cleaners	0.6
Lubricants	0.1-104.5	Water repellents	0.2-116.2
Miscellaneous nonautomotive	12.5-67.5	Wood cleaners	12.3-20.4
Miscellaneous automotive	0.3-0.4	Woodstain/varnishes/finishes	0.1-21.4

NS = not specified  
Source: ATSDR (1995)

## 3.5 CHAPTER SUMMARY

Table 3-4 summarizes the findings of 1,1,1-trichloroethane.

**Table 3-4. 1,1,1-Trichloroethane (Methyl Chloroform) Summary**

	Estimates	Support
Uses	Metal cleaning and degreasing, many other solvent applications, chemical intermediate, many household products	Well documented in recent studies
Production	3.13 x 10 <sup>8</sup> kg	1992 data
Releases	49.45 x 10 <sup>6</sup> lbs in 1994, mostly to air	TRI (U.S. EPA, 1996) data is primary source, so data are current but uncertain due to self reporting and exemptions
Properties/Fate	Volatile, no significant bio-concentration, slow bio-degradation	Well documented in recent studies
Media Levels	Air: outdoor urban - 0.545-5.45 : g/m <sup>3</sup> outdoor rural - <1.09 : g/m <sup>3</sup> Drinking Water: 0.01-3.5 ppb Groundwater: 0-18 ppb Some data on food and in many household items	Data is dated and represent uncertain number of samples
General Population Exposure	Inhalation: rural - 12.2 : g/d urban/suburban - 46.5 : g/d Water ingestion: surface water - 0.8 : g/d; groundwater - 4.2 : g/d	Values based on limited data
Special Population Exposures	Workers in dry cleaning, chemistry labs, lab tech, painting	Data limited

## 4.0 1,2-DICHLOROETHYLENE

### 4.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 4.1.1 Nomenclature

CAS No.: 540-59-0

Synonyms: 1,2-dichloroethene; acetylene dichloride; ethene, 1,2-dichloro

Trade Names: Diform, NCI.C5603

#### 4.1.2 Formula and Molecular Weight

Structural Formula:  $C_2H_2Cl_2$   
Molecular Weight: 96.95

#### 4.1.3 Chemical and Physical Properties

Description: Colorless liquid (usually a mixture of cis and trans isomers); slightly acid, chloroform-like odor (NIOSH Pocket Guide Chem. Haz., 1994).

Boiling Point: 55°C (Merck Index, 9th Ed., 1976).

Melting Point: -50°C (Patty. Indus. Hyg. & Tox., 3rd Ed., 1981-82).

Density: 1.27 @ 25°C (liquid) (CHRIS Hazard Chem. Data Vol. II, 1984-5).

Spectroscopy Data: IR: 3645 (Sadtler Research Laboratories Prism Collection); Mass: 203 (Atlas of Mass Spectral Data) (Weast. 1985. CRC Handbook Data Organic CPDS, Vol. I, II).

Solubility: Soluble in alcohol, ether, acetone (cis- and trans-1,2-dichloroethylenes) (CRC Handbook Chem. & Physics, 1994-1995). Soluble in most organic solvents (Merck Index, 11th Ed., 1989)

Volatility: Vapor Pressure: 324 torr at 25°C (Patty. Indus. Hyg. & Tox, 3rd. Ed., Vol. 2A, 2B, 2C, 1981-1982).

Stability: Gradually decomposed by air, light, and moisture, forming HCl (Merck Index, 10th Ed., 1983).

Reactivity: The reaction of 1,2-dichloroethylene and potassium hydroxide produces chloroacetylene, which is explosive and spontaneously flammable in air. It is highly toxic. The addition of sodium, caustic, or caustic solution to 1,2-dichloroethylene may form monochloroacetylene which is spontaneously flammable in air (Fire Protect Guide Hazard Matls, 10th Ed., 1991). May release explosive chloroacetylene by the contact with copper or copper alloys (Tox & Hazard Indus Chem Safety Manual, 1988). Incompatible with alkalies, difluoromethylene dihypofluorite, and nitrogen tetroxide (Sax, 1984). Reactive with strong oxidizers, strong alkalis, potassium hydroxide, copper (Note: usually contains inhibitors to prevent polymerization) (NIOSH Pocket Guide Chem Haz, 1994).

Octanol/Water

Partition Coefficient: No data

#### **4.1.4 Technical Products and Impurities**

1,2-Dichloroethylene is produced in the following grades: technical; As cis, trans; and as a mixture of both (Sax, 1987). Technical 1,2-dichloroethylene consists of 60%, 40% cis- trans-isomers (ACGIH, 1985).

## **4.2 PRODUCTION AND USE**

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996) and ATSDR (1996a).

### **4.2.1 Production**

No information concerning U.S. production, import, or export volumes was identified.

### **4.2.2 Uses**

1,2-Dichloroethylene has been used as a solvent for fats, phenol, camphor; for retarding fermentation (Merck Index, 11th Ed., 1989); solvent for natural rubber; coolant in refrigeration plants; low temperature solvent; and a special-purpose solvent (HSDB, 1996; ATSDR, 1996a). It has also been used in extraction of dyes, caffeine, fats from animal flesh; perfumes; lacquers; thermoplastics; and organic synthetics (Sax, 1987). Although cis- and trans-isomers of 1,2-dichloroethylene have had use as solvents and chemical intermediates, neither of the isomers has developed wide industrial usage in the U.S., partly because of their flammability (Patty. Indus Hyg & Tox, 3rd Ed., Vol. 2A, 2B, 2C, 1981-82). 1,2-dichloroethylene obtained as a byproduct is used as feed stock for the synthesis of tri- and perchloroethylene (Ullmann's Encyc Indust Chem, 5th Ed., Vol. A1, 1985-present). It also has miscellaneous uses such as a liquid dry cleaning

agent; cleaning agent for printed circuit boards; for food packaging adhesive; and germicidal fumigant. The extent of these continued uses has not been confirmed (ATSDR, 1996a).

In applications where dichloroethylenes could be used as solvents and for low temperature extraction processes, they have been replaced with methylene chloride (Ullmann's Ency Indus Chem, 5th Ed., 1985-present).

### **4.2.3 Disposal**

1,2-Dichloroethylene is a potential candidate for rotary kiln incineration at a temperature range of 820 to 1,600°C and residence times of seconds for liquids and gases and hours for solids; for fluidized bed incineration at a temperature range of 450 to 980°C and residence times of seconds for liquids and gases, and longer for solids; and for liquid injection incineration at a temperature range of 650 to 1,600°C and a residence time of 0.1 to 2 seconds (trans-1,2-dichloroethylene) (USEPA. 1981. Engineering Handbook for Hazardous Waste Incineration). This compound should be susceptible to removal from wastewater by air stripping (USEPA/ORD. 1980. Innovative and Alternative Technology Assessment Manual). Incineration is a disposal method, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids produced. The recommendable method is incineration (Un. Treat Disposal Methods Waste Chem Data Series No. 5, 1985).

At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge) consult with environmental regulatory agencies for guidance on acceptable disposal practices (HSDB Scientific Review Panel; HSDB, 1996).

## **4.3 POTENTIAL FOR HUMAN EXPOSURE**

### **4.3.1 Natural Occurrence**

No information on natural occurrence of 1,2-dichloroethylene was identified.

### **4.3.2 Occupational**

Occupational potential for exposure is reported in Section 5 and Section 6 for the cis and trans isomers, respectively.

### **4.3.3 Environmental**

Most of the 1,2-dichloroethylene released into the environment will eventually enter the groundwater or the atmosphere (ATSDR, 1996a). Releases to the environment are a result of process and fugitive emissions from production and use as a chemical intermediate; leaching from landfills; evaporation from wastewater streams, landfills, and solvents; emissions from heating or combustion PVC and vinyl copolymers; and formation via anaerobic biodegradation of some chlorinated solvents (ATSDR, 1996a).

#### 4.3.3.1 *Environmental Releases*

**Air:** Releases of 1,2-dichloroethylene to air are usually the result of emissions from industrial production and use facilities, contaminated waste disposal sites, and emissions from pyrolysis/combustion of certain plastic resins. TRI estimates for releases to the air in 1991 totaled 44,782 pounds (>99 percent of total TRI estimated environmental releases) (ATSDR, 1996a).

**Water:** 1,2-dichloroethylene may be released to surface waters, groundwater, and has been detected in drinking water. It may be released to surface waters through runoff from contaminated waste disposal sites, wastewater from industrial sources, and from some POTWs. According to TRI estimates for 1993, a total of 28 pounds of 1,2-dichloroethylene (<0.1 percent of total releases to the environment) were released to water from reporting manufacturing and processing facilities (ATSDR, 1996a).

1,2-dichloroethylene may be released to groundwater due to leaching from contaminated waste disposal sites and cracked sewer interceptors carrying industrial waste contaminated with this chemical. It may also be released to groundwater as a result of anaerobic degradation of highly chlorinated ethenes (TCE, PCE) and ethanes present in groundwater (ATSDR, 1996a). 1,2-dichloroethylene's presence in drinking water may be attributed to raw water source contamination; however, there is little documentation of direct groundwater contamination.

**Other Media:** The cis and trans isomers of 1,2-dichloroethylene are released to soil from disposal of waste contaminated with this chemical. Additionally, they may also be found in landfills from anaerobic biodegradation of PCE, TCE, 1,1,1-trichloroethane, and 1,1,2,2-tetrachloroethane (ATSDR, 1996a). TRI estimates for 1993 indicated that no 1,2-dichloroethylene was released to land from manufacturing and processing facilities (ATSDR, 1996a). Available data are not sufficient to estimate the amount of 1,2-dichloroethylene released to soil and to sediments.

#### 4.3.3.2 *Monitored Environmental Media Levels*

**Air:** 1,2-dichloroethylene has been detected in ambient air samples in various urban locations throughout the U.S. It has also been detected in the gas from various landfills in the U.S. Levels found in the ambient air ranged from <0.1 to 2.6 ppb, and levels in the gas from landfills ranged from 70 ppb (mean) to 75,600 ppb (maximum values; trans isomer) (ATSDR, 1996a). 1,2-dichloroethylene detected in the indoor air of 2 studies were 0.015 ppb and 8.1 ppb, respectively (ATSDR, 1996a). The data reported in most studies were not isomer-specific. In the EPA National Ambient Database update, outdoor ambient concentrations of 1,2-dichloroethylene averaged 0.326 ppb. A median value of 0.037 ppb was also reported. These reported levels were based on 161 data points (ATSDR, 1996a). According to ATSDR (1996a), the efficiency of waste treatment plants has improved and loadings to receiving waters have decreased. But, this decrease has often resulted in increased emissions to the atmosphere as the volatile constituents are removed through processes such as air stripping (ATSDR, 1996a).

**Water:** Concentrations of 1,2-dichloroethylene found in water reported in ATSDR (1996a) are described below. These ranges are based on various studies.

- C Surface water: not detected - 1,370.5 ppb (maximum value)
- C Groundwater: 0.25-0.28 ppb (average value) - 50,000 ppb (maximum value; trans isomer)
- C Drinking water: trace - 64 ppb (maximum value - groundwater source)
- C Leachate: 1.4-470 (cis isomer) ppb - 45-800 ppb (average concentration of leachate; maximum value)
- C Aqueous Lagoon: 50 ppb (trans isomer)
- C Wastewater at various industries: 1.6 ppb (cis isomer) - 2,265 ppb (trans isomer; median value)
- C Rainwater: 0.230 ppb (1 sample)

A maximum concentration of 33 ppb for cis isomer was found in a shallow unconfirmed aquifer receiving waste water from metal plating operations. The EPA Contract Laboratory Program (CLP) data base has reported trans isomer mean concentrations ranging from 5 to 4,000 ppb at 8 of 357 hazardous waste sites.

**Other Media:** Trans 1,2-dichloroethylene concentrations ranging from 22 to 55 g/L have been detected in municipal sludge from various treatment throughout the United States (1996a), while 0.04 ppm (mean value) to 0.05 ppm (maximum value) of 1,2-dichloroethylene were found in fish tissues from Commencement Bay in Tacoma, Washington (1996a). Monitoring data for levels of 1,2-dichloroethylene in soil are very limited. The mean concentration range of 5 to 4,000 ppb was reported at 87 of 357 hazardous waste sites (ATSDR, 1996a). However, the trans isomer was reported in all cases (ATSDR, 1996a). According to ATSDR (1996a), the available data for 1,2-dichloroethylene in soil are limited to data from hazardous waste site monitoring.

### **4.3.3.3 Environmental Fate and Transport**

#### **4.3.3.3.1 Summary**

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of 1,2-dichloroethylene released to surface soils is volatilization. Some 1,2-dichloroethylene may leach downward in the soil column because of the high water solubility and low  $K_{oc}$  values of the two isomers. Also, 1,2-dichloroethylene is formed under anaerobic conditions in soil, groundwater, and sediments as a breakdown product from microbial reductive dehalogenation of the common industrial solvents trichloroethylene, tetrachloroethylene, and 1,1,2,2-tetrachloroethane. The fate of 1,2-dichloroethylene in subsurface soils and groundwater is slow anaerobic degradation with the formation of vinyl chloride as a degradation product.

**Fate in the Atmosphere:** In the atmosphere, 1,2-dichloroethylene is expected to be present in the vapor phase rather than sorbed to particulate matter. Removal by scavenging

during wet precipitation is expected because of the high solubility of the two isomers. The predominant degradation process affecting both isomers is photo-oxidation by hydroxyl radicals. Predicted half-lives for this reaction are 3.6 and 8 days for the trans- and cis- isomers, respectively.

**Fate in Aquatic Environments:** The dominant fate of 1,2-dichloroethylene released to surface waters is volatilization (predicted half-life of 3 hours). Bioconcentration and sorption to sediments and suspended solids are not expected to be significant transport/partitioning processes. Although biodegradation is not expected to be a significant degradation process, any 1,2-dichloroethylene that reaches the sediment will undergo slow anaerobic biodegradation.

#### **4.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:** The relatively low predicted soil adsorption coefficients ( $K_{oc}$ ) for cis- and trans-1,2-dichloroethylene, 36 and 49, respectively, indicate that adsorption of the 1,2-dichloroethylene isomers to soil, sediment, and suspended solids is not a significant fate process. As a consequence, these isomers should show high mobility in soil (HSDB, 1996; Howard, 1993).

**Volatilization:** The dominant removal mechanism for the dichloroethylene isomers in surface waters is volatilization. The Henry's Law constants for cis- and trans- dichloroethylene are 0.00408 and 0.00938, respectively. Based on these values, the estimated half-lives for volatilization of cis- and trans-dichloroethylene from a model river 1 m deep with a 1 m/sec current and a 3 m/sec wind speed are 3.1 and 3.0 hours, respectively. Similarly, the volatilization half-lives from a 1 m deep body of water predicted from laboratory volatilization studies are 5.0 and 6.2 hours, respectively. Because of their high vapor pressures, both isomers are also expected to readily volatilize from soil surfaces and also from suspended particulate matter in the atmosphere (HSDB, 1996; Howard, 1993).

**Bioconcentration:** Bioconcentration factors of 15 and 22 are predicted for cis- and trans-dichloroethylene, respectively, based on their respective octanol/water partition coefficients. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996; Howard, 1993).

