



Candidate Contaminant List Regulatory Determination Support Document for Hexachlorobutadiene

**Contaminant Candidate List
Regulatory Determination Support Document
for Hexachlorobutadiene**

U.S. Environmental Protection Agency
Office of Water (4607M)
Standards and Risk Management Division
Washington, DC 20460

<http://www.epa.gov/SAFEWATER/ccl/cclregdetermine.html>

EPA-815-R-03-11
July 2003

Disclaimer

This document is designed to provide supporting information regarding the regulatory determinations for hexachlorobutadiene as part of the Contaminant Candidate List (CCL) evaluation process. This document is not a regulation, and it does not substitute for the Safe Drinking Water Act (SDWA) or the Environmental Protection Agency's (EPA's) regulations. Thus, it cannot impose legally-binding requirements on EPA, States, or the regulated community, and may not apply to a particular situation based upon the circumstances. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

ACKNOWLEDGMENTS

This document was prepared in support of the EPA's Office of Ground Water and Drinking Water regulatory determination for hexachlorobutadiene as part of the Contaminant Candidate List (CCL) evaluation process. Karen Wirth and Tom Carpenter served as EPA's Co-Team Leaders for the CCL regulatory determination process and Ephraim King as Standards and Risk Management Division Director. Harriet Colbert served as Work Assignment Manager. The CCL Work Group provided technical guidance throughout. In particular, Karen Wirth, Dan Olson, and Joyce Donohue provided scientific and editorial guidance. External expert reviewers and many stakeholders provided valuable advice to improve the CCL Program and this document. The Cadmus Group, Inc., served as the primary contractor providing support for this work. The major contributions of Matt Collins, Emily Brott, Ashton Koo, Richard Zeroka, and Brent Ranalli are gratefully acknowledged. George Hallberg served as Cadmus' Project Manager.

This page intentionally left blank.

USEPA, Office of Water Report: EPA 815-R-03-011, July 2003

**CONTAMINANT CANDIDATE LIST
REGULATORY DETERMINATION SUPPORT DOCUMENT
FOR HEXACHLOROBUTADIENE**

EXECUTIVE SUMMARY

Hexachlorobutadiene was a 1998 Contaminant Candidate List (CCL) regulatory determination priority contaminant. Hexachlorobutadiene was one of the contaminants considered by EPA for a regulatory determination. The available data on occurrence, exposure, and other risk considerations suggest that regulating hexachlorobutadiene may not present a meaningful opportunity to reduce health risk. EPA presented preliminary CCL regulatory determinations and further analysis in the June 3, 2002 *Federal Register* Notice (USEPA, 2002a; 67 FR 38222), and confirmed the final CCL regulatory determinations in the July 18, 2003 *Federal Register* Notice (USEPA, 2003a; 68 FR 42898).

To make this regulatory determination for hexachlorobutadiene, EPA used approaches guided by the National Drinking Water Advisory Council's (NDWAC) Work Group on CCL and Six-Year Review. The Safe Drinking Water Act (SDWA) requirements for National Primary Drinking Water Regulation (NPDWR) promulgation guided protocol development. The SDWA Section 1412(b)(1)(A) specifies that the determination to regulate a contaminant must be based on a finding that each of the following criteria are met: (i) "the contaminant may have adverse effects on the health of persons"; (ii) "the contaminant is known to occur or there is substantial likelihood that the contaminant will occur in public water systems with a frequency and at levels of public health concern"; and (iii) "in the sole judgement of the Administrator, regulation of such contaminant presents a meaningful opportunity for health risk reduction for persons served by public water systems." Available data were evaluated to address each of the three statutory criteria.

Hexachlorobutadiene is a volatile organic compound (VOC) not known to naturally occur. It is commonly used as a solvent and in the production of rubber compounds (ATSDR, 1995; see Section 2.0). Hexachlorobutadiene is not specifically manufactured as a commercial product in the United States, but significant quantities of the chemical are generated here as a waste by-product from the chlorination of hydrocarbons. It is also imported for use as a chemical intermediate in some manufacturing processes and as a component of a number of commercial products. Its use in these products, such as transformer and hydraulic fluids, gyroscope fluids, heat transfer liquids, solvents, and laboratory reagents, is widespread.

Hexachlorobutadiene was monitored from 1987 to 1999 under the SDWA Unregulated Contaminant Monitoring (UCM) program. Hexachlorobutadiene is also monitored or regulated by other federal programs including the Clean Water Act Priority Pollutants list, the Clean Air Act Hazardous Air Pollutant list, the Comprehensive Environmental Response, Compensation, and Liability

Act (CERCLA), the Resource Conservation and Recovery Act (RCRA), and the Toxic Release Inventory (TRI).

Because of concerns about human health risk, EPA issued a drinking water health advisory (HA) for hexachlorobutadiene in 1989 at 1 µg/L. Other federal agencies and organizations have issued recommendations for occupational exposure.

The United States Geological Survey's (USGS) National Water Quality Assessment (NAWQA) program studies to date have reported no detections of hexachlorobutadiene in ambient water. However, releases of hexachlorobutadiene to the environment reported through the Toxic Release Inventory (TRI), and its occurrence in site samples recorded in the Agency for Toxic Substances and Disease Registry's (ATSDR) Hazardous Substance Release and Health Effects Database (HazDat) and at CERCLA National Priorities List (NPL) hazardous waste sites, provides evidence for the widespread use and environmental release of hexachlorobutadiene.

Hexachlorobutadiene has also been detected in PWS samples collected under SDWA. Occurrence estimates are low for both rounds of UCM monitoring with less than 0.2% of all samples showing detections. Significantly, the values for the 99th percentile and median concentrations of all samples are less than the Minimum Reporting Level. Systems with detections only constitute 0.350% of Round 1 systems and 0.180% for Round 2. Detections greater than the Health Reference Level (HRL) of 0.9 µg/L are less: 0.114% and 0.018% of Round 1 and Round 2 systems, respectively. National estimates for the population served by PWSs with detections are also low, especially for detections greater than the HRL. For both rounds, these estimates are less than 0.5% of the national PWS population.

The available toxicological data indicate that HCBBD has the potential to cause adverse health effects in animals. In particular, the primary target organ for HCBBD is the kidney. Data on human health effects, however, are limited to a few studies of occupational exposure to HCBBD. These data, collected from inhalation exposure, are often confounded by simultaneous exposures to other chemicals in an occupational setting. Such equivocal data has made it difficult to establish a relationship between HCBBD exposure and toxic/cytogenetic effects in human. Hexachlorobutadiene is classified as a possible human carcinogen.

Monitoring data indicate that hexachlorobutadiene is infrequently detected in public water supplies. In addition to the fact that these detections are low, it is important to note that when hexachlorobutadiene is detected, it very rarely exceeds the HRL or a value of one-half the HRL. For example, under Round 2 monitoring, the 20-State cross-section analysis shows that only 4 out of 22,736 of the reporting PWSs had detections above the HRL. Therefore regulation of hexachlorobutadiene is unlikely to represent a meaningful opportunity for health risk reduction.