#### **4.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** The results of most aerobic biodegradation studies indicate that 1,2-dichloroethylene is recalcitrant to aerobic degradation in soil and water (i.e., half-lives on the order of months); however, one study reported half-lives on the order of days to weeks. Several studies have demonstrated that both isomers will undergo slow anaerobic biodegradation in soils and sediments with half-lives on the order of months or longer. Vinyl chloride is a degradation product (HSDB, 1996; Howard, 1993; Howard et al., 1991).

**Photodegradation:** In the atmosphere, cis- and trans-1,2-dichloroethylene react with photochemically produced hydroxyl radicals resulting in half-lives of 8 and 3.6 days, respectively. The only product positively identified from this reaction is formyl chloride. Photo-

oxidation through reaction with ozone is much slower, on the order of months. Because cis- and trans-1,2-dichloroethylene absorb only a small amount of UV light in the environmentally significant range, direct photolysis is an insignificant fate process (HSDB, 1996; Howard, 1993; Howard et al., 1991).

**Hydrolysis:** The two isomers of 1,2-dichloroethylene contain no hydrolyzable groups (Howard et al., 1991)

## **4.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **4.4.1 General U.S. Population**

The general population may be exposed to low levels ranging from 0.013 to 0.076 ppb of 1,2-dichloroethylene through inhalation of contaminated air in urban areas (ATSDR, 1996a). ATSDR (1996a) calculated the corresponding average daily intake of 1 to 6  $\mu\text{g}/\text{day}$  based on an average air intake of 20  $\text{m}^3/\text{day}$ . HSDB (1996) has reported the following assumed concentrations for average daily intake:

- Air intake - assume air concentration of 68 ppt (5.4  $\mu\text{g}$ )
- Water intake - assume water concentration from contaminated sources of 1.1 ppb (2.2  $\mu\text{g}$ ) when drinking water is contaminated

The general population with potentially the highest exposures are those living near production/processing facilities, municipal wastewater treatment plant, hazardous waste sites, and municipal landfills. Potential exposure exists in air downwind of these sites and in the contaminated drinking water from groundwater down gradient from the sites (ATSDR, 1996a).

Cis-1,2-dichloroethylene has been identified in 146 of the 1,430 current or former EPA National Priorities List (NPL) hazardous waste sites and trans -1,2-dichloroethylene has been identified in at least 563 of the current or former NPL sites (ATSDR, 1996a). Although the number of sites evaluated for this chemical is not known, the frequency of these sites has been determined and is presented in Figure 4-1.

### **4.4.2 Occupational Exposure**

According to a 1981-1983 NIOSH survey, a statistical estimate of 215 workers in the U.S. are potentially exposed to 1,2-dichloroethylene (mixture of cis and trans isomers) in the workplace (ATSDR, 1996a). An estimated 61 workers are potentially exposed to the cis isomer (ATSDR, 1996a). An estimate for potential occupational exposure to the trans isomer was not estimated from the survey.

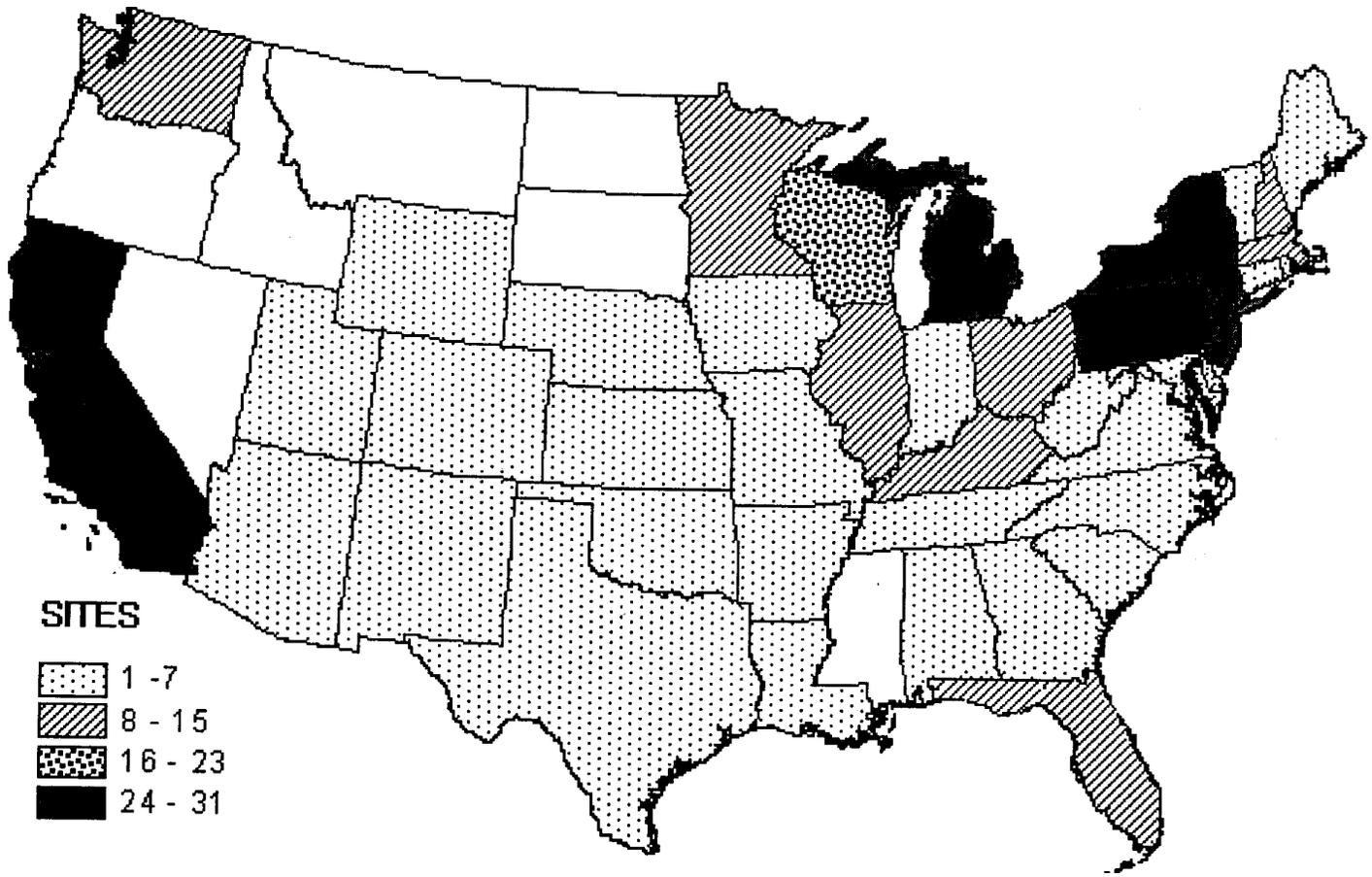


Figure 4-1. Frequency of NPL Sites with 1,2-Dichloroethene (Unspecified) Contamination  
 (Source: ATSDR, 1996a)

### 4.4.3 Consumer Exposure

Readily available data were not found on consumer exposures for 1,2-dichloroethylene.

## 4.5 CHAPTER SUMMARY

Table 4-1 summarizes the findings of 1,2-dichloroethylene.

**Table 4-1. 1,2-Dichloroethylene Summary**

	Estimates	Support
Uses	Many solvent applications	Well documented
Production	No recent information was identified	
Releases	44.8 x 10 <sup>3</sup> lbs/year to air (>99% of total environmental releases)	TRI (U.S. EPA, 1996) data
Properties/Fate	Volatile; insoluble in water; relatively stable in air; flammable; significant bioconcentration not expected	Well documented
Media Levels	Air: <0.545-14.16 : g/m <sup>3</sup> Ambient air: 0.202 : g/m <sup>3</sup>  Surface water: ND-1,370 ppb Groundwater: 0.25-0.28 ppb (average value) Drinking water: trace-64 ppb	ATSDR (1996a) 161 data points, from EPA National Ambient Database
General Population Exposure	Inhalation: 1 to 6 ug/d	ATSDR (1996a)
Special Population Exposures	215 workers are potentially exposed	Data from early 1980s

## 5.0 CIS-1,2-DICHLOROETHYLENE

### 5.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 5.1.1 Nomenclature

CAS No.:	156-59-2
Synonyms:	1,2-cis-dichloroethene; cis-dichloroethylene; ethene, 1,2-dichloro-, ethylene; 1,2-dichloro-
Trade Names:	Acetalyne dichloride

#### 5.1.2 Formula and Molecular Weight

Structural Formula:	$C_2H_2Cl_2$
Molecular Weight:	96.95

#### 5.1.3 Chemical and Physical Properties

Description:	Liquid (Merck Index, 11th Ed., 1989); colorless (Tox & Hazard Indus Chem Safety manual, 1982); Sweetish (Ullmann's Encyc Indust Chem, 5th Ed., Vol A1, 1985-present).
Boiling Point:	60.3°C @ 760 mm Hg (CRC Handbook Chem & Physics, 75th Ed., 1994-1995).
Melting Point:	-80.5°C (CRC Handbook Chem & Physics, 75th Ed., 1994-1995).
Density:	1.2837 @ 20°C/4°C (CRC Handbook Chem & Physics, 75th Ed., 1994-1995).
Spectroscopy Data:	Index of refraction: 1.4490 20°C/D; maximum absorption (vapor): greater than 200 nm (CRC Handbook Chem & Physics, 75th Ed., 1994-1995). Sadtler reference number: 3645 (IR, Prism) (Weast, 1979). Refractive index: 1.4519 @ 15°C (Flick. Indust Solvents Handbook, 1985). Mass: 203 (Atlas of Mass Spectral Data) (Weast, 1985).
Solubility:	Water solubility = 0.35 g/100 g @ 25°C (Kirk-Othmer, 4th Ed., Vol. 1, 1991-present). Soluble in alcohol, acetone, ether, benzene, and chloroform (Weast. Hdbk Chem & Phys, 67th Ed., 1986-87).

Volatility:	Vapor Pressure: 273 mm Hg @ 30°C. Vapor Density: 3.54 g/l (at bp, 760 mm Hg) (Flick. Indust Solvents Hdbk, 1985).
Stability:	Decomposes slowly on exposure to air, light, and moisture.
Reactivity:	May release explosive chloroacetylene by the contact with copper or copper alloys (1,2-dichloroethylene (ITII. Tox & Hazard Indus Chem Safety Manual, 1988). Reacts with strong oxidizers (1,2-dichloroethylene (Sittig. Handbook Toxic Hazard Chem & Carcinog, 2nd Ed., 1985).
Octanol/Water Partition Coefficient:	log Kow = 1.86 (Hansch. Log P Database, 1987)

#### 5.1.4 Technical Products and Impurities

No data were identified.

### 5.2 PRODUCTION AND USE

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 5.2.1 Production

The U.S. production in 1977 was at least  $5.0 \times 10^8$  g (captive production) (SRI). More recent production data were unavailable. No data were identified for import and export volumes.

#### 5.2.2 Uses

Cis-1,2-dichloroethylene is used as a solvent (isomeric mixture) for perfumes, dyes, and lacquers; solvent (as mixture) for thermoplastics, fats, and phenols; solvent (as mixture) for camphor and natural rubber; chemical intermediate (as isomeric mixture) for chlorinated compound; and an agent in retarding fermentation (SRI). It is also used as a solvent in waxes, resins, and acetylcellulose and used in the extraction of rubber, as a refrigerant, in the manufacture of pharmaceuticals and artificial pearls and in the extraction of oils and fats from fish and meat (Sittig. Handbook Toxic Hazard Chem & Carcinog, 2nd Ed., 1985).

Although cis- and trans-isomers of 1,2-dichloroethylene have had use as solvents and chemical intermediates, neither isomer has developed wide industrial usage in the U.S., partly because of their flammability (Patty. Indus Hyg & Tox, 3rd Ed., 1981-82). 1,2-dichloroethylenes obtained as byproducts are used as feed stock for the synthesis of tri- and perchloroethylene (Ullmann's Encyc. Indust. Chem., 5th Ed., Vol 1a, 1985-present).

In applications where dichloroethylenes could be used as solvents and for low temperature extraction processes, they have been replaced by methylene chloride (Ullmann's Encyc Indust Chem, 5th Ed., Vol A1, 1985-present).

### **5.2.3 Disposal**

1,2-dichloroethylene may be disposed of by atomizing in a suitable combustion chamber equipped with an appropriate effluent gas cleaning device (NIOSH/OSHA. Occupat Health Guide Chem Hazards, 1981). Incineration is a disposal method, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids produced (Sittig. Handbook Toxic Hazard Chem & Carcinog, 2nd Ed, 1985). This compound should be susceptible to removal from wastewater by air stripping (USEPA/ORD. 1980. Innovative and Alternative Technology Assessment Manual).

At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (Including waste sludge) consult with environmental regulatory agencies for guidance on acceptable disposal practices (HSDB Scientific Review Panel; HSDB, 1996).

## **5.3 POTENTIAL FOR HUMAN EXPOSURE**

### **5.3.1 Natural Occurrence**

Cis-1,2-dichloroethylene is not known to occur naturally.

### **5.3.2 Occupational**

Occupational exposure to cis-1,2-dichloroethylene is expected to be through dermal contact with the vapor and liquids and through inhalation of contaminated air at the work place (HSDB, 1996).

### **5.3.3 Environmental**

#### **5.3.3.1 *Environmental Releases***

Cis-1,2-dichloroethylene may be released to the environment in emissions and wastewater during its production and use as a solvent and extract (HSDB, 1996). The cis isomer is apparently more commonly found than the trans isomer, but is usually mistakenly listed as the trans isomer. The Michigan Department of Health has reported that it has the capability of distinguishing between the two isomers and where concentrations are high, they occasionally find traces of the trans isomer (HSDB, 1996). Under aerobic conditions that may exist in landfills or sediments, 1,2-dichloroethylenes may be present as breakdown products from reduction dehalogenation of trichloroethylene and tetrachloroethylene (HSDB, 1996).

### 5.3.3.2 *Monitored Environmental Media Levels*

According to HSDB (1996), an assessment of the sources of the cis-1,2-dichloroethylene is complicated because the cis isomer was a priority pollutant, unlike the trans isomer. These isomers cannot be differentiated using the EPA standard method analysis. Therefore, monitoring reports have erroneously listed the trans isomer when the cis isomer is present (HSDB, 1996). (See Section 4.0 (1,2-Dichloroethylene) for more information on environmental levels.)

**Air:** For urban/suburban areas in the U.S., reported levels for 669 sites/samples were 68 ppt (median values) and 3,500 ppt (maximum value). Source areas (101 sites/samples) reported levels were 300 ppt (median) and 6,700 ppt (maximum value) (HSDB, 1996).

**Water:** Cis-1,2-dichloroethylene was found in Miami drinking water at 16 ppb, Cincinnati and Philadelphia at 0.1 ppb, but was not found in 7 other drinking waters surveyed (HSDB, 1996). Raw water from a well in Wisconsin contained 83.3 ppb of this chemical. The Biscayne Aquifer (near the Miami inactive drum recycling hazardous waste site) that supplies drinking water to Dade County, Florida, contained 0-26 ppb. Shallow groundwater near the site had reported levels of 839 and 13.3-17.9 ppb (HSDB, 1996).

**Other Media:** Data were not available for levels in food, plants, fish, animals, and milk.

### 5.3.3.3 *Environmental Fate and Transport*

#### 5.3.3.3.1 Summary

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of 1,2-dichloroethylene released to surface soils is volatilization. Some 1,2-dichloroethylene may leach downward in the soil column because of the high water solubility and low  $K_{oc}$  values of the two isomers. Also, 1,2-dichloroethylene is formed under anaerobic conditions in soil, groundwater, and sediments as a breakdown product from microbial reductive dehalogenation of the common industrial solvents trichloroethylene, tetrachloroethylene, and 1,1,2,2,-tetrachloroethane. The fate of 1,2-dichloroethylene in subsurface soils and groundwater is slow anaerobic degradation with the formation of vinyl chloride as a degradation product.

**Fate in the Atmosphere:** In the atmosphere, 1,2-dichloroethylene is expected to be present in the vapor phase rather than sorbed to particulate matter. Removal by scavenging during wet precipitation is expected because of the high solubility of the two isomers. The predominant degradation process affecting both isomers is photo-oxidation by hydroxyl radicals. Predicted half-lives for this reaction is 8 days for the cis- isomers.

**Fate in Aquatic Environments:** The dominant fate of 1,2-dichloroethylene released to surface waters is volatilization (predicted half-life of 3 hours). Bioconcentration and sorption to sediments and suspended solids are not expected to be significant transport/partitioning

processes. Although bio-degradation is not expected to be a significant degradation process, any 1,2-dichloroethylene that reaches the sediment will undergo slow anaerobic biodegradation.

#### **5.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:** The relatively low predicted soil adsorption coefficients ( $K_{oc}$ ) for cis-1,2-dichloroethylene of 36 indicate that adsorption of the cis-1,2-dichloroethylene isomer to soil, sediment, and suspended solids is not a significant fate process. As a consequence, these isomers should show high mobility in soil (HSDB, 1996; Howard, 1993).

**Volatilization:** The dominant removal mechanism for the dichloroethylene isomers in surface waters is volatilization. The Henry's Law constants for cis-dichloroethylene is 0.00408. Based on this value, the estimated half-life for volatilization of cis-dichloroethylene from a model river 1 m deep with a 1 m/sec current and a 3 m/sec wind speed is 3.1 hours. Similarly, the volatilization half-life from a 1 m deep body of water predicted from laboratory volatilization studies is 5.0 hours. Because of its high vapor pressures, this isomer is also expected to readily volatilize from soil surfaces and also from suspended particulate matter in the atmosphere (HSDB, 1996; Howard, 1993).

**Bioconcentration:** Bioconcentration factors of 15 is predicted for cis-dichloroethylene, based on its respective octanol/water partition coefficient. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996; Howard, 1993).

#### **5.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** The results of most aerobic biodegradation studies indicate that 1,2-dichloroethylene is recalcitrant to aerobic degradation in soil and water (i.e., half-lives on the order of months); however, one study reported half-lives on the order of days to weeks. Several studies have demonstrated that both isomers will undergo slow anaerobic biodegradation in soils and sediments with half-lives on the order of months or longer. Vinyl chloride is a degradation product (HSDB, 1996; Howard, 1993; Howard et al., 1991).

**Photodegradation:** In the atmosphere, cis-1,2-dichloroethylene reacts with photochemically produced hydroxyl radicals resulting in half-life of 8 days. The only product positive identified from this reaction is formyl chloride. Photo-oxidation through reaction with ozone is much slower, on the order of months. Because cis-1,2-dichloroethylene absorb only a small amount of UV light in the environmentally significant range, direct photolysis is an insignificant fate process (HSDB, 1996; Howard, 1993; Howard et al., 1991).

**Hydrolysis:** This isomer of 1,2-dichloroethylene contain no hydrolyzable groups (Howard et al., 1991)

## **5.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **5.4.1 General U.S. Population**

The general population is exposed to cis-1,2-dichloroethylene in urban air and from contaminated drinking water from groundwater sources. For the average daily intake, HSDB (1996) has reported the following: air intake, assume a concentration of 68 ppt (5.4  $\mu\text{g}$ ); water intake, assume water concentration from contaminated sources of 0.23-2.7 ppb (0.5-5.4  $\mu\text{g}$ ) when drinking water is contaminated (HSDB, 1996).

### **5.4.2 Occupational Exposure**

Occupational exposure to cis-1,2-dichloroethylene is expected to be through dermal contact with the vapor and liquids and through inhalation of contaminated air at the work place (HSDB, 1996). Data for occupational exposures and exposed population estimates were not found.

### **5.4.3 Consumer Exposure**

Data for consumer exposures were not found.

## 6.0 TRANS-1,2-DICHLOROETHYLENE

### 6.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 6.1.1 Nomenclature

CAS No.: 156-60-5  
Synonyms: Ethylene, 1,2-dichloro-; sym-dichloroethylene  
Trade Names: No data

#### 6.1.2 Formula and Molecular Weight

Structural Formula:  $C_2H_2Cl_2$   
Molecular Weight: 96.95

#### 6.1.3 Chemical and Physical Properties

Description: Colorless, light liquid; sweetish odor (Ullmann's Encyc Indust Chem, 5th Ed., Vol A1, 1985-present).

Boiling Point: 48.0-48.5°C @ 760 mm Hg (Flick. Indust Solvents Hdbk, 1985).

Melting Point: -50°C (Flick. Indust Solvents Hdbk, 1985).

Density: 1.2565 @ 20°C/4°C (CRC Handbook Chem & Physics, 75th Ed, 1994-1995).

Spectroscopy Data: Refractive index: 1.4490 @ 15°C/D (Flick. Indust Solvents Hdbk, 1985), IR: 3646 (Sadler Research Laboratories Prism Collection); NMR: 6742 (Sadler Research Laboratories Spectral Collection); MASS: 203 (Atlas of Mass Spectral Data) (Weast, 1985).

Solubility: Soluble in alcohol, ether, acetone, benzene, and chloroform (Weast, 1986-97). Water solubility: 0.63 g/100 g @ 25°C (Flick. Indust Solvents Hdbk, 1985).

Volatility: Vapor Pressure: 395 mm Hg at 30°C (Flick. Indust Solvents Hdbk, 1985).  
Vapor Density: 3.67 g/l at (bp at 760 mm Hg) (Flick. Indust Solvents Hdbk, 1985).

Stability: Gradually decomposed by air, light, and moisture, forming HCl (HSDB Scientific Review Panel; HSDB, 1996); potential phosgene formation (Merck Index, 10th Ed., 1983).

Reactivity: May release explosive chloroacetylene by the contact with copper or copper alloys (1,2-dichloroethylene) (ITII. Tox & Hazard Indus Chem Safety Manual, 1988). Reacts with strong oxidizers (Sittig. Handbook Toxic Hazard Chem & Carcinog, 2nd Ed., 1985). Incompatible with alkalis, difluoromethylene dihypofluorite, and nitrogen tetroxide (Sax. Danger Props Indus Mater, 6th Ed., 1984).

Octanol/Water

Partition Coefficient:  $\log K_{ow} = 2.06$  (Hansch. Log P Database, 1987).

#### **6.1.4 Technical Products and Impurities**

No data were identified.

### **6.2 PRODUCTION AND USE**

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank during September 1996.

#### **6.2.1 Production**

No data concerning U.S. production, import, or export volumes were identified.

#### **6.2.2 Uses**

Trans-1,2-dichloroethylene is more widely used in industry than either the cis isomer or the commercial mixture (HSDB, 1996). It is used as a solvent for waxes, resins, and acetylcellulose. It is also used in the extraction of rubber, as a refrigerant, in the manufacture of pharmaceuticals and artificial pearls and in the extraction of oils and fats from fish and meat (Sittig. Handbook Toxic Hazard Chem & Carcinog, 2nd Ed., 1985). 1,2-dichloroethylenes obtained as byproducts are used as feed stock for the synthesis of tri- and perchloroethylene. In applications where dichloroethylenes could be used as solvents and for low temperature extraction processes, they have been replaced by methylene chloride (Ullmann's Encyc Indust Chem, 5th Ed., Vol. A1, 1985-present). Although this chemical has had use as a solvent and chemical intermediate, it has not developed wide industrial usage in the U.S., partly because of its flammability (Patty. Indus Hyg and Tox, 3rd Ed., Vol. 2A, 1981-82).

### 6.2.3 Disposal

A method of disposal is incineration, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids produced (Sittig. Handbook Toxic Hazard Chem & Carcinog, 2nd Ed., 1985). Trans-1,2-dichloroethylene is a potential candidate for rotary kiln incineration at a temperature range of 820 to 1,600°C and residence times of seconds for liquids and gases and hours for solids. It is also a potential candidate for fluidized bed incineration at a temperature range of 450 to 980°C and residence times of seconds for liquids and gases, and longer for solids and a potential candidate for liquid injection incineration at a temperature range of 650 to 1,600°C and a residence time of 0.1 to 2 seconds (USEPA. 1981. Engineering Handbook for Hazardous Waste Incineration). This compound should be susceptible to removal from wastewater by air stripping (USEPA/ORD. 1980. Innovative and Alternative Technology Assessment Manual).

At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (Including waste sludge) consult with environmental regulatory agencies for guidance on acceptable disposal practices (HSDB Scientific Review Panel, HSDB, 1996).

## 6.3 POTENTIAL FOR HUMAN EXPOSURE

### 6.3.1 Natural Occurrence

Trans-1,2-dichloroethylene is not known to occur naturally.

### 6.3.2 Occupational

Potential occupational exposures exist in production and manufacturing facilities from the use of trans-1,2-dichloroethylene as a solvent and extractant.

### 6.3.3 Environmental

#### 6.3.3.1 Environmental Releases

Trans-1,2-dichloroethylene may be released to the environment in air emissions and wastewater during its production and use. Dichloroethylenes can be found as breakdown products from the reduction dehalogenation of common industrial solvents such as trichloroethylene, tetrachloroethylene, and 1,1,2,2-tetrachloroethane under aerobic high organic mix conditions, that may exist in landfills, aquifers, or sediment. The cis isomer is the isomer found most. However, it mistakenly reported as the trans isomer because EPA standard methods analytical procedures do not distinguish between isomers (HSDB, 1996). See Section 4.0 (1,2-Dichloroethylene) for more information on environmental levels.

**Air:** Trans-1,2-dichloroethylene has been identified in ambient air near production and manufacturing facilities from its use.

**Water:** Trans-1,2-dichloroethylene has been detected in drinking water, surface water, and groundwater.

**Other Media:** Trans-1,2-dichloroethylene has been identified in the effluent of many manufacturing facilities, POTW effluents (and sludges), urban runoff, and sediment and soil samples (HSDB, 1996).

### **6.3.3.2 Monitored Environmental Media Levels**

**Air:** The atmospheric concentration near source areas in Edison, New Jersey, was 930 ppt (HSDB, 1996).

**Water:** Trans-1,2-dichloroethylene was found in drinking water in Miami at 1 PPB; in private wells in Illinois at nondetected to 64 ppb with a median of 8 ppb (HSDB, 1996). It was found in a groundwater plume of predominantly trichloroethylene that was believed to originate from an old industrial source. In Tacoma, Washington, two utility production wells had levels of 200 ppb trans-1,2-dichloroethylene. Groundwater monitoring wells (789 wells) near a degreasing plant in Connecticut contained levels of this chemical ranging from 1.2 - 320.9 ppb (HSDB, 1996).

**Other Media:** In an EPA survey of wastewater from 4,000 industrial and publicly owned treatment works, the highest effluent concentration among several industries was for iron and steel manufacturing at 3,013 ppb, with a median contamination of 2,265.9 ppb. Median concentrations in the effluents of other industries were: organics and plastics (14.6 ppb); inorganic chemicals (3.9 ppb); rubber processing (19.0 ppb); auto and other laundries (60.6 ppb); explosives (3.9 ppb); electronics (140.7 ppb); mechanical products (13.7 ppb); transportation equipment (29.3 ppb); POTWs (16.3 ppb) (Shackelford et al., *Analyt Chem Acta*, Vol. 146, 1983; HSDB, 1996). In another survey of industrial occurrences, wastewater discharges had the following mean concentrations: metal finishing (260 ppb); photographic equipment (2,200 ppb maximum concentration); nonferrous metal manufacturing (75 ppb); rubber processing (150 ppb).

### **6.3.3.3 Environmental Fate and Transport**

#### **6.3.3.3.1 Summary**

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of 1,2-dichloroethylene released to surface soils is volatilization. Some 1,2-dichloroethylene may leach downward in the soil column because of the high water solubility and low  $K_{oc}$  values of the two isomers. Also, 1,2-dichloroethylene is formed under anaerobic conditions in soil, groundwater, and sediments as a breakdown product from microbial reductive dehalogenation of the common industrial solvents trichloroethylene, tetrachloroethylene, and 1,1,2,2,-tetrachloroethane. The fate of 1,2-

dichloroethylene in subsurface soils and groundwater is slow anaerobic degradation with the formation of vinyl chloride as a degradation product.

**Fate in the Atmosphere:** In the atmosphere, 1,2-dichloroethylene is expected to be present in the vapor phase rather than sorbed to particulate matter. Removal by scavenging during wet precipitation is expected because of the high solubility of the two isomers. The predominant degradation process affecting both isomers is photo-oxidation by hydroxyl radicals. Predicted half-lives for this reaction is 3.6 days for the trans- isomers.

**Fate in Aquatic Environments:** The dominant fate of 1,2-dichloroethylene released to surface waters is volatilization (predicted half-life of 3 hours). Bioconcentration and sorption to sediments and suspended solids are not expected to be significant transport/partitioning processes. Although biodegradation is not expected to be a significant degradation process, any 1,2-dichloroethylene that reaches the sediment will undergo slow anaerobic biodegradation.

#### **6.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:** The relatively low predicted soil adsorption coefficients ( $K_{oc}$ ) for trans-1,2-dichloroethylene, 49, indicate that adsorption of this 1,2-dichloroethylene isomer to soil, sediment, and suspended solids is not a significant fate process. As a consequence, this isomer should show high mobility in soil (HSDB, 1996; Howard, 1993).

**Volatilization:** The dominant removal mechanism for the dichloroethylene isomers in surface waters is volatilization. The Henry's Law constants for trans-dichloroethylene is 0.00938. Based on this value, the estimated half-life for volatilization of trans-dichloroethylene from a model river 1 m deep with a 1 m/sec current and a 3 m/sec wind speed is 3.0 hours. Similarly, the volatilization half-life from a 1 m deep body of water predicted from laboratory volatilization studies is 6.2 hours. Because of its high vapor pressure, this isomer is also expected to readily volatilize from soil surfaces and also from suspended particulate matter in the atmosphere (HSDB, 1996; Howard, 1993).

**Bioconcentration:** Bioconcentration factors of 15 and 22 are predicted for cis- and trans-dichloroethylene, respectively, based on their respective octanol/water partition coefficients. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996; Howard, 1993).

#### **6.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** The results of most aerobic biodegradation studies indicate that 1,2-dichloroethylene is recalcitrant to aerobic degradation in soil and water (i.e., half-lives on the order of months); however, one study reported half-lives on the order of days to weeks. Several studies have demonstrated that both isomers will undergo slow anaerobic biodegradation in soils and sediments with half-lives on the order of months or longer. Vinyl chloride is a degradation product (HSDB, 1996; Howard, 1993; Howard et al., 1991).