TABLE OF CONTENTS

ACKNOWLEDGMENTS	i
EXECUTIVE SUMMARY	iii
TABLE OF CONTENTS	v
LIST OF TABLES	vii
LIST OF FIGURES	ix
1.0 INTRODUCTION	1
1.1 Purpose and Scope	1
1.2 Statutory Framework/Background	1
1.3 Statutory History of Hexachlorobutadiene	2
1.4 Regulatory Determination Process	3
1.5 Determination Outcome	4
2.0 CONTAMINANT DEFINITION	5
2.1 Physical and Chemical Properties	5
2.2 Environmental Fate/Behavior	5
3.0 OCCURRENCE AND EXPOSURE	5
3.1 Use and Environmental Release	6
3.1.1 Production and Use	6
3.1.2 Environmental Release	7
3.2 Ambient Occurrence	8
3.2.1 Data Sources and Methods	8
3.2.2 Results	9
3.3 Drinking Water Occurrence	10
3.3.1 Data Sources, Data Quality, and Analytical Approach	10
3.3.1.1 UCM Rounds 1 and 2	11
3.3.1.2 Developing a Nationally Representative Perspective	11
3.3.1.2.1 Cross-Section Development	12
3.3.1.2.2 Cross-Section Evaluation	13
3.3.1.3 Data Management and Analysis	14
3.3.1.4 Occurrence Analysis	15
3.3.2 Results	18
3.3.2.1 Occurrence Estimates	18
3.3.2.2 Regional Patterns	20
3.4 Conclusion	24

4.0 HEALTH EFFECTS	24
4.1 Hazard Characterization and Mode of Action Implications	24
4.2 Dose-Response Characterization and Implications in Risk Assessment	28
4.3 Relative Source Contribution	30
4.4 Sensitive Populations	30
4.5 Exposure and Risk Information	32
4.6 Conclusion	32
5.0 TECHNOLOGY ASSESSMENT	32
5.1 Analytical Methods	32
5.2 Treatment Technology	33
6.0 SUMMARY AND CONCLUSIONS - DETERMINATION OUTCOME	34
REFERENCES	37
APPENDIX A: Abbreviations and Acronyms	43

LIST OF TABLES

Table 2-1: Physical and chemical properties 6
Table 3-1: Environmental releases (in pounds) for hexachlorobutadiene in the United States, 1988-
1998 8
Table 3-2: Cross-section States for Round 1 (24 States) and Round 2 (20 States) 14
Table 3-3: Summary occurrence statistics for hexachlorobutadiene 22

This page intentionally left blank.

LIST OF FIGURES

Figure 3-1: Geographic distribution of cross-section States for Round 1 (top) and Round 2 (bottom) 17

Figure 3-2: States with PWSs with detections of hexachlorobutadiene for all States with data in URCIS (Round 1) and SDWIS/FED (Round 2) 25

Figure 3-3: States with PWSs with detections of hexachlorobutadiene (any PWSs with results greater than the Minimum Reporting Level [MRL]) for Round 1 (above) and Round 2 (below) cross-section States 26

Figure 3-4: Cross-section States (Round 1 and Round 2 combined) with PWSs with detections of hexachlorobutadiene (above) and concentrations greater than the Health Reference Level (below) 27

This page intentionally left blank.

1.0 INTRODUCTION

1.1 Purpose and Scope

This document presents scientific data and summaries of technical information prepared for and used in the Environmental Protection Agency's (EPA) regulatory determination for hexachlorobutadiene. Information regarding hexachlorobutadiene's physical and chemical properties, environmental fate, occurrence and exposure, and health effects is included. Analytical methods and treatment technologies are also discussed. Furthermore, the regulatory determination process is described to provide the rationale for the decision.

1.2 Statutory Framework/Background

The Safe Drinking Water Act (SDWA), as amended in 1996, requires the United States Environmental Protection Agency (USEPA) to publish a list of contaminants (referred to as the Contaminant Candidate List, or CCL) to assist in priority-setting efforts. The contaminants included on the CCL were not subject to any current or proposed National Primary Drinking Water Regulations (NPDWR), were known or anticipated to occur in public water systems, and were known or suspected to adversely affect public health. These contaminants therefore may require regulation under SDWA. The first Drinking Water CCL was published on March 2, 1998 (USEPA, 1998a; 63 FR 10273), and a new CCL must be published every five years thereafter.

The 1998 CCL contains 60 contaminants, including 50 chemicals or chemical groups, and 10 microbiological contaminants or microbial groups. The SDWA also requires the Agency to select 5 or more contaminants from the current CCL and determine whether or not to regulate these contaminants with an NPDWR. Regulatory determinations for at least 5 contaminants must be completed 3½ years after each new CCL.

Language in SDWA Section 1412(b)(1)(A) specifies that the determination to regulate a contaminant must be based on a finding that each of the following criteria are met:

Statutory Finding i: the contaminant may have adverse effects on the health of persons;

Statutory Finding ii: the contaminant is known to occur or there is substantial likelihood that the contaminant will occur in public water systems with a frequency and at levels of public health concern; and

Statutory Finding iii: in the sole judgement of the Administrator, regulation of such contaminant presents a meaningful opportunity for health risk reduction for persons served by public water systems.

The geographic distribution of the contaminant is another factor evaluated to determine whether it occurs at the national, regional or local level. This consideration is important because the Agency is

charged with developing national regulations and it may not be appropriate to develop NPDWRs for regional or local contamination problems.

EPA must determine if regulating this CCL contaminant will present a meaningful opportunity to reduce health risk based on contaminant occurrence, exposure, and other risk considerations. The Office of Ground Water and Drinking Water (OGWDW) is charged with gathering and analyzing the occurrence, exposure, and risk information necessary to support this regulatory decision. The OGWDW must evaluate when and where this contaminant occurs, and what would be the exposure and risk to public health. EPA must evaluate the impact of potential regulations as well as determine the appropriate measure(s) for protecting public health.

For each of the regulatory determination contaminants, EPA first publishes in the *Federal Register* the draft determinations for public comment. EPA responds to the public comments received, and then finalizes regulatory determinations. If the Agency finds that regulations are warranted, the regulations must then be formally proposed within 24, and promulgated 18 months later. EPA has determined that there is sufficient information to support a regulatory determination for hexachlorobutadiene.

1.3 Statutory History of Hexachlorobutadiene

Hexachlorobutadiene has been monitored under the SDWA Unregulated Contaminant Monitoring (UCM) program since 1987. It was among 14 VOCs included for discretionary monitoring (USEPA, 1987; 52 FR 25690). Monitoring for hexachlorobutadiene under UCM continued throughout the 1990s, but ceased for small public water systems (PWSs) under a direct final rule published January 8, 1999 (USEPA, 1999a; 64 FR 1494). Monitoring ended for large PWSs with promulgation of the new Unregulated Contaminant Monitoring Regulation (UCMR) issued September 17, 1999 (USEPA, 1999b; 64 FR 50556) and effective January 1, 2001. At the time the UCMR lists were developed, the Agency concluded there were adequate monitoring data for a regulatory determination. This obviated the need for continued monitoring under the new UCMR list.

EPA previously recommended guidelines for exposure to hexachlorobutadiene in drinking water through a health advisory (USEPA, 1989; ATSDR, 1995). As part of the CCL process, health effects data have been reviewed. These are summarized in Section 4.0 of this document.

Hexachlorobutadiene is regulated or monitored by other federal programs as well. It is included on the Clean Water Act Priority Pollutants list for which EPA establishes ambient water quality criteria. It is also listed as a Hazardous Air Pollutant under the Clean Air Act and subject to Best Available Control Technology limits. Both the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA or "Superfund") and the Resource Conservation and Recovery Act (RCRA) include it as a hazardous substance and a hazardous constituent, respectively. CERCLA's listing requires reporting of releases over a certain "reportable quantity" which, for hexachlorobutadiene, is one pound (ATSDR, 1995). Also, hexachlorobutadiene is a Toxic Release Inventory (TRI) chemical. The TRI was established by the Emergency Planning and Community Right-to-Know Act (EPCRA).