**Photodegradation:** In the atmosphere, trans-1,2-dichloroethylene react with photochemically produced hydroxyl radicals resulting in a half-life of 3.6 days. The only product positive identified from this reaction is formyl chloride. Photo-oxidation through reaction with ozone is much slower, on the order of months. Because trans-1,2-dichloroethylene absorb only a small amount of UV light in the environmentally significant range, direct photolysis is an insignificant fate process (HSDB, 1996; Howard, 1993; Howard et al., 1991).

**Hydrolysis:** Trans-1,2-dichloroethylene contains no hydrolyzable groups (Howard et al., 1991)

## **6.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **6.4.1 General U.S. Population**

The general population is exposed to trans-1,2-dichloroethylene in urban air and contaminated drinking water from ground water sources.

### **6.4.2 Occupational Exposure**

Occupational exposure will be through dermal contact with the vapor and liquid or through inhalation. Data for occupational exposures and exposed population estimates were not found.

### **6.4.3 Consumer Exposure**

Data for consumer exposures were not found.

## 7.0 1,1,1,2-TETRACHLOROETHANE

### 7.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 7.1.1 Nomenclature

CAS No.: 630-20-6  
Synonyms: Ethane, 1,1,1,2-tetrachloro-  
Trade Names: NCI-C52459

#### 7.1.2 Formula and Molecular Weight

Structural Formula:  $C_2H_2Cl_4$   
Molecular Weight: 167.85

#### 7.1.3 Chemical and Physical Properties

Description: Yellowish-red liquid (NIOSH Pocket Guide Chem Haz, 1994).

Boiling Point: 130.5°C @ 760 mm Hg (CRC Handbook Chem & Physics, 75th Ed., 1994-1995).

Melting Point: -70.2°C (CRC Handbook Chem & Physics, 75th Ed., 1994-1995).

Density: 1.4506 @ 20°C/4°C (CRC Handbook Chem & Physics, 75th Ed., 1994-1995).

Spectroscopy Data: Index of Refraction: 1.4821 @ 20°C/D (Weast, 1986-87); Mass: 1074 (Atlas of Mass Spectral Data) (Weast, 1985).

Solubility: Water solubility is  $1.1 \times 10^3$  mg/l @ 25°C (McKay and Shiu, 1981; J. Phys. Chem. Ref. Data, Vol. 19). Soluble in alcohol, ether, acetone, benzene, chloroform (Weast, 1986-87).

Volatility: Vapor Pressure - 14 Torr at 25°C (Willing, WL. 1977. Environ Sci Technol, Vol. 11).  
Vapor Density - No data.

Stability: Decomposes when heated and emits toxic fumes of chlorine (Sax, 6th Ed., 1984); when in contact with flame, incandescent material,

or red hot metal surfaces, it decomposes to form hydrochloric acid, carbon monoxide, and carbon dioxide (Encyc. Occupat. Health and Safety, 1983).

Reactivity: Mixtures of sodium-potassium alloy and bromoform, tetrachloroethane, or pentachloroethane can explode on standing at room temperature. They are especially sensitive to impact (NFPA. 1986. Fire Protect Guide Hazard Matls, 9th Ed.) Reacts with dinitrogen tetroxide; potassium hydroxide nitrogen tetroxide; 2,4-dinitrophenyl disulfide (NIOSH Pocket Guide Chem Haz, 1994).

Octanol/Water

Partition Coefficient: Log Kow = 2.66 (IARC Monographs, 1972-present)

#### **7.1.4 Technical Products and Impurities**

1,1,1,2-tetrachloroethane is available at 99% purity and is used for a laboratory standard for selected EPA methods (The Aldrich Catalog/Handbook of Fine Chemicals, 1994-95). It is not available in commercial quantities.

### **7.2 PRODUCTION AND USE**

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### **7.2.1 Production**

As of 1982, this chemical was not produced commercially in USA; no data are available for other years. This chemical is not produced on an industrial scale and is mainly the byproduct from the production of chlorinated ethanes. No data are available concerning import and export volumes.

#### **7.2.2 Uses**

1,1,1,2-tetrachloroethane is used as a solvent in cleaning, degreasing, and extraction processes; in manufacture of insecticides, herbicides, soil fumigants, bleaches, paints and varnishes and as a laboratory reagent (NRC. 1977. Drinking Water & Health; IARC Monograph, V.41, 1986). 1,1,1,2-tetrachloroethane is used primarily as a feedstock for the production of solvents such as trichloroethylene and tetrachloroethylene (Kirk-Othmer. 1991-present. Encyc Chem Tech, 4th Ed., Vol 1).

### 7.2.3 Disposal

1,1,1,2-tetrachloroethane is a potential candidate for fluidized bed incineration at a temperature range of 450 to 980°C and residence times of seconds for liquids and gases and longer for solids; for rotary kiln incineration at a temperature range of 820 to 1,600°C and residence times of seconds for liquids and gases and hours for solids; and for liquid injection incineration at a temperature range of 650 to 1,600°C and a residence time of 0.1 to 2 seconds (USEPA. 1981. Engineering Handbook for Hazardous Waste Incineration. EPA 68-03-3025). Incineration is a method of disposal, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids produced. Recommendable methods are incineration and evaporation. Not recommendable method: discharge to sewer.

At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices (HSDB Scientific Review Panel; HSDB, 1996).

## 7.3 POTENTIAL FOR HUMAN EXPOSURE

### 7.3.1 Natural Occurrence

Available data do not indicate that 1,1,1,2-tetrachloroethane occurs naturally.

### 7.3.2 Occupational

1,1,1,2-tetrachloroethane is not produced on an industrial scale but is formed as an incidental byproduct. Potential occupational exposure would occur from exposure to air emissions or contact with the vapor or liquid in the workplace.

### 7.3.3 Environmental

#### 7.3.3.1 *Environmental Releases*

According to available data, it appears that 1,1,1,2-tetrachloroethane is currently not produced in the U.S. However, since the chemical may be formed incidentally during the manufacture of other chlorinated ethanes, it may be released into the environment as air emissions or in wastewater (HSDB, 1996). It has not been confirmed if this chemical is currently used in the U.S. However, if used, environmental releases as a result of use would be expected.

#### 7.3.3.2 *Monitored Environmental Media Levels*

**Air:** Field studies were conducted in Arizona and California to better characterize the abundance of selected chemicals in the atmosphere. Average daily dosages from exposure to haloethane, including 1,1,1,2-tetrachloroethane, was determined to be 142 µg/day (Singh, H.B. et al., 1981; Atmos. Environ. Vol. 15, No. 4; HSDB, 1996). 1,1,1,2-tetrachloroethane was not

detected in two rural/remote sites in the U.S. For 602 urban/suburban sites in the U.S., a median level of 2.2 ppt and a maximum level of 63 ppt were found. In source areas, 43 sites/samples in the U.S., the mean concentration was 0.071 ppt and the maximum level 3.1 ppt. However, 1,1,1,2-tetrachloroethane was not detected in over 75 percent of the samples (Brodzinsky and Singh, SRI Contract 68-02-34; Class and Ballschmiter, 1986, Chemosphere, Vol. 15; HSDB, 1996).

**Water:** In the U.S. Groundwater Supply Survey, 1,1,1,2-tetrachloroethane was not detected (detection limit 0.2 ppb) in the drinking water of 945 supplies where groundwater was the source (Westrick et al., 1984; J. Amer. Water Works Assoc., Vol. 76; HSDB, 1996).

**Other Media:** Wastewater was analyzed in a survey conducted by the EPA of 4,000 industrial and publicly owned treatment works. 1,1,1,2-tetrachloroethane was identified in the discharges from several industrial categories. The median concentrations reported as follows: organics and plastic (27.4 ppb); inorganic chemicals (14.8 ppb); and electronics (272.6 ppb) (Shackelford, W.M. et al., 1983, Analyt. Chem. Acta., Vol. 146; HSDB, 1996).

### **7.3.3.3 Environmental Fate and Transport**

#### **7.3.3.3.1 Summary**

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of 1,1,1,2-tetrachloroethane released to surface soils is volatilization. Because of its moderate mobility in soils, tetrachloroethylene introduced into soil (e.g., landfills) has the potential to migrate through the soil into groundwater.

**Fate in the Atmosphere:** In the atmosphere, 1,1,1,2-tetrachloroethane is expected to be present primarily in the vapor phase rather than sorbed to particulates because of its moderate vapor pressure. Removal by scavenging during wet precipitation is expected because of the moderate solubility of 1,1,1,2-tetrachloroethane in water (1,100 mg/L). The major degradation process affecting vapor phase 1,1,1,2-tetrachloroethane is photo-oxidation by hydroxyl radicals and the chlorine radicals formed by the hydroxyl radical reaction (half-life on the order of years). Due to its persistence, 1,1,1,2-tetrachloroethane will disperse over long distances and slowly diffuse into the stratosphere where it would be rapidly degraded.

**Fate in Aquatic Environments:** The dominant fate of 1,1,1,2-tetrachloroethane released to surface waters is volatilization (predicted half-life of hours). Bioconcentration and sorption to sediments and suspended solids are not expected to be significant transport/partitioning processes.

### **7.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:** A  $K_{oc}$  of 93 is predicted for 1,1,1,2-tetrachloroethane based on its measured water solubility. An experimentally determined  $K_{oc}$  for 1,1,1,2-tetrachloroethane is reported to be 399. Based on the predicted and measured  $K_{oc}$ s, 1,1,1,2-tetrachloroethane is expected to exhibit moderate mobility and may leach slowly to the groundwater particularly in soils with low organic content (HSDB, 1996).

**Volatilization:** The dominant removal mechanism for 1,1,1,2-tetrachloroethane in surface waters is volatilization. The half-life will depend on wind and mixing conditions and is estimated to range from 4 to 11 hours in rivers, lakes, and ponds based on laboratory experiments. Because of its moderate vapor pressure (14 torr at 25 degrees C) and relatively low soil adsorption coefficient ( $K_{oc}$  of 93 to 399), 1,1,1,2-tetrachloroethane is expected to volatilize from dry soil surfaces and also from suspended particulate matter in the atmosphere (HSDB, 1996).

**Bioconcentration:** No experimental data are available on the bioconcentration of 1,1,1,2-tetrachloroethane. A bioconcentration factor of 12 is predicted for 1,1,1,2-tetrachloroethane based on its measured water solubility of 1,100 mg/L. Actual BCFs measured in fish studies are less than 10 for structurally similar halogenated aliphatic compounds. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996).

### **7.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** Little information is available on the biodegradability of 1,1,1,2-tetrachloroethane. Based on the results of a river die-away test for 1,1,1,2-tetrachloroethane and several studies examining the biodegradability of 1,1,1-trichloroethane, 1,1,1,2-tetrachloroethane is estimated to undergo biodegradation at a slow rate. The estimated half-lives are one to six months under aerobic conditions and 4 to six months under anaerobic conditions (Howard et al., 1991).

**Photodegradation:** Based upon an estimated rate constant for the vapor phase photo-oxidation reaction with photochemically produced hydroxyl radicals, the half-life of 1,1,1,2-tetrachloroethane in the atmosphere is 550 days. No data are readily available on the photolysis of 1,1,1,2-tetrachloroethane (HSDB, 1996).

**Hydrolysis:** Hydrolysis of 1,1,1,2-tetrachloroethane is not significant at environmental temperatures and pHs; the half-life for this process (at 25 C, pH 7) is 46.8 years (HSDB, 1996).

## **7.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **7.4.1 General U.S. Population**

Potential exposure, if any, to the general population would probably be through inhalation of ambient air contaminated with 1,1,1,2-tetrachloroethane (HSDB, 1996).

## 7.4.2 Occupational Exposure

Data are not available for the estimated occupationally exposed populations.

## 7.4.3 Consumer Exposure

According to Kirk-Othmer (1991), 1,1,1,2-tetrachloroethane is used primarily as a feedstock for the production of solvents such as trichloroethylene and tetrachloroethylene (HSDB, 1996). The IARC Monographs in 1986 have reported use in the manufacture of products such as paints and varnishes. It has not been confirmed if this use is current or if these products are/were consumer or industrial products (HSDB, 1996).

## 7.5 CHAPTER SUMMARY

Table 7-1 summarizes the findings of 1,1,1,2-tetrachloroethane.

**Table 7-1. 1,1,1,2-Tetrachloroethane Summary**

	Estimates	Support
Uses	Many solvent applications; chemical intermediate	Recent information
Production	As of 1982, not produced in U.S.; no other data are available	
Releases	No available data	
Properties/Fate	Volatile; water soluble; no significant bioconcentration; moderate mobility	Recent information
Media Levels	Air: 0.012 : g/m <sup>3</sup> - median value at 602 urban/suburban sites Water: Non detect (detection limit = 0.2 ppb) in 945 groundwater supplies	
General Population Exposure	No available data	
Special Population Exposures	No available data	

## 8.0 1,1-DICHLOROETHANE

### 8.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 8.1.1 Nomenclature

CAS No.: 75-34-3

Synonyms: Ethane, 1,1-dichloro-; ethylidene chloride; ethylidene dichloride

Trade Names: NCI-C04535

#### 8.1.2 Formula and Molecular Weight

Molecular Formula:  $C_2H_4Cl_2$

Molecular Weight: 98.97

#### 8.1.3 Chemical and Physical Properties

Description: Oily liquid, chloroform-like odor, taste as of chloroform (Merck Index, 11th Ed., 1989); colorless liquid (Sax. Danger Props Indus Mater, 6th Ed., 1984); colorless, oily liquid, chloroform-like odor (NIOSH Pocket Guide Chem Haz, 1994); aromatic ethereal odor (Sax. Hawley's Condensed Chem Dict, 11th Ed., 1987).

Boiling Point: 57.3°C (Merck Index, 11th Ed., 1989).

Melting Point: -96.9°C (CRC Handbook Chem & Physics, 75th Ed., 1994-1195).

Density: 1.175 @ 20°C/4°C (Merck Index, 11th Ed., 1989).

Spectroscopy Data: Index of Refraction: 1.4167 @ 20°C (Merck Index, 11th Ed., 1989); Sadtler Reference Number: 3205 (IR, prism); J118 (NMR) (Weast, 1979); Mass: 68 (National Bureau of Standards EPA-NIH Mass Spectra Data Base) (Weast, 1985).

Solubility: 0.55 g/100 ml water at 20°C; soluble in ethanol, ethyl ether (Patty. Indus Hyg & Tox, 3rd Ed., Vol 2A, 2B, 2C, 1981-82)

Volatility: Vapor Pressure: 3.44 (air = 1) (Sax. Danger Props Indus Mater, 6th Ed., 1984).

Vapor Density: 234 torr at 25°C (Patty. Indus Hyg & Tox, 3rd Ed., Vol 2A, 2B, 3C, 1981-82).

Stability: No data.

Reactivity: Reacts with strong oxidizers, strong caustics (NIOSH Pocket Guide Chem Haz, 1994).

Octanol/Water

Partition Coefficient: Log Kow = 1.9 (ITC/USEPA. Information Review #209 (Draft) Chloroethanes, 1980).

#### **8.1.4 Technical Products and Impurities**

1,1-dichloroethane is produced as reagent grade, 99.7% pure, with the following impurities: ethyl chloride 0.02%, butylene oxide 0.08%, trichloroethylene 0.08%, ethylene dichloride 0.01%, unknown 0.14% (expressed as volume percentage by weight of sample (ITC/USEPA. 1980. Information Review #209).

### **8.2 PRODUCTION AND USE**

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### **8.2.1 Production**

No information was identified for U.S. production, import, or export volumes.

#### **8.2.2 Uses**

1,1-dichloroethane is used as a solvent for plastics, oils, and fats; cleaning agent; degreaser; in rubber cementing; as a fumigant and insecticide spray; in fabric spreading; in fire extinguishing; and in medication: formerly used as an anesthetic (Browning. 1965. Tox & Metab Indus Solv). It is also used as an extractant for heat-sensitive substances (NIOSH OSHA. 1981. Occupat Health Guide Chem Hazards). Other uses include as a coupling agent in antiknock gasoline; in paint, varnish and paint removers; metal degreasing; and in ore flotation (Verschueren. 1983. Handbook Environ Data Org Chem). 1,1-dichloroethane is usually used as an intermediate in the production of 1,1,1-trichloroethane by thermal chlorination or photochlorination and in the production of vinyl chloride (Kirk-Othmer, 1991-present).

#### **8.2.3 Disposal**

Generators of waste containing this contaminant (i.e., EPA hazardous waste number U076) must conform with USEPA regulations in storage, transportation, treatment, and disposal of waste (40 CFR 240-280, 300-306, 702-799). 1,1-dichloroethane may be disposed of by atomizing in a suitable combustion chamber equipped with an appropriate effluent gas cleaning

device (NIOSH OSHA. 1981. Occupat Health Guide Chem Hazards). It is a potential candidate for liquid injection incineration, with a temperature range of 650 to 1,600°C and a residence time of 0.1 to 2 seconds; for rotary kiln incineration, with a temperature range of 820 to 1,600 °C and a residence time of seconds; and for fluidized bed incineration, with a temperature range of 450 to 980°C and a residence time of seconds (USEPA. 1981. Engineering Handbook for Hazardous Waste Incineration). The following wastewater treatment technologies have been investigated for 1,1-dichloroethane: concentration process: stripping, solvent extraction, activated carbon, and resin adsorption (USEPA. 1982. Management of Hazardous Waste Leachate. EPA Contract No. 68-03-2766).

### **8.3 POTENTIAL FOR HUMAN EXPOSURE**

#### **8.3.1 Natural Occurrence**

There are no known natural sources of 1,1-dichloroethane; however, it has been reported that 1,1,1-trichloroethane is biodegraded to 1,1-dichloroethane in anaerobic environments such as landfills (ATSDR, 1990).

#### **8.3.2 Occupational**

In addition to members of the general populations living near emission point sources and hazardous waste sites, human exposure to 1,1-dichloroethane is expected to be highest among certain occupational groups (ATSDR, 1990). These groups are workers in the chemical and allied products industry (ATSDR, 1990).

#### **8.3.3 Environmental**

##### **8.3.3.1 Environmental Releases**

The primary disposition of 1,1-dichloroethane in the environment is the result of production, storage, consumption, transport, and disposal from its use as chemical intermediate, solvent, finish remover, and degreaser (ATSDR, 1990). Releases from industrial processes are almost exclusively to the atmosphere. 1,1-dichloroethane has been detected generally at low levels in ambient air, surface water, groundwater, drinking water, and human breath. Concentrations are largest in environmental media near source areas (ATSDR, 1990). Another source of this chemical in the environment is the reduction (biotic or abiotic) of 1,1,1-trichloroethane to 1,1-dichloroethane in groundwater (HSDB, 1996).

**Air:** The majority (99 percent) of all releases of 1,1-dichloroethane to the environment are emissions to the atmosphere (ATSDR, 1990). Releases from the production of 1,1,1-trichloroethane and 1,2-dichloroethane account for approximately 52 percent and 35 percent, respectively of these releases (ATSDR, 1990). Approximately 52,000 kg of 1,1-dichloroethane are released to the air from POTWs (ATSDR, 1990).

**Water:** Releases of 1,1-dichloroethane to surface waters from industrial solvent use and from POTWs are approximately 2,000 kg/yr (ATSDR, 1990). The largest sources of these

releases are believed to be from its use as a cleaning solvent or chemical intermediate and from POTWs (ATSDR, 1990). Approximately 1,000 kg/yr of 1,1-dichloroethane are released in the effluents of POTWs (ATSDR, 1990).

**Other Media:** Releases to land from solvent use and POTWs were estimated at 6,000 kg in 1978 (ATSDR, 1990). According to ATSDR (1990), approximately 4,000 kg/yr of 1,1-dichloroethane are released to land as sludge from POTWs.

### **8.3.3.2 Monitored Environmental Media Levels**

**Air:** Atmospheric levels of 1,1-dichloroethane have been detected at urban, rural, and industrial sites across the U.S. The reported median concentration is 55 ppt (ATSDR, 1990). In the urban/suburban parts of the U.S., reported concentrations were 61 ppt (median value) and 100 ppt (maximum values) for the analysis of 455 samples (HSDB, 1996). The concentrations in source areas (101 samples) were 11 ppt (median value) and 1,400 ppt (maximum value) (HSDB, 1996).

**Water:** Data summarized from the EPA STORET data base in 1982 have shown concentrations for 1,1-dichloroethane ranging from <10 ppb (not detected) to 1,900 ppb (ATSDR, 1990). The highest reading was from the upper Mississippi River Basin; however, the reported monitoring results indicated that in surface water the levels were mostly <10 ppb.

According to a study summarizing groundwater data from numerous State agencies, 18 percent of monitored drinking water wells contained 1,1-dichloroethane; the highest reported concentration in wells was 11,300 ppb and a maximum surface concentration of 0.2 ppb (ATSDR, 1990; HSDB, 1996). In Iowa, 127 wells from 58 public water supplies contained 1,2-dichloroethane residues 1 to 24 ppb (HSDB, 1996).

Finished water supplies in the U.S. from groundwater sources that were tested for EPA contaminants had a maximum concentration of 4.2 ppb; detectable levels of 1,1-dichloroethane was found in 10.8 percent of 158 non-random samples. Groundwater samples taken from 178 hazardous waste disposal sites contained an average concentration of 0.31 ppm with a maximum concentration of 56.1 ppm and had a frequency of 18 percent (ATSDR, 1990).

**Other Media:** Data for levels in soil were not found. The reported mean concentration was 33 ppt for oysters obtained from the Mississippi River delta (HSDB, 1996). Information were not found for ambient concentrations of 1,1-dichloroethane in soil, current disposal of waste products containing this chemical in landfills, foods, plants, fish, or animals (HSDB, 1996; ATSDR, 1990).

### 8.3.3.3 *Environmental Fate and Transport*

#### 8.3.3.3.1 Summary

The summary is based on the data presented in the subsequent fate and transport sections.

**Fate in Terrestrial Environments:** The dominant fate of 1,1-dichloroethane released to surface soils is volatilization. Because of its high mobility in soils, 1,1-dichloroethane introduced into soil (e.g., landfills) has the potential to migrate through the soil into groundwater. Biodegradation under anaerobic conditions in soil and groundwater may occur at a relatively slow rate (half-lives on the order of months or longer).

**Fate in the Atmosphere:** In the atmosphere, 1,1-dichloroethane is expected to be present in the vapor phase rather than sorbed to particulate matter. Removal of 1,1-dichloroethane during wet precipitation is expected because of its relatively high water solubility. 1,1-Dichloroethane will degrade by reaction with photochemically produced hydroxyl radicals. Because photo-oxidation is not a rapid process (predicted half-lives ranging from 10 to 100 days), considerable dispersion of 1,1-dichloroethane in the atmosphere may occur.

**Fate in Aquatic Environments:** The dominant fate of 1,1-dichloroethane released to surface waters is volatilization (predicted half-life of 1 to 10 days). Bioconcentration, biodegradation, and sorption to sediments and suspended solids are not expected to be significant fate processes.

#### 8.3.3.3.2 Transport and Partitioning

**Soil Adsorption/Mobility:** The very low predicted soil adsorption coefficients ( $K_{oc}$ ) for 1,1-dichloroethane ( $K_{oc}$  of 43) indicates that sorption of 1,1-dichloroethane to soil, sediment, and suspended solids is not a significant fate process. As a consequence, these isomers should show high mobility in soil (HSDB, 1996).

**Volatilization:** The dominant removal mechanism for the 1,1-dichloroethane isomers in surface waters is volatilization. The half-life will depend on wind and mixing conditions and is estimated to range from 1 to 10 days in rivers, lakes, and ponds based on laboratory experiments. Because of its high vapor pressure and relatively low soil adsorption coefficient, 1,1-dichloroethane is expected to volatilize rapidly from soil surfaces and also from suspended particulate matter in the atmosphere (HSDB, 1996).

**Bioconcentration:** A bioconcentration factor of 1.3 is predicted for 1,1-dichloroethane based on the reported water solubility of 5,500 mg/L. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996).

### **8.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** The results of aerobic biodegradation studies indicate that 1,1-dichloroethane is recalcitrant to aerobic degradation in soil and water (i.e., half-lives on the order of months). Although no studies examining the anaerobic biodegradation of 1,1-dichloroethane are available, the estimated half-life under anaerobic conditions has been estimated to range from months to years (HSDB, 1996; Howard et al., 1991).

**Photodegradation:** Based on measured rate data for the vapor phase reaction with hydroxyl radicals, the estimated half-life of 1,1-dichloroethane in the troposphere ranges from 10 to 100 days (HSDB, 1996; Howard et al., 1991).

**Hydrolysis:** No information specifically addressing the hydrolytic half-life of 1,1-dichloroethane is available. Considering the volatility of 1,1-dichloroethane from water and the fact that the hydrolytic half-lives of structurally similar chlorinated ethanes are on the order of months to years, indicates that hydrolysis is not an important fate process (HSDB, 1996; Howard et al., 1991).

## **8.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **8.4.1 General U.S. Population**

The primary route of exposure for the general population to 1,1-dichloroethane is the inhalation of air contaminated with this chemical. An additional potential route of exposure is ingestion of 1,1-dichloroethane contaminated drinking water. Specifically, persons near industrial facilities and hazardous waste may be potentially exposed from inhalation of ambient air and ingestion of drinking water (ATSDR, 1990). EPA has identified 1,1-dichloroethane in 248 of the 1,177 NPL sites; the number of sites evaluated for this chemical was not reported (ATSDR, 1990). The frequency of these sites within the U.S. are presented in Figure 8-1.

The U.S. EPA assumed median ambient air concentration of 55 ppt and an average inhalation rate of 20 m<sup>3</sup>/day and estimated the average inhalation exposure to 1,1-dichloroethane from the general population to be 4 µg/day (ATSDR, 1990).

### **8.4.2 Occupational Exposure**

Populations potentially exposed in the workplace in the early 1980s were estimated by NIOSH to have ranged from 715 to 1,957 workers (ATSDR, 1990). Occupational exposures are primarily the result of the use of 1,1-dichloroethane as a chemical intermediate, solvent, and a component of fumigant formulations (ATSDR, 1990).

### **8.4.3 Consumer Exposure**

No data were found for consumer exposure estimates.



## 8.5 CHAPTER SUMMARY

Table 8-1 summarizes the findings of 1,1-dichloroethane.

**Table 8-1. 1,1-Dichloroethane Summary**

	Estimates	Support
Uses	Many solvent uses; fumigant; chemical intermediate; degreaser	Well documented
Production	No available information	
Releases	Predominantly air - 52,000 kg released to air from POTWs	ATSDR (1990)
Properties/Fate	Volatile; slightly soluble in water; no significant bioconcentration or biodegradation expected	
Media Levels	Air: urban/suburban - 0.332 : g/m <sup>3</sup> (median) Water: surface water <10 ppb to 1,900 ppb Groundwater: varies 1 to 24 ppb (Iowa; 127 wells)	455 samples
General Population Exposure	Primarily through air or potentially contaminated groundwater Air = 4 : g/d	ATSDR (1990)
Special Population Exposures	Chemical and allied product workers	ATSDR (1990)

## SECTION C. METABOLITES OF TRICHLOROETHYLENE AND PARENT COMPOUNDS

### 9.0 CHLORAL

#### 9.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996) and IARC (1995).

##### 9.1.1 Nomenclature

CAS No.:	75-87-6
Synonyms:	2,2,2-trichloroacetaldehyde; acetaldehyde, trichloro-; anhydrous chloral; trichloroacetaldehyde; trichloroethanol
Trade Name:	Grasex

##### 9.1.2 Formula and Molecular Weight

Structural Formula:	$C_2HCl_3-0$
Molecular Weight:	147.40

##### 9.1.3 Chemical and Physical Properties

Description:	Colorless, oily liquid with an irritating odor (Encyc. Occupat. Health & Safety, 1983).
Boiling Point:	97.8°C @ 760 mm Hg (Merck Index, 10th Ed., 1983).
Melting Point:	-57.5°C (Merck Index, 10th Ed., 1983).
Density:	1.5121 @ 20°C/4°C (Weast. Hdbk. Chem. & Phys., 67th Ed., 1986-87).
Spectroscopy Data:	Index of refraction: 1.45572 @ 20°C/D (Weast. Hdbk. Chem. & Phys., 67th Ed., 1986-87); IR: 4626, IR: 4426 (Sadtler Research Laboratories Prism Collection); IR: 6507 (Coblentz Society Spectral Collection); UV: 5-3 (Organic Electronic Spectral Data); Mass: 814 (Atlas of Mass Spectral Data) (Weast. CRC Hdbk. Data Organic CPDS., Vol. I, II, 1985)

Solubility:	Highly soluble in water; soluble in alcohol, ether (Merck Index, 10th Ed., 1983); chloral hydrate is extremely soluble in water (825 g/100 g water (Seidell, A. (1941) Solubilities of Organic Compounds); soluble in chloroform (Condensed Chem. Dictionary, 10th Ed., 1981).
Volatility:	Vapor Pressure: 35 mm Hg @ 20°C (Encyc. Occupat. Health & Safety, 1983; IARC, 1995). Vapor Density: 5.1 (air = 1) (Patty. Indus. Hyg. & Tox, 1981-1982).
Stability:	Unstable (Goodman (1985) Pharm. Basis Therap., 7th Ed.).
Reactivity:	Forms chloral hydrate when dissolved in water and forms chloral alcoholate when dissolved in alcohol (Merck Index, 10th Ed., 1983).
Octanol/Water Partition Coefficient:	No data.

#### 9.1.4 Technical Products and Impurities

Chloral is produced in a technical grade with a minimum of 94% purity (Hawley (1981) Condensed Chem. Dictionary, 10th Ed.). Instead of water, various alcohols can be added to chloral to form hemiacetals. Chloral alcoholate and chloral betaine are simple adducts and laboratory anesthetic alpha-chloralose is a complex adduct. Chloral is an unstable oil that does not lend itself well to pharmaceutical formulations; therefore, in medicine it was introduced in the form of chloral hydrate (Goodman (1985) Pharm. Basis Therap, 7th Ed.) The typical impurities (max.) are as follows: water, 0.06%; 2,2-dichloroethane, 0.3%; 2,2,3-trichlorobutanol, 0.01%; hydrogen chloride, 0.06%; and chloroform (IARC, 1995).

## 9.2 PRODUCTION AND USE

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996) and IARC (1995).