EPCRA requires certain industrial sectors to publically report the environmental release or transfer of chemicals included in this inventory (USEPA, 2000d).

Finally, the National Institute for Occupational Safety and Health (NIOSH) recommends an occupational exposure limit of 0.02 parts hexachlorobutadiene per million in air (0.02 ppm) for an 8-hour workday over a 40-hour workweek. The American Conference of Governmental Industrial Hygienists (ACGIH) makes the same workplace recommendations (ATSDR, 1995).

1.4 Regulatory Determination Process

In developing a process for the regulatory determinations, EPA sought input from experts and stakeholders. EPA asked the National Research Council (NRC) for assistance in developing a scientifically sound approach for deciding whether or not to regulate contaminants on the current and future CCLs. The NRC's Committee on Drinking Water Contaminants recommended that EPA: (1) gather and analyze health effects, exposure, treatment, and analytical methods data for each contaminant; (2) conduct a preliminary risk assessment for each contaminant based on the available data; and (3) issue a decision document for each contaminant describing the outcome of the preliminary risk assessment. The NRC noted that in using this decision framework, EPA should keep in mind the importance of involving all interested parties.

One of the formal means by which EPA works with its stakeholders is through the National Drinking Water Advisory Council (NDWAC). The NDWAC comprises members of the general public, State and local agencies, and private groups concerned with safe drinking water, and advises the EPA Administrator on key aspects of the Agency's drinking water program. The NDWAC provided specific recommendations to EPA on a protocol to assist the Agency in making regulatory determinations for current and future CCL contaminants. Separate but similar protocols were developed for chemical and microbial contaminants. These protocols are intended to provide a consistent approach to evaluating contaminants for regulatory determination, and to be a tool that will organize information in a manner that will communicate the rationale for each determination to stakeholders. The possible outcomes of the regulatory determination process are: a decision to regulate, a decision not to regulate, or a decision that some other action is needed (e.g., issuance of guidance).

The NDWAC protocol uses the three statutory requirements of SDWA Section 1412(b)(1)(A)(i)-(iii) (specified in section 1.2) as the foundation for guiding EPA in making regulatory determination decisions. For each statutory requirement, evaluation criteria were developed and are summarized below.

To address whether a contaminant may have adverse effects on the health of persons (statutory requirement (i)), the NDWAC recommended that EPA characterize the health risk and estimate a health reference level for evaluating the occurrence data for each contaminant.

Regarding whether a contaminant is known to occur, or whether there is substantial likelihood that the contaminant will occur, in public water systems with a frequency, and at levels, of public health concern (statutory requirement (ii)), the NDWAC recommended that EPA consider: (1) the actual and estimated national percent of public water systems (PWSs) reporting detections above half the health reference level; (2) the actual and estimated national percent of PWSs with detections above the health reference level; and (3) the geographic distribution of the contaminant.

To address whether regulation of a contaminant presents a meaningful opportunity for health risk reduction for persons served by public water systems (statutory requirement (iii)) the NDWAC recommended that EPA consider estimating the national population exposed above half the health reference level and the national population exposed above the health reference level.

The approach EPA used to make regulatory determinations followed the general format recommended by the NRC and the NDWAC to satisfy the three SDWA requirements under section 1412(b)(1)(A)(i)-(iii). The process was independent of many of the more detailed and comprehensive risk management factors that will influence the ultimate regulatory decision making process. Thus, a decision to regulate is the beginning of the Agency regulatory development process, not the end.

Specifically, EPA characterized the human health effects that may result from exposure to a contaminant found in drinking water. Based on this characterization, the Agency estimated a health reference level (HRL) for each contaminant.

For each contaminant EPA estimated the number of PWSs with detections $>1/2$ HRL and $>$ HRL, the population served at these benchmark values, and the geographic distribution, using a large number of occurrence data (approximately seven million analytical points) that broadly reflect national coverage. Round 1 and Round 2 UCM data, evaluated for quality, completeness, bias, and representativeness, were the primary data used to develop national occurrence estimates. Use and environmental release information, additional drinking water data sets (e.g., State drinking water data sets, EPA National Pesticide Survey, and Environmental Working Group data reviews), and ambient water quality data (e.g., NAWQA, State and regional studies, and the EPA Pesticides in Ground Water Database) were also consulted.

The findings from these evaluations were used to determine if there was adequate information to evaluate the three SDWA statutory requirements and to make a determination of whether to regulate a contaminant.

1.5 Determination Outcome

After reviewing the best available public health and occurrence information, EPA has made a determination not to regulate hexachlorobutadiene with an NPDWR. EPA's determination is based on the finding that hexachlorobutadiene is not known to occur at levels of public health concern. All CCL regulatory determinations and further analysis are formally presented in the *Federal Register* Notices

(USEPA, 2002a; 67 FR 38222; and USEPA, 2003a; 68 FR 42898). The following sections summarize the data used by the Agency to reach its decision.

2.0 CONTAMINANT DEFINITION

Hexachlorobutadiene, a volatile organic compound (VOC) also known as perchlorobutadiene, is a colorless liquid with a turpentine-like odor. It is not known to naturally occur, but instead forms in the production of other chemicals (ATSDR, 1995). It is commonly used as a solvent and in the production of rubber compounds. Hexachlorobutadiene is also used as hydraulic and transformer fluid, a heat transfer liquid, a pesticide, in gyroscopes, and in the production of lubricants (ATSDR, 1995; USEPA, 1989; Howard, 1989).

2.1 Physical and Chemical Properties

Table 2-1 lists summary information regarding hexachlorobutadiene's physical and chemical properties. Also included are its CAS Registry Number and molecular formula.

2.2 Environmental Fate/Behavior

When hexachlorobutadiene is released to the environment, it is expected to volatilize quickly. Its vapor pressure indicates that it will probably evaporate from surfaces, with the lowest evaporation rate from soils because of its relatively high $\log K_{oc}$ value (indicating its strong sorption potential). Its half life in surface water ranges from 3-300 days, with a longer atmospheric half life that can be greater than a year (Howard, 1989).

With a relatively high $\log K_{oc}$, it has a strong sorption potential and therefore will not rapidly migrate through the soil, though there is evidence it will leach through sandy soils. In the unsaturated zone, it may biodegrade. However, based on laboratory tests, hexachlorobutadiene under anaerobic conditions will probably not biodegrade (Howard, 1989).

Hexachlorobutadiene's high Henry's Law constant suggests it will quickly volatilize from water. But because of its high K_{oc} , volatilization may be decreased because of adsorption to bed sediments, suspended sediments, and biota. Volatilization will be quicker from turbulent streams when compared with lakes. Hexachlorobutadiene may biodegrade in natural waters (Howard, 1989).

3.0 OCCURRENCE AND EXPOSURE

This section examines the occurrence of hexachlorobutadiene in drinking water. While no complete national database exists of unregulated or regulated contaminants in drinking water from public water systems (PWSs) collected under SDWA, this report aggregates and analyzes existing State data that have been screened for quality, completeness, and representativeness. Populations served by PWSs exposed to hexachlorobutadiene are estimated, and the occurrence data are examined for regional or

other special trends. To augment the incomplete national drinking water data and aid in the evaluation of occurrence, information on the use and environmental release, as well as ambient occurrence of hexachlorobutadiene, is also reviewed.