### 9.2.1 Production

The principal use of chloral in the U.S. was in the manufacture of DDT. According to IARC (1995), when the use of DDT was banned in the U.S. in 1972, the demand for chloral in the U.S. rapidly declined. DDT is still produced in the U.S. for use in tropical countries (IARC, 1995).

- U.S. Production: (1969)  $2.83 \times 10^{10}$  g; (1975)  $2.27 \times 10^{10}$  g (SRI).

- Import Volumes: (1984)  $1.02 \times 10^8$  g (Bureau of the Census. U.S. Imports for Consumption and General Imports, 1984).
- Export Volumes: (1972 and 1975) negligible.

### **9.2.2 Uses**

Chloral is used in the spraying and pouring of polyurethanes (NRC, 1977); as a chemical intermediate for the herbicide trichloroacetic acid and chloral hydrate (HSDB, 1996); used to induce swelling of starch granules at room temperature (Kirk-Othmer, 1978-present); and as an intermediate in DDT and other insecticides, including: methoxychlor, dichlorvos, naled, and trichlorofon (Sittig. (1985) Handbook Toxic hazard Chem & Carcinog, 2nd Ed.; IARC, 1995). Estimated use in the U.S. in 1975 was in the manufacture of DDT (40%); methoxychlor, dichlorvos, and naled (10%); and miscellaneous other applications (50%) (IARC, 1995).

### **9.2.3 Disposal**

Chloral is a potential candidate for liquid injection incineration at a temperature range of 650 to 1,600°C and a residence time of 0.1 to 2 seconds; for rotary kiln incineration at a temperature range of 820 to 1,600°C and residence times of seconds for liquids and gases, and hours for solids; and for fluidized bed incineration at a temperature range from 450 to 980°C and residence times of seconds for liquids and gases, and longer for solids. (USEPA (1981) Engineering Handbook for Hazardous Waste Incineration).

At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices (HSDB Technical Review Panel; HSDB, 1996).

## **9.3 POTENTIAL FOR HUMAN EXPOSURE**

### **9.3.1 Natural Occurrence**

Chloral is not known to occur as a natural product (IARC, 1995).

### **9.3.2 Occupational**

Exposure to chloral is thought to be primarily via inhalation and dermal contact with the vapor (HSDB, 1996). Chloral has been detected in the work environment during spraying and casting of polyurethane foam, identified as an auto-oxidation product of trichloroethylene during extraction of vegetable oil, and also identified at the output of etching chambers in semiconductor processing (IARC, 1995).

### 9.3.3 Environmental

#### 9.3.3.1 Environmental Releases

Chloral may be released to the environment from the synthesis of methoxychlor and DVPP, and also from wood processing plants in the chlorination portion of the bleaching process (HSDB, 1996). It is a reactive intermediate metabolite of trichloroethylene (IARC, 1995).

#### 9.3.3.2 Monitored Environmental Media Levels

**Air:** No data.

**Water:** Chloral is formed during aqueous chlorination of humic substances and amino acids (IARC, 1995). It may therefore occur in drinking water as a result of chlorine disinfection of raw waters containing natural organic substances. The concentration of chloral measured in drinking water in the U.S. is summarized in Table 9-1.

Chloral was reported in the drinking water supplies of several U.S. cities as follows: Philadelphia, PA - 5 µg/l; Seattle, WA - 3.5 µg/l; Cincinnati, OH - 2 µg/l; Terrebonne Parish, LA - 1 µg/l; New York City, NY - 0.02 µg/l; Grand Forks, ND - 0.01 µg/l (HSDB, 1996). In surface water samples taken from water of New Orleans/Baton Rouge, chloral was reported at a mean concentration of 1.0 µg/l (HSDB, 1996).

Chloral has also been detected in the spent chlorination liquor from bleaching of sulfite pulp after oxygen treatment at concentrations of <0.1 to 0.5 g/ton of pulp. Trace amounts have also been reported from photocatalytic degradation of trichloroethylene in water (IARC, 1995).

**Other Media:** Chloral is a reactive intermediate metabolite of trichloroethylene (IARC, 1995).

**Table 9-1. Concentrations of Chloral (As Chloral Hydrate) in Drinking Water in the United States**

Water Type (Location)	Concentration (µg/L)
Tap water (reservoir)	7.2-18.2
Surface, reservoirs, lake, and groundwater	1.7-3.0
Tap water	0.01-5.0
Distribution system	0.14-6.7
Surface water	6.3-28

Source: IARC, 1995.

### 9.3.3.3 *Environmental Fate and Transport*

#### 9.3.3.3.1 Summary

**Fate in Terrestrial Environments:** The dominant fate of chloral released to soils is rapid hydrolysis by soil water to form chloral hydrate. Volatilization is likely to be important only in the event of a spill onto relatively dry soil.

**Fate in the Atmosphere:** Chloral should react rapidly with the moisture in air to form chloral hydrate. Although photo-oxidation by hydroxyl radicals will likely occur to some extent, the reaction rate is much slower than for hydrolysis; the half-life for the vapor phase reaction of chloral with photochemically produced hydroxy radicals is estimated to be 10.8 hours.

**Fate in Aquatic Environments:** The dominant fate of any chloral released to water is rapid hydrolysis to form chloral hydrate. Although this hydrolysis reaction is reversible, the equilibrium constant favors the formation of chloral hydrate (27,000 to 1). Chloral is thus essentially removed from the water. Volatilization, sorption to suspended solids, and bioconcentration are not expected to be significant.

#### 9.3.3.3.2 Transport and Partitioning

**Soil Adsorption/Mobility:** No data are available concerning the sorption of chloral to soil. However, since chloral reacts rapidly with water to form chloral hydrate, it should also react rapidly with soil moisture. Since chloral hydrate is extremely soluble in water (8,250 g/L) and is not expected to sorb to soil, chloral hydrate has the potential to leach through soils (HSDB, 1996).

**Volatilization:** Chloral has a relatively high vapor pressure (35 torr at 25 degrees C) and should therefore volatilize rapidly from dry surfaces. Chloral reacts rapidly with water to form chloral hydrate thus precluding any significant volatilization of chloral from water (HSDB, 1996).

**Bioconcentration:** No data are available concerning the bioconcentration of chloral. However, since chloral reacts rapidly with water to form chloral hydrate, bioconcentration would not be expected to be a significant fate process. Since chloral hydrate is extremely soluble in water (8,250 g/L), bioconcentration in aquatic organisms should not be significant for chloral hydrate (HSDB, 1996).

#### 9.3.3.3.3 Transformation and Degradation Processes

**Biodegradation:** No data are available concerning the biodegradability of chloral. However, since chloral reacts rapidly with water to form chloral hydrate, biodegradation would not be expected to be a significant fate process.

**Photodegradation:** The half-life for the vapor phase reaction of chloral with photochemically produced hydroxy radicals is estimated to be 10.8 hours. No data are available

on the photolytic sensitivity of chloral. However, acetaldehyde has a UV absorption maximum at 293 nm which suggests that chloral will also absorb some UV light (HSDB, 1996).

**Hydrolysis:** Chloral reacts exothermically with water to form chloral hydrate. Because the equilibrium constant for this reaction is  $3.6 \times 10^{-5}$ , very little chloral will remain in solution (HSDB, 1996)

## **9.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

### **9.4.1 General U.S. Population**

The general population can be exposed to chloral during its production and use, from drinking chlorinated water, and from pharmaceutical use (IARC, 1995).

### **9.4.2 Occupational Exposure**

Results of the National Occupational Exposure Survey conducted between 1981 and 1983 indicate that 2,757 employees in the U.S. were potentially exposed to chloral (IARC, 1995). The estimate was based on a survey of companies and did not involve measurements of actual exposure.

### **9.4.3 Consumer Exposure**

No data concerning consumer exposure were found.

## **9.5 CHAPTER SUMMARY**

Table 9-2 summarizes the findings of chloral.

**Table 9-2. Chloral Summary**

	Estimates	Support
Uses	Chemical intermediate for manufacture of pesticides; used in spraying and pouring of polyurethanes	Well documented
Production	2.3 x 10 <sup>7</sup> kg	1975 data
Releases	No available data	
Properties/Fate	Soluble in water; rapid hydrolysis to chloral hydrate; no significant bio-concentration expected	
Media Levels	Air: no data Drinking water supplies: six U.S. cities - 0.02 ug/l to 5 mg/l	
General Population Exposure	No available data	
Special Population Exposures	2,757 employees potentially exposed	Data from early 1980s

## 10.0 CHLORAL HYDRATE

### 10.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 10.1.1 Nomenclature

CAS No. 302-17-0

Synonyms: 1,1,1-trichloro-2,2-dihydroxyethane; 2,2,2-trichloro-1,1-ethanediol; trichloroacetaldehyde hydrate; trichloroacetaldehyde monohydrate; trichloroethylidene glycol; 2,2,2-trichloroethane-1,1-diol

Trade Names: Kessodrate, Noctec, Phaldrone, Sontec, Chloralvan, Chloralex

#### 10.1.2 Formula and Molecular Weight

Molecular Formula:  $C_2H_3Cl_3O_2$

Molecular Weight: 165.42

#### 10.1.3 Chemical and Physical Properties

Description: Transparent, colorless crystals (Sax, 1984); aromatic, penetrating and slightly acid odor; slightly bitter, caustic taste (Merck Index, 11th Ed., 1989).

Boiling Point: 96.3°C @ 764 mm Hg (decomp) (CRC Handbook Chem. & Physics, 1991-1992).

Melting Point: -57°C (Merck Index, 11th Ed., 1989).

Density: 1.908 @ 20°C/4°C (CRC Handbook Chem. & Physics, 1991-1992).

Spectroscopy Data: IR: 5423 (Coblentz Society Spectral Collection); NMR: 10362 (Sadler Research Laboratories Spectral Collection); Mass: 1054 (Atlas of Mass Spectral Data) (Weast, 1985); intense mass spectral peaks: 82 m/z, 111 m/z, 146 m/z (Pfleger, 1985).

Solubility: 2.4 g/ml water @ 0°C; 14.3 g/ml water @ 40°C; 8.3 g/ml water at 25°C. Sparingly soluble in turpentine, petroleum ether, benzene, toluene, carbon tetrachloride; 1 g/68 g carbon disulfide; 1 g/1.3 ml alcohol; 1 g/1.4 ml olive oil; freely soluble

in acetone, methyl ethyl ketone; 1 g/2 ml chloroform; 1 g/1.5 ml ether; 1 g/0.5 ml glycerol (Merck Index, 11th Ed., 1989).

Volatility: No data.

Stability: Slowly volatilizes on exposure to air (Merck Index, 11th Ed., 1989). Aqueous solutions of chloral hydrate decomposed rapidly when exposed to ultraviolet light, with the formation of hydrochloric acid, trichloroacetic acid, and formic acid. A 1% solution lost about 5% of its strength after storage at room temperature for 20 weeks; aqueous solutions are likely to develop mold growth (Martindale. Extra Pharmacopeia, 28th Ed., 1982).

Reactivity: No data.

Octanol/Water

Partition Coefficient:  $\log K_{ow} = 0.99$  (Hansch. Log P Database, 1987)

#### 10.1.4 Technical Products and Impurities

Dosage forms for chloral hydrate are the following: capsules: 250 and 500 mg, and 1 g; elixir: 500 mg/5 ml; suppositories: 325, 500, and 650 mg; syrup: 250 and 500 mg/5 ml (Remington's Pharm. Sci., 17Ed., 1985). Noctec capsules contain 250 or 500 mg chloral hydrate per capsule; Noctec syrup contains 500 mg chloral hydrate per 5 cc (AHFS drug Information 92 Plus Suppl's). Chloral hydrate is produced in technical and USP grades (Sax, 1987). For chloropent injection; intravenous anesthetic; each ml contains chloral hydrate 42.5 mg; magnesium sulfate 21.2 mg; pentobarbital 8.86 mg; ethyl alcohol 14.25%; propylene glycol 33.8%; and purified water, qs (for cattle and horses) (Vet Pharm. & Biolog., 1982-1983). Chloral hydrate capsules contain not less than 95.0% and not more than 110.0% of the labeled amount of chloral hydrate; chloral hydrate syrup contains not less than 95.0% and not more than 110.09% of the labeled amount of chloral hydrate (USPC. USP XXII & NF XVII 1990, Plus Suppl's).

## 10.2 PRODUCTION AND USE

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

### 10.2.1 Production

U.S. Production: (1972)  $1.14 \times 10^{10}$  g (anhydrous chloral); (1975)  $5.9 \times 10^8$  g (SRI).

Import Volume: (1972)  $2.83 \times 10^7$  g; (1975)  $4.8 \times 10^7$  g (SRI); (1984)  $5.41 \times 10^6$  g;  $4.67 \times 10^{12}$  g (Bureau of the Census. U.S. Imports for Consumption and General Imports, 1984; 1986).

Export Volume: No data.

### 10.2.2 Uses

Chloral hydrate is used in medication as a hypnotic and sedative (Merck Index, 11th Ed., 1989; IARC, 1995). It is also used as a rubefacient in topical preparations (AHFS Drug Information 92 Plus Suppl's); veterinary medication (Vet Pharm. & Biolog., 1982-1983); and as a glue peptizing agent (Kirk-Othmer, 1980).

### 10.2.3 Disposal

Chloral hydrate is a waste chemical stream constituent which may be subjected to ultimate disposal by controlled incineration, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene; an acid scrubber is necessary to remove the halo acids produced (USEPA. 1981. Engineering Handbook of Hazardous Waste Leachate). Solvent extraction is a wastewater treatment technology that has been investigated for chloral hydrate (USEPA. 1982. Engineering Handbook of Hazardous Waste Leachate).

## 10.3 POTENTIAL FOR HUMAN EXPOSURE

### 10.3.1 Natural Occurrence

Chloral hydrate is not known to occur as a natural product (IARC, 1995).

### 10.3.2 Occupational

Specific information concerning potential for occupational exposure were not found.

### 10.3.3 Environmental

#### 10.3.3.1 *Environmental Releases*

Specific data on environmental releases of chloral hydrate were not found.

#### 10.3.3.2 *Monitored Environmental Media Levels*

**Air:** No data.

**Water:** Chloral hydrate may occur in drinking water as a result of chlorine disinfection of raw waters containing natural organic substances. The concentration of chloral measured in drinking water (as chloral hydrate) in the U.S. is summarized in Section 9, Table 9-1.

**Other Media:** Chloral hydrate has been detected in human milk (HSDB, 1996). Data were not available in HSDB (1996) on the mechanism whereby the breast milk became contaminated.

### **10.3.3.3 *Environmental Fate and Transport***

#### **10.3.3.3.1 Summary**

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** Since chloral hydrate is very soluble in water (8,250 g/L), it is not expected to sorb to soil and thus has the potential to leach through soils. No information is available on the biodegradation of chloral hydrate.

**Fate in the Atmosphere:** Any chloral hydrate released to the atmosphere is expected to be readily scavenged during precipitation events. Chloral hydrate may also undergo photolysis, but the available data are not adequate to determine its relative importance.

**Fate in Aquatic Environments:** Because of its very high water solubility, chloral hydrate is not expected to volatilize, sorb to suspended solids or sediments, or bioconcentrate. No information is available on the biodegradation of chloral hydrate.

#### **10.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:** No data are available concerning the sorption of chloral hydrate to soil. However, since chloral hydrate is very soluble in water (8,250 g/L), it is not expected to sorb to soil and thus has the potential to leach through soils (HSDB, 1996).