3.1 Use and Environmental Release

3.1.1 Production and Use

Hexachlorobutadiene has never been specifically manufactured as a commercial product in the United States. However, significant quantities of the chemical are generated in the U.S. as waste by-product from the chlorination of hydrocarbons, and lesser quantities are imported

Table 2-1: Physical and chemical properties

Identification	
CAS number	87-68-3
Molecular Formula	C ₄ Cl ₆
Physical and Chemical Properties	
Boiling Point	215 °C
Melting Point	- 21 °C
Molecular Weight	260.76 g/mol
Log K _{oc}	3.67
Log K _{ow}	4.78
Water Solubility	2 - 2.55 mg/L at 20 °C
Vapor Pressure	0.15 mm Hg at 25 °C
Henry's Law Constant †	0.04 - 1.1

after ATSDR, 1994

† note: this quantity is expressed in a dimensionless form.

mostly from Germany as commercial product. Hexachlorobutadiene is used as an intermediate product in rubber manufacturing and chlorofluorocarbon and lubricant production, as well as for transformer and hydraulic fluids, fluid for gyroscopes, heat transfer liquid, solvents, laboratory reagents, and as a wash liquor for removing C₄ and higher hydrocarbons. The chemical is also used as a fumigant in Russia, France, Italy, Greece, Spain, and Argentina (ATSDR, 1995; Howard, 1989).

Eight million pounds of hexachlorobutadiene were generated as a waste by-product in the U.S. in 1975, with 0.1 million pounds released into the environment. By 1982, the annual U.S. by-product generation of the chemical had jumped to 27 million pounds. In contrast, the annual import rate of hexachlorobutadiene dropped from 500,000 lbs/yr imported annually in the late 70's, to 145,000 lbs/yr imported in 1981 (ATSDR, 1994; Howard, 1989).

3.1.2 Environmental Release

Hexachlorobutadiene is listed as a toxic release inventory (TRI) chemical. In 1986, the Emergency Planning and Community Right-to-Know Act (EPCRA) established the Toxic Release Inventory (TRI) of hazardous chemicals. Created under the Superfund Amendments and Reauthorization Act (SARA) of 1986, EPCRA is also sometimes known as SARA Title III. The EPCRA mandates that larger facilities publicly report when TRI chemicals are released into the environment. This public reporting is required for facilities with more than 10 full-time employees that annually manufacture or produce more than 25,000 pounds, or use more than 10,000 pounds, of TRI chemical (USEPA, 1996; USEPA, 2000d).

Under these conditions, facilities are required to report the pounds per year of hexachlorobutadiene released into the environment both on- and off-site. The on-site quantity is subdivided into air emissions, surface water discharges, underground injections, and releases to land (see Table 3-1). For hexachlorobutadiene, air emissions constitute most of the on-site releases. Also, over the period for which data is available (1988-1998) surface water discharges generally increased, peaked in 1992-93, and then decreased significantly through the late 1990s. These TRI data for hexachlorobutadiene were reported from eight States (CA, IL, KS, LA, NJ, NY, TX, UT); however, hexachlorobutadiene contamination has often been found in remote areas far from apparent physical discharge sources (USEPA, 2000b; Howard, 1989).

Although the TRI data can be useful in giving a general idea of release trends, it is far from exhaustive and has significant limitations. For example, only industries which meet TRI criteria (at least 10 full-time employees and manufacture and processing of quantities exceeding 25,000 lbs/yr, or use of more than 10,000 lbs/yr) are required to report releases. These reporting criteria do not account for releases from smaller industries. Threshold manufacture and processing quantities also changed from 1988-1990 (dropping from 75,000 lbs/yr in 1988 to 50,000 lbs/yr in 1989 to its current 25,000 lbs/yr in 1990) creating possibly misleading data trends. Finally, the TRI data is meant to reflect releases and should not be used to estimate general exposure to a chemical (USEPA, 2000c; USEPA, 2000a).

While TRI releases were reported in only eight States, the use of hexachlorobutadiene is widespread. It is included in the Agency for Toxic Substances and Disease Registry's (ATSDR) Hazardous Substance Release and Health Effects Database (HazDat) and has been detected in site samples in fourteen States (AL, AZ, CT, IA, LA, MI, MN, NJ, NY, OH, PA, RI, SC, WA; ATSDR, 2000). These States are distributed nationwide and include 11 States, and two regions (New England and the Pacific Northwest), not reporting TRI releases yet manifesting hexachlorobutadiene detections in the environment.

The National Priorities List (NPL) of hazardous waste sites, created in 1980 by CERCLA, is a listing of some of the most health-threatening waste sites in the United States. Hexachlorobutadiene was detected in eleven of the Final NPL sites in 1999. These sites are located in eight States: AK, CO, IN, LA, NJ, OH, PA, WA. Again, note there is little overlap between these States and the eight TRI reporting States (USEPA, 1999c).

In summary, although hexachlorobutadiene is not manufactured in the United States, both its use in industry and occurrence in the environment are widespread. Significant quantities of hexachlorobutadiene are generated in the United States as a waste by-product, and smaller quantities are imported for industrial needs. Hexachlorobutadiene is present in hazardous waste sites in at least 8 States (at NPL sites), has been detected in site samples in at least 14 States (listed in ATSDR's HazDat), and has been released into the environment directly in at least 8 States (based on TRI data).

Table 3-1: Environmental releases (in pounds) for hexachlorobutadiene in the United States, 1988-1998

Year	On-Site Releases				Off-Site Releases	Total On- & Off-site Releases
	Air Emissions	Surface Water Discharges	Underground Injection	Releases to Land		
1998	2,421	5	0	0	510	2,936
1997	1,415	9	299	0	200	1,923
1996	2,381	256	952	0	310	3,899
1995	3,310	661	434	0	252	4,657
1994	1,410	351	201	0	430	2,392
1993	1,747	1,200	520	0	12	3,479
1992	4,134	1,911	738	0	5	6,788
1991	3,410	681	200	2	4,263	8,556
1990	4,906	715	330	0	45	5,996
1989	4,628	622	330	1	26,343	31,924
1988	2,508	153	220	0	19,640	22,521

after USEPA, 2000b

3.2 Ambient Occurrence

To understand the presence of a chemical in the environment, an examination of ambient occurrence is useful. In a drinking water context, ambient water is source water existing in surface waters and aquifers before treatment. The most comprehensive and nationally representative data describing ambient water quality in the United States are being produced through the United States Geological Survey's (USGS) National Water Quality Assessment (NAWQA) program. (NAWQA, however, is a relatively young program and complete national data are not yet available from their entire array of sites across the nation.)

3.2.1 Data Sources and Methods

To examine water quality status and trends in the United States, the USGS instituted the NAWQA program in 1991. NAWQA is designed and implemented in such a manner as to allow consistency and comparison between representative study basins located around the country, facilitating interpretation of natural and anthropogenic factors affecting water quality (Leahy and Thompson, 1994).

The NAWQA program consists of 59 significant watersheds and aquifers referred to as “study units.” The study units represent approximately two thirds of the overall water usage in the United States and a similar proportion of the population served by public water systems. Approximately one half of the nation’s land area is represented (Leahy and Thompson, 1994).

To facilitate management and make the program cost-effective, approximately one third of the study units at a time engage in intensive assessment for a period of 3 to 5 years. This is followed by a period of less intensive research and monitoring that lasts between 5 and 7 years. This way all 59 study units rotate through intensive assessment over a ten-year period (Leahy and Thompson, 1994). The first round of intensive monitoring (1991-96) targeted 20 watersheds. This first group was more heavily slanted toward agricultural basins. A national synthesis of results from these study units and other research initiatives focusing on pesticides and nutrients is being compiled and analyzed (Kolpin et al., 2000; Larson et al., 1999).

For volatile organic chemicals (VOCs), the national synthesis will compile data from the first and second rounds of intensive assessments. Study units assessed in the second round represent conditions in more urbanized basins, but initial results are not yet available. However, VOCs were analyzed in the first round of intensive monitoring and data are available for these study units (Squillace et al., 1999). The minimum reporting limit (MRL) for most VOCs, including hexachlorobutadiene, was 0.2 µg/L (Squillace et al., 1999).

Furthermore, the NAWQA program has compiled, by study unit, data collected from local, State, and other Federal agencies to augment its own data. The data set provides an assessment of VOCs in untreated ambient ground water of the conterminous United States for the period 1985-1995 (Squillace et al., 1999). Data were included in the compilation if they met certain criteria for collection, analysis, well network design, and well construction (Lapham et al., 1997). They represent both rural and urban areas, but should be viewed as a progress report as NAWQA data continue to be collected that may influence conclusions regarding occurrence and distribution of VOCs (Squillace et al., 1999).

3.2.2 Results

Initial results published for the 20 NAWQA study units undergoing intensive assessment from 1991-96 indicate that hexachlorobutadiene was not detected in ground water (Squillace et al., 1999). Hexachlorobutadiene also was not detected in rural or urban wells of the local, State, and federal data set compiled by NAWQA. These data represent untreated ambient ground water of the coterminous United States for the years 1985-1995 (Squillace et al., 1999).

Furthermore, a review of highway and urban runoff studies found no detections of hexachlorobutadiene (Lopes and Dionne, 1998). This review was undertaken as part of the National Highway Runoff Data and Methodology Synthesis and examined 44 studies implemented since 1970.

3.3 Drinking Water Occurrence

The Safe Drinking Water Act (SDWA), as amended in 1986, required public water systems (PWSs) to monitor for specified “unregulated” contaminants, on a five year cycle, and to report the monitoring results to the States. Unregulated contaminants do not have an established or proposed National Primary Drinking Water Regulation (NPDWR), but they are contaminants that were formally listed and required for monitoring under federal regulations. The intent was to gather scientific information on the occurrence of these contaminants to enable a decision as to whether or not regulations were needed. All non-purchased community water systems (CWSs) and non-purchased non-transient non-community water systems (NTNCWSs), with greater than 150 service connections, were required to conduct this unregulated contaminant monitoring. Smaller systems were not required to conduct monitoring under federal regulations, but were required to be available to monitor if the State decided such monitoring was necessary. Many States collected data from smaller systems. Additional contaminants were added to the Unregulated Contaminant Monitoring (UCM) program in 1991 (USEPA, 1991; 56 FR 3526) for required monitoring that began in 1993 (USEPA, 1992; 57 FR 31776).

Hexachlorobutadiene has been monitored under the SDWA UCM program since 1987 (USEPA, 1987; 52 FR 25690). Monitoring for hexachlorobutadiene under UCM continued throughout the 1990s, but ceased for small public water systems (PWSs) under a direct final rule published January 8, 1999 (USEPA, 1999a; 64 FR 1494). Monitoring ended for large PWSs with promulgation of the revised Unregulated Contaminant Monitoring Regulation (UCMR) issued September 17, 1999 (USEPA, 1999b; 64 FR 50556) and effective January 1, 2001. At the time the UCMR lists were developed, the Agency concluded there were adequate monitoring data for a regulatory determination. This obviated the need for continued hexachlorobutadiene monitoring under the new UCMR list.

3.3.1 Data Sources, Data Quality, and Analytical Approach

Currently, there is no complete national record of unregulated or regulated contaminants in drinking water from public water systems collected under SDWA. Many States have submitted their unregulated contaminant PWS monitoring data to EPA databases; but there are issues of data quality, completeness, and representativeness. Nonetheless, a significant amount of State data are available for UCM contaminants that can provide estimates of national occurrence. The contaminant occurrence analyses findings presented in this report are based on a national cross-section of aggregated state data (i.e., a representative subset if there is available state data) derived from the SDWIS/FED database.

The National Contaminant Occurrence Database (NCOD) is an interface to the actual occurrence data stored in the Safe Drinking Water Information System (Federal version; SDWIS/FED) and can be queried to provide a summary of the data in SDWIS/FED for a particular contaminant. The data used

in this report were derived from the data in SDWIS/FED and another database called the Unregulated Contaminant Information System (URCIS). Note, however, that the SDWIS/FED data in this report have been reviewed, edited, and filtered to meet various data quality objectives for the purposes of this analysis. Hence, not all data from a particular source were used, only data meeting the quality objectives described below. The sources of these data, their quality and national aggregation, and the analytical methods used to estimate a given contaminant's national occurrence (from these data) are discussed in this section (for further details see USEPA, 2001a, 2001b).

3.3.1.1 UCM Rounds 1 and 2

The 1987 UCM contaminants include 34 volatile organic compounds (VOCs), divided into two groups: one with 20 VOCs for mandatory monitoring, and the other with 14 VOCs for discretionary monitoring (USEPA, 1987; 52 FR 25690). Hexachlorobutadiene was among the 14 VOCs included for discretionary monitoring. The UCM (1987) contaminants were first monitored coincident with the Phase I regulated contaminants, during the 1988-1992 period. This period is often referred to as "Round 1" monitoring. The monitoring data collected by the PWSs were reported to the States (as primacy agents), but there was no protocol in place to report these data to EPA. These data from Round 1 were collected by EPA from many States over time.

The Round 1 data were put into a database called the Unregulated Contaminant Information System, or URCIS. Most of the Phase 1 regulated contaminants were also VOCs. Both the unregulated and regulated VOCs are analyzed using the same sample and the same laboratory methods. Hence, the URCIS database includes data on all of these 62 contaminants: the 34 UCM (1987) VOCs; the 21 regulated Phase 1 VOCs; 2 regulated synthetic organic contaminants (SOCs); and 5 miscellaneous contaminants that were voluntarily reported by some States (e.g., isomers of other organic contaminants).

The 1993 UCM contaminants include 13 SOCs and 1 inorganic contaminant (IOC) (USEPA, 1992; 57 FR 31776). Monitoring for the UCM (1993) contaminants began coincident with the Phase II/V regulated contaminants in 1993 through 1998. This is often referred to as "Round 2" monitoring. The UCM (1987) contaminants were also included in the Round 2 monitoring. As with other monitoring data, PWSs reported these results to the States. EPA, during the past several years, requested that the States submit these historic data to EPA.

The details of the actual individual monitoring periods are complex. The timing of required monitoring was staggered related to different size classes of PWSs, and the program was implemented somewhat differently by different States. While Round 1 includes the period from 1988-1992, it also includes results from samples analyzed prior to 1988 that were "grandfathered" into the database. For further details see EPA (2001a, 2001b).

3.3.1.2 Developing a Nationally Representative Perspective

The Round 1 and Round 2 databases contain contaminant occurrence data from a total of 40 and 35 primacy entities (largely States), respectively. However, data from some States are incomplete and biased. Furthermore, the national representativeness of the data is problematic because the data were not collected in a systematic or random statistical framework. These State data could be heavily skewed to low-occurrence or high-occurrence settings. Hence, the State data were evaluated based on pollution-potential indicators and the spatial/hydrologic diversity of the nation. This evaluation enabled the construction of a cross-section from the available State data sets that provides a reasonable representation of national occurrence.

A national cross-section comprised of the Round 2 state contaminant occurrence databases was established using the approach developed for the EPA report *A Review of Contaminant Occurrence in Public Water Systems* (USEPA, 1999d). This approach was developed to support occurrence analyses for EPA's Chemical Monitoring Reform (CMR) evaluation, and was supported by peer reviewers and stakeholders. The approach cannot provide a "statistically representative" sample because the original monitoring data were not collected or reported in an appropriate fashion. However, the resultant "national cross-section" of states should provide a clear indication of the central tendency of the national data. The remainder of this section provides a summary description of how the national cross-section from the SDWIS/FED (Round 2) database was developed. The details of the approach are presented in other documents (USEPA, 2001a, 2003b); readers are referred to these for more specific information.