**Volatilization:** Although vapor pressure data for chloral hydrate are not readily available, chloral hydrate has been reported to slowly volatilize from surfaces when exposed to air. Because of its very high water solubility, volatilization from water is not expected to be significant (HSDB, 1996).

**Bioconcentration:** No data are available concerning the bioconcentration of chloral hydrate. However, since chloral hydrate is very soluble in water (8,250 g/L), bioconcentration in aquatic organisms should not be significant (HSDB, 1996).

#### **10.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** No information is available on the biodegradation of chloral hydrate (HSDB, 1996).

**Photodegradation:** Although no studies have apparently been published that quantitatively have examined direct atmospheric photolysis of chloral hydrate, a 1 percent

aqueous solution of chloral hydrate was reported to have lost 5 percent of its strength after storage for 20 weeks at room temperature. Hydrochloric acid, trichloroacetic acid, and formic acid were formed as products (HSDB, 1996).

**Hydrolysis:** Hydrolysis is not expected to be a significant fate process for chloral hydrate.

#### 10.4 HUMAN EXPOSURE AND POPULATION ESTIMATES

Human exposure to chloral hydrate can occur during its production and use, from pharmaceutical use, and from drinking chlorinated water (IARC, 1995). Specific exposure data and data on estimates of exposed populations were not found. The general population may be potentially exposed from ingestion of drinking water contaminated with chloral hydrate. The occupational population may be exposed in the workplace during production and use. The consumer population may be potentially exposed from use of pharmaceuticals.

#### 10.5 CHAPTER SUMMARY

Table 10-1 summarizes the findings of chloral hydrate.

**Table 10-1. Chloral Hydrate Summary**

	Estimates	Support
Uses	Pharmaceutical	Well documented
Production	5.9 x 10 <sup>5</sup> kg	1975 data
Releases	No available data	
Properties/Fate	Water soluble; no significant bioconcentration expected; no information on biodegradation	
Media Levels	No available data	
General Population Exposure	No available data	
Special Population Exposures	No available data	

## 11.0 MONOCHLOROACETIC ACID

### 11.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 11.1.1 Nomenclature

CAS No.: 79-11-8

Synonyms: Acetic acid; chloro-; alpha-chloroacetic acid; chloracetic acid; chloroethanoic acid; monochloroacetic acid; monochloroethanoic acid

Trade Names: NCI-C60231

#### 11.1.2 Formula and Molecular Weight

Molecular Formula:  $C_2H_3ClO_2$

Molecular Weight: 94.50

#### 11.1.3 Chemical and Physical Properties

Description: Colorless or white crystals (Merck Index, 11th Ed., 1989).  
Characteristic penetrating odor similar to vinegar.

Boiling Point: All three forms (alpha, beta, gamma) boil at 189° C (Merck Index, 11th Ed., 1989).

Melting Point: Exists in three physical modifications: alpha 63° C; beta 55-56° C; gamma 50° C (Merck Index, 11th Ed., 1989).

Density: 1.4043 @ 40° C/4° C (Gardner's Chem Synonyms, Trade Names, 1987).

Spectroscopy Data: Index of Refraction: 1.4351 @ 55° C/D; Sadtler Ref. Number: 2094 (IR, Prism (Weast, 1988-89); IR: 5567 (Coblentz Society Spectral Collection) (Weast, 1985); NMR: 128 (Sadtler Research Laboratories Spectral Collection) (Weast, 1985); Mass; 196 (Weast, 1985).

Solubility: Very soluble in water, slightly soluble in chloroform (Weast, 1988-89); Soluble in acetone, carbon disulfide (Weast, 1979); soluble in benzene (Merck Index, 1989); soluble in ethanol, diethyl ether (Worthing, Pesticide Manual, 1979); soluble in carbon tetrachloride (Encyc. Occupat. Health & Safety, 1983).

Volatility: Vapor Pressure: 1 mm Hg @ 43.0° C (Patty, Indus. Hyg. & Tox., 3rd Ed., 1981-82).

Vapor Density: 3.26 (air = 1) (Sax, 1984).

Stability: No data.

Reactivity: Highly reactive; chemically reacts with ammonia to form glycine and with aniline to form a precursor for indigo dyes (Encyc. Occupat. Health & Safety, 1983).

Octanol/Water

Partition Coefficient: log Kow = 0.22 (Hansch, 1981)

#### **11.1.4 Technical Products and Impurities**

Monochloroacetic acid is produced in technical and medicinal grades with 99.5% purity. Data were not available for impurities.

### **11.2 PRODUCTION AND USE**

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### **11.2.1 Production**

U.S. Production: (1978)  $3.50 \times 10^{10}$  g (SRI); (1982) probably greater than  $6.81 \times 10^6$  g (SRI); Chemical Int. For sodium carboxymethyl cellulose, 60%; for herbicides, 30%; for other derivatives (e.g., glycine, thioglycolic acid, pharmaceuticals, and indigoid dyes), 10% (SRI, 1979).

Import Volumes: (1978)  $1.25 \times 10^{10}$  g (SRI); (1982)  $1.35 \times 10^{10}$  g (SRI).

#### **11.2.2 Uses**

Monochloroacetic acid is used as a chemical intermediate for pharmaceuticals (e.g., vitamin A); chemical intermediate for indigoid dyes; and as a herbicide (Merck Index, 1989). It is also used as a preservative, bacteriostat, intermediate in production of synthetic caffeine; carboxymethyl cellulose; ethyl chloracetate; glycine; scariosine; thioglycolic acid; EDTA; 2,4-D; 2,4,5-T (Hawley's Condensed Chem. Dict., 11th Ed., 1987). It has also been recommended as a defoliant (Pesticide Manual, 4th Ed., 1974, p.106).

#### **11.2.3 Disposal**

No data were identified.

## 11.3 POTENTIAL FOR HUMAN EXPOSURE

### 11.3.1 Natural Occurrence

No information on the natural occurrence of chloroacetic acid was found.

### 11.3.2 Occupational

No specific information on potential for occupational exposure of chloroacetic acid was found.

### 11.3.3 Environmental

#### 11.3.3.1 Environmental Releases

Chloroacetic acid may enter the environment in emissions and wastewater from its production and use as a chemical intermediate primarily in the manufacture of chlorophenoxy herbicides and carboxymethyl cellulose. Such releases of the chemical would be limited to industrial settings (HSDB, 1996). Chloroacetic acid has been used as a pre-emergent herbicide and defoliant, and if it is still used for these applications, its use would constitute an emission source and ground contamination of a more general nature (HSDB, 1996).

Total Toxic Release (TRI) releases for years 1987 to 1994 are shown in Table 11-1. The receiving media are air, water, land, and for underground injection, POTW transfer, and other transfer. These releases are reported from manufacturing and processing facilities. Only certain facilities are required to report, and therefore may not capture all releases.

**Table 11-1. Release of Chloroacetic Acid (lbs/yr)**

Year	Number of Reporting Facilities	Fugitive Air Releases	Stack Air Releases	Surface Water Release	Underground Injection	Land Disposal	POTW Transfer	Other Transfers	Total
1987	34	24229	4383	29956	280	0	1380	4010	64272
1988	37	21660	5159	850	10	0	10727	9406	47849
1989	35	20616	4229	1524	10	0	9717	4096	40227
1990	37	20660	4759	1691	0	0	1785	6779	35711
1991	36	60745	446920	1696	0	123675	3279	6444	642795
1992	31	10778	1024	3199	0	0	1792	3147	19971
1993	29	5796	767	8719	0	750	1433	2219	19713
1994	32	5983	710	10178	0	950	1015	6259	25127

Source: TRI, 1996.

### 11.3.3.2 *Monitored Environmental Media Levels*

**Air:** Data were not found for monitored levels in air.

**Water:** Between the spring of 1988 and the winter of 1989, grab samples were collected at the clearwell effluents (after disinfection) from 35 treatment facilities and analyzed by gas chromatography/mass spectroscopy (GC/MS). The concentration of monochloroacetic acid was <1.0 to 1.2 µg/L (U.S. EPA, 1994). Chloroacetic acid was also found in a study where concentrated humic acid from a coastal North Carolina lake was chlorinated (U.S. EPA, 1994).

**Other Media:** Data were not found for monitored levels in other media.

### 11.3.3.3 *Environmental Fate and Transport*

#### 11.3.3.3.1 Summary

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of chloroacetic acid released to or into soils is biodegradation. Although no soil biodegradation studies with chloroacetic acid have been reported, studies with wastewater and river water inocula indicate that biodegradation in soil will be a relatively rapid process. This ready biodegradability should minimize the possibility of any significant leaching of chloroacetic acid into groundwater.

**Fate in the Atmosphere:** Because of its high water solubility and slow rates of photo-oxidation and photolysis, any chloroacetic acid released into the atmosphere will likely be scavenged during precipitation events before any significant photodegradation occurs.

**Fate in Aquatic Environments:** The dominant fate of chloroacetic acid released to surface waters is biodegradation (predicted half-life of days). Bioconcentration and sorption to sediments and suspended solids are not expected to be significant transport/partitioning processes.

#### 11.3.3.3.2 Transport and Partitioning

**Soil Adsorption/Mobility:** The relatively low predicted soil adsorption coefficient ( $\log K_{oc}$ ) for chloroacetic acid (0.08) indicates that adsorption to soil, sediment, and suspended solids is not a significant fate process. As a consequence, chloroacetic acid has the potential for high mobility in soil; however, the extent of migration will be minimized because of the ready biodegradability of chloroacetic acid (HSDB, 1996; U.S. EPA, 1996).

**Volatilization:** The very low predicted Henry's Law constant for chloroacetic acid ( $<10^{-7}$  atm-m<sup>3</sup>/mol) indicates that minimal volatilization is expected from water bodies. Because of its relatively low vapor pressure (<1 torr), minimal volatilization from soil surfaces is expected (HSDB, 1996; U.S. EPA, 1996).

**Bioconcentration:** A bioconcentration factor of 0.86 is predicted for chloroacetic acid based on its very low measured log octanol/water partition coefficient of 0.22. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996; U.S. EPA, 1996).

#### **11.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** Chloroacetic acid is expected to undergo ultimate biodegradation in aerobic environmental settings with a half-life on the order of days. Degradation under anaerobic conditions is expected to proceed more slowly with a predicted half-life on the order of weeks. In laboratory tests using sewage or acclimated sludge inocula, chloroacetic acid readily undergoes biodegradation with greater than 70-90 percent degradation being reported in 5-10 days. The results of river water studies indicate 73 percent mineralization (i.e., conversion to carbon dioxide) in 8-10 days (HSDB, 1996; U.S. EPA, 1996; Howard et al., 1991).

**Photodegradation:** Photolysis in the atmosphere or in aquatic environments is expected to proceed very slowly with predicted half-lives on the order of months to years. Chloroacetic acid does not appreciably absorb UV light above 290 nm and thus will not directly photolyze. The presence of sensitizers such as p-cresol and tryptophan that generate superoxide radicals has been shown to increase the rate of photodechlorination by up to 16-fold. Based on the estimated reaction rate constant of chloroacetic acid with hydroxyl radicals, the estimated half-life of chloroacetic acid in the atmosphere is on the order of weeks to months (HSDB, 1996; Howard et al., 1991).

**Hydrolysis:** Based upon the results of darkened controls during photolysis experiments, the half-life of chloroacetic acid is on the order of years (HSDB, 1996; Howard et al., 1991)

#### **11.4 HUMAN EXPOSURE AND POPULATION ESTIMATES**

Data were not found for human exposure and population estimates.

#### **11.5 CHAPTER SUMMARY**

Table 11-1 summarizes the findings of monochloroacetic acid.

**Table 11-2. Monochloroacetic Acid Summary**

	Estimates	Support
Uses	Chemical intermediate; herbicide	Well documented
Production	6.81 x 10 <sup>3</sup> kg/yr	1982 data
Releases	25,127 lbs - all media	1994 TRI data
Properties/Fate	Very soluble in water; no significant bioconcentration or biodegradation expected	
Media Levels	Air: no available data Water samples from treatment facilities - <1.0 to 1.2 ug/l	35 facilities
General Population Exposure	No available data	
Special Population Exposures	No available data	

## 12.0 DICHLOROACETIC ACID

### 12.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from IARC Monographs, Volume 63, 1995.

#### 12.1.1 Nomenclature

CAS No.: 79-43-6

Synonyms: Bichloracetic acid; DCA; CDA (acid); DCAA; dichloracetic acid; dichlorethanoic acid; dichloroethanoic acid; 2,2-dichloroethanoic acid

#### 12.1.2 Formula and Molecular Weight

Molecular Formula:  $C_2H_2Cl_2O_2$

Molecular Weight: 128.94

#### 12.1.3 Chemical and Physical Properties

Description: Colorless to slightly yellowish liquid with a pungent acid-like odor (Merck Index, 1989; Hoechst Chemicals, 1990).

Boiling Point: 194°C

Melting Point: 13.5°C

Density: 1.5634 @ 20°C/4°C

Spectroscopy Data: Infrared (prism [2806]; grating [36771]), nuclear magnetic resonance (proton [116], C-13 [500]), and mass spectral data have been reported (Sadler Research Laboratories, 1980; IARC, 1995).

Solubility: Soluble in water, acetone, ethanol, and diethyl ether; also soluble in ketones, hydrocarbons, and chlorinated hydrocarbons (IARC, 1995). In aqueous solution, dichloroacetic acid and dichloroacetate exist as an equilibrium mixture, the proportions of each depending primarily on the pH of the solution. The  $pK_a$  of dichloroacetic acid is 1.48 @ 25°C.

Volatility: Vapor Pressure - 0.19 mbar (19 Pa) @ 20°C (Hoechst Chemicals, 1990).

Vapor Density - No data.

Reactivity: Highly corrosive and attacks metals; releases hydrogen chloride gas (see IARC, 1992) when heated (Hoechst Chemicals, 1990).

Octanol/Water

Partition Coefficient: log P, 0.92 (Hansch, 1995)

#### **12.1.4 Technical Products and Impurities**

Dichloroacetic acid is available commercially at a purity of 99% with a maximum of 0.3% water (Hoechst Chemicals, 1990; Spectrum Chemical Mfg Corp., 1994)

### **12.2 PRODUCTION AND USE**

#### **12.2.1 Production**

Figures for the production and use of dichloroacetic acid in the U.S. or throughout the world are not available (IARC, 1995).

#### **12.2.2 Uses**

Dichloroacetic acid is presently of little economic importance. Its acid chloride and methyl ester, however, are used as intermediates in the manufacture of agrochemicals and the pharmaceutical, chloramphenicol (IARC, 1995). Dichloroacetic acid is also a starting material for the production of glyoxylic acid, dialkyloxy and diaryloxy acids, and sulfonamides. The compound is used as a test reagent for analytical measurements during the manufacture of polyethylene terephthalate and as a medical disinfectant, in particular as a substitute for formaldehyde (IARC, 1995). It has been considered for use in the treatment of lactic acidosis, diabetes mellitus, hyperlipoproteinaemia, and several other disorders; however, it has never been marketed for any of these purposes (Merck Index, 1989).

#### **12.2.3 Disposal**

No information concerning disposal methods for dichloroacetic acid was identified.