3.3.1.2.1 Cross-Section Development

As a first step in developing the cross-section, the State data contained in the URCIS database (that contains the Round 1 monitoring results) and SDWIS/FED database (that contains the Round 2 monitoring results) were evaluated for completeness and quality. For both the URCIS (Round 1) and SDWIS/FED (Round 2) databases, some State data were unusable for a variety of reasons. Some States reported only detections, or the data was recorded with incorrect units. Data sets only including detections are obviously biased, over-representing high-occurrence settings. Other problems included substantially incomplete data sets without all PWSs reporting. Also, data from Washington, D.C. and the Virgin Islands were excluded from this analysis because it was difficult to evaluate them for the current purposes in relation to complete State data (USEPA, 2001a Sections II and III).

The balance of the States remaining after the data quality screening were then examined to establish a national cross-section. This step was based on evaluating the States' pollution potential and geographic coverage in relation to all States. Pollution potential is considered to ensure a selection of States that represent the range of likely contaminant occurrence and a balance with regard to likely high and low occurrence. Geographic consideration is included so that the wide range of climatic and hydrogeologic conditions across the United States are represented, again balancing the varied conditions that affect transport and fate of contaminants, as well as conditions that affect naturally occurring contaminants (USEPA, 2001b Sections III.A. and III.B.).

The cross-section States were selected to represent a variety of pollution potential conditions. Two primary pollution potential indicators were used. The first factor selected indicates pollution potential from manufacturing/population density and serves as an indicator of the potential for VOC contamination within a State. Agriculture was selected as the second pollution potential indicator because the majority of SOCs of concern are pesticides (USEPA, 2001b Section III.A.). The 50 individual States were ranked from highest to lowest based on the pollution potential indicator data. For example, the State with the highest ranking for pollution potential from manufacturing received a ranking of 1 for this factor and the State with the lowest value was ranked as number 50. States were ranked for their agricultural chemical use status in a similar fashion.

The States' pollution potential rankings for each factor were subdivided into four quartiles (from highest to lowest pollution potential). The cross-section States were chosen equally from all quartiles for both pollution potential factors to ensure representation, for example, from: States with high agrochemical pollution potential rankings and high manufacturing pollution potential rankings; States with high agrochemical pollution potential rankings and low manufacturing pollution potential rankings; States with low agrochemical pollution potential rankings and high manufacturing pollution potential rankings; and States with low agrochemical pollution potential rankings and low manufacturing pollution potential rankings (USEPA, 2001b Section III.B.). In addition, some secondary pollution potential indicators were considered to further ensure that the cross-section States included the spectrum of pollution potential conditions (high to low). At the same time, states within the specific quartiles were considered collectively across all quartiles to attempt to provide a geographic coverage across all regions of the United States.

The data quality screening, pollution potential rankings, and geographic coverage analysis established national cross-sections of 24 Round 1 (URCIS) States and 20 Round 2 (SDWIS/FED) States. In each cross-section, the States provide good representation of the nation's varied climatic and hydrogeologic regimes and the breadth of pollution potential for the contaminant groups (Table 3-2 and Figure 3-1).

3.3.1.2.2 Cross-Section Evaluation

To evaluate and validate the method for creating the national cross-sections, the method was used to create smaller State subsets from the 24-State, Round 1 cross-section. Again, States were chosen to achieve a balance from the quartiles describing pollution potential, and a balanced geographic distribution, to incrementally build subset cross-sections of various sizes. For example, the Round 1 cross-section was tested with subsets of 4, 8 (the first 4 State subset plus 4 more States), and 13 (8 State subset plus 5) States. Two additional cross-sections were included in the analysis for comparison; a cross-section composed of 16 States with biased data eliminated from the 24-State cross-section for data quality reasons and a cross-section composed of all 40 Round 1 States (USEPA, 2001b Section III.B.1).

These Round 1 incremental cross-sections were then used to evaluate occurrence for an array of both high and low occurrence contaminants. The comparative results illustrate several points. The

results are quite stable and consistent for the 8-, 13- and 24-State cross-sections. They are much less so for the 4-State, 16-State (biased), and 40-State (all Round 1 States) cross-sections. The 4-State cross-section is apparently too small to provide balance both geographically and with pollution potential, a finding that concurs with past work (USEPA, 1999d). The CMR analysis suggested that a minimum of 6-7 States was needed to provide balance both geographically and with pollution potential, and the CMR report used 8-States out of the available data for its nationally representative cross-section. The 16-State and 40-State cross-sections, both including biased States, provided occurrence results that were unstable and inconsistent for a variety of reasons associated with their data quality problems (USEPA, 2001b Section III.B.1).

The 8-, 13-, and 24-State cross-sections provide very comparable results, are consistent, and are usable as national cross-sections to provide estimates of contaminant occurrence. Including greater data from more States improves the national representation and the confidence in the results-- as long as the States are balanced related to pollution potential and spatial coverage. The 24- and 20-State cross-sections provide the best, nationally representative cross-sections for the Round 1 and Round 2 data.

3.3.1.3 Data Management and Analysis

The cross-section analyses focused on occurrence at the water system level; i.e., the summary data presented discuss the percentage of public water *systems* with detections, not the percentage of *samples* with detections. By normalizing the analytical data to the system level, skewness inherent in the sample data, particularly over the multi-year period covered in the URCIS data, is avoided. System level analysis was used since a PWS with a known contaminant problem usually has to sample more frequently than a PWS that has never detected the contaminant. Obviously, the results of a simple computation of the percentage of samples with detections (or other statistics) can be skewed by the more frequent sampling results reported by the contaminated site. This level of analysis is conservative. For example, a system need only have a single sample with an analytical result greater than the minimum reporting limit (MRL), i.e., a detection, to be counted as a system with a result “greater than the MRL.”

Also, the data used in the analyses were limited to only those data with confirmed water source and sampling type information. Only standard SDWA compliance samples were used; “special” samples, or “investigation” samples (investigating a contaminant problem that would bias results), or samples of unknown type were not used in the analyses. Various quality control and review checks were made of the results, including follow-up questions to the States providing the data. Many of the most intractable data quality problems encountered occurred with older data. These problematic data were, in some cases, simply eliminated from the analysis. For example, when the number of problematic data were insignificant relative to the total number of observations those data were dropped from the analysis (For further details see Cadmus, 2000).

Table 3-2: Cross-section States for Round 1 (24 States) and Round 2 (20 States)

Round 1 (URCIS)		Round 2 (SDWIS/FED)	
Alabama	Minnesota*	Alaska*	New Hampshire
Alaska*	Montana	Arkansas	New Mexico*
Arizona	New Jersey	Colorado	North Carolina*
California	New Mexico*	Kentucky*	North Dakota
Florida	North Carolina*	Maine	Ohio*
Georgia	Ohio*	Maryland*	Oklahoma
Hawaii	South Dakota	Massachusetts	Oregon
Illinois	Tennessee	Michigan	Rhode Island
Indiana	Utah	Minnesota*	Texas
Iowa	Washington*	Missouri	Washington*
Kentucky*	West Virginia		
Maryland*	Wyoming		

* cross-section State in both Round 1 and Round 2

3.3.1.4 Occurrence Analysis

To evaluate national contaminant occurrence, a two-stage analytical approach has been developed. The first stage of analysis provides a straightforward, conservative, non-parametric evaluation of occurrence of the CCL regulatory determination priority contaminants as described above. These Stage 1 descriptive statistics are summarized here. Based in part on the findings of the Stage 1 Analysis, EPA will determine whether more rigorous parametric statistical evaluations, the Stage 2 Analysis, may be warranted to generate national probability estimates of contaminant occurrence and exposure for priority contaminants (for details on this two stage analytical approach see Cadmus, 2000 and USEPA, 2002b).

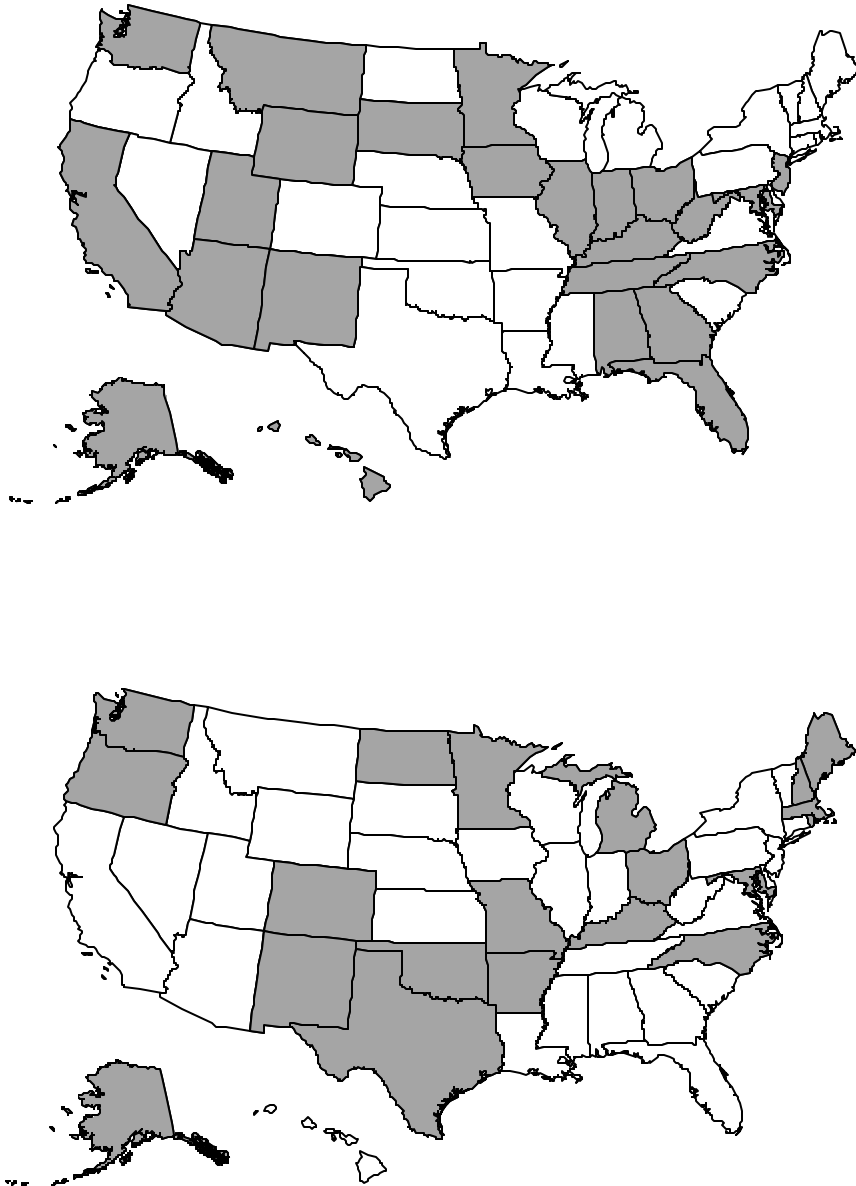
The summary descriptive statistics presented in Table 3-3 for hexachlorobutadiene are a result of the Stage 1 analysis and include data from both Round 1 (URCIS, 1987-1992) and Round 2 (SDWIS/FED, 1993-1997) cross-section States. Included are the total number of samples, the percent samples with detections, the 99th percentile concentration of all samples, the 99th percentile concentration of samples with detections, and the median concentration of samples with detections. The percentages of PWSs and population served indicate the proportion of PWSs whose analytical results showed a detection(s) of the contaminant (simple detection, > MRL) at any time during the monitoring period; or a detection(s) greater than half the Health Reference Level (HRL); or a detection(s) greater than the Health Reference Level. The Health Reference Level, 0.9 µg/L, is a preliminary estimated health effect level used for this analysis. The HRL was derived using the 10⁻⁶ cancer risk as calculated by the linear method and using a body weight to the three quarter power (slope factor 4 x 10⁻² (mg/kg-day)⁻¹).

The 99th percentile concentration is used here as a summary statistic to indicate the upper bound of occurrence values because maximum values can be extreme values (outliers) that sometimes result from sampling or reporting error. The 99th percentile concentration is presented for both the samples with only detections and all of the samples because the value for the 99th percentile concentration of all samples is below the Minimum Reporting Level (MRL) (denoted by “<” in Table 3-3). For the same reason, summary statistics such as the 95th percentile concentration of all samples or the median (or mean) concentration of all samples are omitted because these also are all “<” values. This is the case because only 0.1% to 0.05% of all samples recorded detections of hexachlorobutadiene in Round 1 and Round 2.

As a simplifying assumption, a value of half the MRL is often used as an estimate of the concentration of a contaminant in samples/systems whose results are less than the MRL. With a contaminant with relatively low occurrence such as hexachlorobutadiene in drinking water occurrence databases, the median or mean value of occurrence using this assumption would be half the MRL (0.5 * MRL). However, for these occurrence data this is not straightforward. For Round 1 and Round 2, States have reported a wide range of values for the MRLs. This is in part related to State data management differences as well as real differences in analytical methods, laboratories, and other factors.

The situation can cause confusion when examining descriptive statistics for occurrence. For example, the modal MRL value for the Round 1 samples is 0.50 µg/L—a value twice as large as the median concentration of detections for Round 1 (0.25 µg/L) (This occurs because some States and/or systems reporting detections were using a lower MRL and had positive results lower than the MRL used by other States or systems). For Round 2, most States reported non-detections as zeros resulting in a modal MRL value of zero. By definition the MRL cannot be zero. This is an artifact of State data management systems. Because a simple meaningful

Figure 3-1: Geographic distribution of cross-section States for Round 1 (top) and Round 2 (bottom)



summary statistic is not available to describe the various reported MRLs, and to avoid confusion, MRLs are not reported in the summary table (Table 3-3).

In Table 3-3, national occurrence is estimated by extrapolating the summary statistics for the 24 and 20 State cross-sections to national numbers for systems, and population served by systems, from the *Water Industry Baseline Handbook, Second Edition* (USEPA, 2000e). From the handbook, the total number of community water systems (CWSs) plus non-transient, non-community water systems (NTNCWSs) is 65,030, and the total population served by CWSs plus NTNCWSs is 213,008,182 persons (see Table 3-3). To arrive at the national occurrence estimate for a particular cross-section, the national estimate for PWSs (or population served by PWSs) is simply multiplied by the percentage for the given summary statistic. [i.e. for Round 1, the national estimate for the total number of PWSs with detections (228) is the product of the percentage of Round 1 PWSs with detections (0.35%) and the national estimate for the total number of PWSs (65,030)].