### **12.3 POTENTIAL FOR HUMAN EXPOSURE**

#### **12.3.1 Natural Occurrence**

Dichloroacetic acid is not known to occur as a natural product.

#### **12.3.2 Occupational**

No specific information concerning the potential for human exposure in an occupational setting was found.

### 12.3.3 Environmental

#### 12.3.3.1 Environmental Releases

No information concerning environmental releases of dichloroacetic acid was found.

#### 12.3.3.2 Monitored Environmental Media Levels

**Air:** No data available.

**Water:** Dichloroacetic acid is produced as a by-product during aqueous chlorination of humic substances and therefore it may occur in drinking water after chlorine disinfection of raw waters containing natural substances (IARC, 1995). The concentrations of dichloroacetic acid measured in various water sources and reported in various studies are summarized in Table 12-1. According to IARC (1995), it has been identified as a major chlorinated by-product of the photocatalytic degradation of tetrachloroethylene in water and a minor by-product of the degradation of trichloroethylene.

**Other Media:** In humans, dichloroacetic acid is a reactive intermediate metabolite of trichloroethylene and an end-metabolite of 1,1,1,2-tetrachloroethane. Dichloroacetic acid has also been reported as a biotransformation product of methoxyflurane (IARC, 1995) and dichlorvos (IARC, 1995). It may occur in the tissues and fluids of animals treated with dichlorvos for helminthic infections (IARC, 1995).

**Table 12-1. Concentrations of Dichloroacetic Acid in Water**

Water Type (Location)	Concentration Range (µg/L)
Drinking Water (chlorinated tap water (USA))	63.1 - 133
Drinking Water (chlorinated surface, reservoir, lake, and groundwater) (USA)	5.0 - 7.3
Chlorinated Surface Water (USA)	9.4 - 23
Chlorinated Drinking Water (USA)	8 - 79
Swimming Pool (Germany)	indoors: 0.2 - 10.6 open air: 83.5 - 181.0 <sup>a</sup>
Surface Water (downstream from a paper mill) & Austria)	<3 - 522
Biologically Treated Kraft Pulp Mill Effluent (Malaysia)	14 - 18

<sup>a</sup> The higher levels found in open-air swimming pools may be due to the input of organic material by swimmers.

Source: IARC, 1995.

### 12.3.3.3 *Environmental Fate and Transport*

No information is readily available on the environmental fate and transport of dichloroacetic acid. However, its environmental fate is expected to be similar to that of monochloroacetic acid and trichloroacetic acid. The environmental fate and transport of monochloroacetic acid and trichloroacetic acid are discussed in Sections 11.3.3.3 and 13.3.3.3, respectively.

## 12.4 HUMAN EXPOSURE AND POPULATION ESTIMATES

### 12.4.1 General U.S. Population

The general population is potentially exposed to dichloroacetic acid through the ingestion of chlorinated drinking water, contact with surface water contaminated with this chemical, and chlorinated water in swimming pools.

### 12.4.2 Occupational Exposure

The National Occupational Exposure Survey conducted between 1981 and 1983 indicated that 1,592 employees in the United States were potentially exposed to dichloroacetic acid in 39 facilities (IARC, 1995).

### 12.4.3 Consumer Exposure

Data were not found on consumer exposure to dichloroacetic acid.

## 12.5 CHAPTER SUMMARY

Table 12-2 summarizes the findings of dichloroacetic acid.

**Table 12-2. Dichloroacetic Acid Summary**

	Estimates	Support
Uses	Chemical intermediate	
Production	No available data	
Releases	No available data	
Properties/Fate	Water soluble	
Media Levels	Water: 5-133 ug/l	
General Population Exposure	No available data	
Special Population Exposures	1,592 employees potentially exposed	Data from early 1980s

## 13.0 TRICHLOROACETIC ACID

### 13.1 CHEMICAL AND PHYSICAL PROPERTIES

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 13.1.1 Nomenclature

CAS No.:	70-03-9
Synonyms:	Acetic acid; trichloro-, <TCA', trichloroethanoic acid
Trade Names:	AMCHEM Grass Killer, Nata, Natal

#### 13.1.2 Formula and Molecular Weight

Structural Formula:	$C_2HCl_3O_2$
Molecular Weight:	163.40

#### 13.1.3 Chemical and Physical Properties

Description:	Colorless to white, crystalline solid; sharp, pungent odor (NIOSH Pocket Guide Chem. Haz., 1994).
Boiling Point:	195.5°C (CRC Handbook Chem. & Physics, 76th Ed., 1995-96).
Melting Point:	-57.5°C (CRC Handbook Chem. & Physics, 76th Ed., 1995-96).
Density:	1.6126 @ 64°C (CRC Handbook Chem. & Physics, 76th Ed., 1995-96).
Spectroscopy Data:	Index of refraction: 1.4603 @ 61°C (CRC Handbook Chem. & Physics, 76th Ed., 1995-96); IR: 2376 (Coblentz Society Spectral Collection); UV: 1-6 (Organic Electronic Spectral Data); NMR: 6 (Sadler Research Laboratories Spectral Collection); Mass: 1026 (Atlas of Mass Spectral Data) (Weast, CRC Handbook Data Organic CPDS, Vol. I, II, 1985).
Solubility:	In water - 1306 g/100 g @ 25°C; in methanol - 2143 g/100 g @ 25°C; in ethyl ether - 617 g/100 g @ 25°C; in acetone - 850 g/100 g @ 25°C; in benzene - 201 g/100 g @ 25°C in o-xylene - 110 g/100 g @ 25°C (Kirk-Othmer. Encyc. Chem. Tech., 4th Ed., Vol. 1, 1991-present); soluble in ethanol, ethyl ether;

slightly soluble in carbon tetrachloride (CRC Handbook Chem. & Physics, 76th Ed., 1995-96).

- Volatility: Vapor Pressure - 1 mm Hg @ 51.0°C (solid) (CRC Handbook Chem. & Physics, 72nd Ed., 1991-1992).
- Stability: Stable in the absence of moisture (Pesticide Manual, 8th Ed., 1987); 2-year shelf life minimum, may cake however (Herbicide Hdbk, 5th Ed., 1983).
- Reactivity: Reacts with moisture, iron, zinc, aluminum, strong oxidizers (Note: decomposes on heating to form phosgene and hydrogen chloride. Corrosive to metals.) (NIOSH Pocket Guide Chem. Haz., 1994).

Octanol/Water  
Partition Coefficient: No data.

#### 13.1.4 Technical Products and Impurities

Trichloroacetic acid is produced in a technical grade (chemically pure: a grade designation signifying a minimum of impurities, but not 100% purity) and a USP grade (Hawley's Condensed Chem. Dict., 12th Ed., 1993).

### 13.2 PRODUCTION AND USE

The information/data presented in this section and the supporting references were obtained from a retrieval from the Hazardous Substances Data Bank (HSDB, 1996).

#### 13.2.1 Production

- U.S. Production: (1975) greater than  $3.60 \times 10^6$  g; (1976) greater than  $2.27 \times 10^6$  g (SRI).
- Import Volumes: (1984)  $3.67 \times 10^9$  g/chloroacetic acid (Bureau of the Census. U.S. Imports for Consumption and General imports, 1984).
- Export Volumes: (1984)  $8.60 \times 10^9$  g (Halogenated Hydrocarbons, Bureau of the Census. U.S. Exports, 1984).

#### 13.2.2 Uses

Trichloroacetic acid is used as a chemical intermediate for the production of ethylene glycol bis(trichloroacetate) and herbicides, sodium trichloroacetate and monuron-TCA; and used as a lab reagent for biological applications (SRI). TCA has been used as an astringent and antiseptic, and polymerization catalyst (Kirk-Othmer. Encyc. Chem. Tech., 4th Ed., Vol. 1,

1991-present). About 21,000-23,000 t/a of the TCA sodium salt are used worldwide as a selective herbicide (Ullmann's Encyc. Indust. Chem., 5th Ed., 1985-present).

### **13.2.3 Disposal**

Reverse osmosis is a wastewater treatment technology that has been investigated for trichloroacetic acid (USEPA, 1982, Management of Hazardous Waste Leachate). After mixing, transfer into a drum and fill with water for drainage after 24 hours (Tox. & Hazard. Indus. Chem. Safety Manual, 1988).

At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices (HSDB Scientific Review Panel; HSDB, 1996).

## **13.3 POTENTIAL FOR HUMAN EXPOSURE**

### **13.3.1 Natural Occurrence**

Trichloroacetic acid is not known to occur naturally (IARC, 1995).

### **13.3.2 Occupational**

The probable routes of occupational exposure are dermal contact and inhalation. Trichloroacetic acid is the major end metabolite of trichloroethylene and tetrachloroethylene in humans and has been used as a biological marker of exposure to these compounds (IARC, 1995). Additionally, it is a metabolite of 1,1,1-trichloroethane and 1,1,1,2-tetrachloroethane and chloral hydrate is rapidly oxidized to trichloroacetic acid in humans (IARC, 1995).

### **13.3.3 Environmental**

#### **13.3.3.1 Environmental Releases**

The production of trichloroacetic acid and its use in organic synthesis, medicine, pharmaceuticals, and as a herbicide may result in its release to the environment through wastestreams (HSDB, 1996).

#### **13.3.3.2 Monitored Environmental Media Levels**

**Air:** No data.

**Water:** The concentrations of trichloroacetic acid in water are presented in Table 13-1.

**Other Media:** Trichloroacetic acid has been detected in the following foods (IARC, 1995):

**Table 13-1. Concentrations of Trichloroacetic Acid in Water**

Water Type (Location)	Concentration Range (µg/L)
Chlorinated Tap Water (USA) (drinking water)	33.6 - 161
Chlorinated Drinking Water (USA)	4.23 - 53.8
Raw Water (USA)	95 - 2,120
Chlorinated Surface, Reservoir, Lake, and Groundwaters (USA)	4.0 - 6.0
Chlorinated Surface Water (USA)	7.4 - 22
Chlorinated Drinking Water (USA)	15 - 64
Raw Water (USA)	60 - 1,630

Source: IARC, 1995.

- Seed of wheat, barley, and oats after treatment with trichloroacetic acid as postemergent herbicide;
- Fruits and vegetables after irrigation with trichloroacetic acid contaminated water (trace levels); and
- Field bean pods and seeds (0.13 to 0.43 mg/kg)

Concentration of trichloroacetic acid was in irrigation water after the application of the sodium salt (herbicide) to control canary grass on the banks of dry canals in the State of Washington. The levels measured ranged from 53 to 297 ppb (HSDB, 1996).

### 13.3.3.3 *Environmental Fate and Transport*

#### 13.3.3.3.1 Summary

The summary is based on the data presented in the subsequent fate and transport subsections.

**Fate in Terrestrial Environments:** The dominant fate of trichloroacetic acid released onto or into soils is biodegradation. Studies with wastewater and soil indicate that aerobic biodegradation in soil will occur within weeks to months depending on the soil type, moisture and temperature. However, the low reported  $K_{oc}$  for trichloroacetic acid indicates that trichloroacetic acid should have high mobility in soil and, therefore, significant leaching to groundwater could occur, particularly in sandy soils.

**Fate in the Atmosphere:** Because of its moderate vapor pressure (<1 mm Hg at 25 degrees C), trichloroacetic acid should exist predominantly in the vapor phase in the atmosphere. Vapor phase trichloroacetic acid is degraded in the atmosphere by reaction with photochemically produced hydroxyl radicals; the half-life for this reaction is estimated to be about 31 days.

**Fate in Aquatic Environments:** The dominant fate of trichloroacetic acid released into surface waters is biodegradation (predicted weeks to months). Bioconcentration, sorption to sediments and suspended solids, and volatilization are not expected to be significant transport/partitioning processes.

#### **13.3.3.3.2 Transport and Partitioning**

**Soil Adsorption/Mobility:** The relatively low predicted soil adsorption coefficient ( $K_{oc} = 1$ ) for trichloroacetic acid indicates that adsorption to soil, sediment, and suspended solids is not a significant fate process. Several laboratory and field soil studies confirm that trichloroacetic acid shows little sorption to soils. As a consequence, trichloroacetic acid has the potential for high mobility in soil (HSDB, 1996).

**Volatilization:** The very low predicted Henry's Law constant for trichloroacetic acid ( $<10^{-7}$  atm-m<sup>3</sup>/mol) indicates that minimal volatilization is expected from water bodies. Because of its relatively low vapor pressure ( $<1$  mm Hg), minimal volatilization from soil surfaces is expected (HSDB, 1996).

**Bioconcentration:** Bioconcentration factors measured in carp range from 0.4 to 1.7. Therefore, bioconcentration in aquatic organisms should not be significant and there is little potential for biomagnification in the food chain (HSDB, 1996).

#### **13.3.3.3.3 Transformation and Degradation Processes**

**Biodegradation:** Trichloroacetic acid has been demonstrated to be undergo biodegradation under aerobic conditions in soil and in laboratory tests with activated sludge inocula (half-lives on the order of weeks to months). However, a noticeable lag period was observed (i.e., a period in which slow degradation was followed by rapid degradation). Degradation appears to be favored by warm moist conditions conducive to high microbiological activity (HSDB, 1996).

**Photodegradation:** Based on the estimated reaction rate constant of trichloroacetic acid with hydroxyl radicals, the estimated half-life of trichloroacetic acid in the atmosphere is about 31 days. No information is available on the photolysis of trichloroacetic acid. However, monochloroacetic acid does not appreciably absorb UV light above 290 nm and thus will not directly photolyze; the presence of sensitizers such as p-cresol and tryptophan that generate superoxide radicals has been shown to increase the rate of photodechlorination by up to 16-fold (HSDB, 1996; Howard et al., 1991).

**Hydrolysis:** No information is available on the hydrolytic half-life of trichloroacetic acid. However, the hydrolytic half-life of monochloroacetic acid is on the order of years based on the results of darkened controls during photolysis experiments (HSDB, 1996; Howard et al., 1991)

## 13.4 HUMAN EXPOSURE AND POPULATION ESTIMATES

### 13.4.1 General U.S. Population

Based on available data, the general population could be potentially exposed to trichloroacetic acid through ingestion of drinking water and foods contaminated with this chemical.

### 13.4.2 Occupational Exposure

Estimates from a NIOSH survey conducted between 1981 and 1983 show that 35,124 employees in the U.S. were potentially exposed occupationally to trichloroacetic acid (IARC, 1995). This potentially exposed population were employees in seven different industries and 1,562 plants (IARC, 1995).

Trichloroacetic acid (3-116 mg/g creatinine) was found in the urine of employees in the metal degreasing industry. These employees were exposed to trichloroethylene (HSDB, 1996).

### 13.4.3 Consumer Exposure

Data were not found for consumer exposures.

## 13.5 CHAPTER SUMMARY

Table 13-2 summarizes the findings of trichloroacetic acid.

**Table 13-2. Trichloroacetic Acid Summary**

	Estimates	Support
Uses	Chemical intermediate; herbicide	Well documented data
Production	More than 2,270 kg	1976 data
Releases	No available data	
Properties/Fate	Water soluble; no significant bioconcentration is expected	
Media Levels	Air: no data Drinking water: 4.2 to 161 ug/l Raw water: 60 to 1,630 ug/l	
General Population Exposure		
Special Population	35,124 employees potentially	Data from early 1980s

#### **14.0 DICHLORO-VINYL CYSTEINE**

No information is readily available for this chemical.

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