Because the State data used for the cross-section are not a strict statistical sample, national extrapolations of these Stage 1 analytical results can be problematic, especially for contaminants with very low occurrence like hexachlorobutadiene and other CCL regulatory determination priority contaminants. For this reason, the nationally extrapolated estimates of occurrence based on Stage 1 results are not presented in the *Federal Register* Notice. The presentation in the *Federal Register* Notice of only the actual results of the cross-section analysis maintains a straight-forward presentation, and the integrity of the data, for stakeholder review. The nationally extrapolated Stage 1 occurrence values are presented here, however, to provide additional perspective. A more rigorous statistical modeling effort, the Stage 2 analysis, could be conducted on the cross-section data (USEPA, 2002b). The Stage 2 results would be more statistically robust and more suitable to national extrapolation. This approach would provide a probability estimate and would also allow for better quantification of estimation error.

Round 1(1987-1992) and Round 2 (1993-1997) data were not merged because they represent different time periods, different States (only eight States are represented in both rounds), and each round has different data management and data quality problems. The two rounds are only merged for the simple spatial analysis overview presented in Section 3.3.2.2 and Figures 3-2 and 3-4.

3.3.2 Results

3.3.2.1 Occurrence Estimates

While States with detections of hexachlorobutadiene are widespread (Figure 3-2), the percentages of PWSs by State with detections are low (Table 3-3). In aggregate, the cross-sections show only 0.2% - 0.4% of PWSs in both rounds experienced detections (> MRL), affecting 0.9% - 2.4% of the population served (approximately 2 - 5 million people). Percentages of PWSs with detections greater than half the Health Reference Level (> ½ HRL) are slightly lower: 0.1% - 0.2%. The percentage of PWSs exceeding the Health Reference Level (> HRL) for both rounds is very small (see also Figure 3-

4). Between 0.02% and 0.1% of PWSs in Rounds 1 and 2 experienced detections > HRL, affecting a population of approximately 10,000 - 750,000.

There are some qualifying notes for both rounds of data that warrant discussion. The Round 1 estimates of PWSs affected by hexachlorobutadiene are influenced by the State of Florida (Table 3-3; Figures 3-3 and 3-4). This State reports that 5.4% of its PWSs experienced detections greater than the HRL during Round 1, a value considerably greater than the next highest State (1.5%). This suggests that Florida's data for hexachlorobutadiene is incomplete and may be biased. Out of 855 Florida PWSs reporting contaminant data for Round 1 monitoring, only 112 provided data for hexachlorobutadiene (USEPA, 2001a). Also, the 5.4% of systems reporting detections all reported concentrations greater than the Health Reference Level. These figures suggest that perhaps only systems experiencing problems submitted data for hexachlorobutadiene, biasing Florida's results for occurrence measures examined in this report.

The large values for the Round 2 national estimates of population served with detections greater than the MRL and greater than half the HRL are influenced by the inclusion of one PWS serving a very large population (1.5 million people). While the percentage of systems with detections of hexachlorobutadiene are similar (both rounds show low values, 0.2% - 0.4% PWSs > MRL), the difference in population served results in a larger difference in the population extrapolations.

Note that for the Round 1 cross-section, the total number of PWSs (and the total population served by the PWSs) is not the sum of the number of ground water and surface water systems (or the populations served by those systems). Because some public water systems are seasonally classified as either surface or ground water, some systems may be counted in both categories. The population numbers for the Round 1 cross-section are also incomplete. Not all of the PWSs for which occurrence data was submitted reported the population they served. (However, the population numbers presented in Table 3-3 for the Round 1 cross-section are reported from 94% of the systems.)

The national estimates extrapolated from Round 1 and Round 2 PWS numbers and populations are not additive either. In addition to the Round 1 classification and reporting issues outlined above, the proportions of surface water and ground water PWSs, and populations served by them, are different between the Round 1 and 2 cross-sections and the national estimates. For example, approximately 49% of the population served by PWSs in the Round 1 cross-section States are served by surface water PWSs (Table 3-3). Nationally, however, that proportion changes to 60%.

Both Round 1 and Round 2 national cross-sections show a proportionate balance in PWS source waters compared to the national inventory. Nationally, 91% of PWSs use ground water (and 9% surface waters); Round 1 shows 89%, and Round 2 shows 90% of systems using ground water. The relative populations served are not as closely comparable. Nationally, about 40% of the population is served by PWSs using ground water (and 60% by surface water). Round 2 data is most representative with 37% of the cross-section population served by ground water; Round 1 shows about 55%.

There are differences in the occurrence results between Round 1 and Round 2, as should be expected. The differences are not great, however, particularly when comparing the proportions of systems affected. The results range from 0.2% - 0.4% of PWSs with detections of hexachlorobutadiene and range from 0.02% to 0.1% of PWSs with detections greater than the Health Reference Level of 0.9 µg/L. These are not substantively different, given the data sources.

The differences in the population extrapolations appear greater, but still constitute relatively small proportions of the population. The most pronounced difference is in the estimate of the population served by PWSs with detections greater than the Health Reference Level, ranging from 10,000 to 750,000. In both cases, this is less than 0.5% of the population. The difference in this category is largely driven by the Florida data in Round 1, as discussed above.

The Round 2 cross-section provides a better proportional balance related to the national population of PWSs and may have fewer reporting problems than Round 1 (i.e., incomplete population numbers, Florida). The larger estimate of the national population served by PWSs with detections greater than the Health Reference Level using Round 1 data can also provide an upper bound estimate in considering the data.

3.3.2.2 Regional Patterns

Occurrence results are displayed graphically by State in Figures 3-2, 3-3, and 3-4 to assess whether any distinct regional patterns of occurrence are present. Combining Round 1 and Round 2 data (Figure 3-2), there are forty-seven States reporting. Six of those States have no data for hexachlorobutadiene, while another 21 have no detections of the chemical. The remaining 20 States have detected hexachlorobutadiene in drinking water and are well distributed throughout the United States.

The simple spatial analysis presented in Figures 3-2, 3-3, and 3-4 suggests that special regional analyses are not warranted. Florida's possible bias is notable, however. While no clear geographical patterns of occurrence are apparent, comparisons with environmental use and release information are useful (see also section 3.1). Five of the eight Toxic Release Inventory States that reported releases of hexachlorobutadiene into the environment between 1988 and 1998 have also detected the chemical in PWS sampling. Of the remaining three (Kansas, Louisiana, and California), Kansas hasn't reported any data for either Round 1 or 2. Also, of the eight States with detections of hexachlorobutadiene at CERCLA National Priorities List (NPL) hazardous waste sites, five have detected the chemical in drinking water. Finally, six of the States detecting hexachlorobutadiene in PWS samples have also detected it in site samples reported to the ATSDR's HazDat database. It is interesting to note that neither Alabama nor Florida, the two States with the highest percentage of PWSs with detections greater than the Health Reference level, are Toxic Release Inventory States for hexachlorobutadiene nor do they have CERCLA NPL sites with detections of the chemical (Figure 3-4).

Table 3-3: Summary occurrence statistics for hexachlorobutadiene

	24 State Cross-Section ¹ (Round 1)	20 State Cross-Section ² (Round 2)	National System & Population Numbers ³	
Frequency Factors				
Total Number of Samples	42,839	93,585	--	
Percent of Samples with Detections	0.13%	0.05%	--	
99 th Percentile Concentration (all samples)	< (Non-detect)	< (Non-detect)	--	
Health Reference Level	0.9 µg/L	0.9 µg/L	--	
Minimum Reporting Level (MRL)	Variable*	Variable*	--	
99 th Percentile Concentration of Detections	10 µg/L	1.5 µg/L	--	
Median Concentration of Detections	0.25 µg/L	0.30 µg/L	--	
Total Number of PWSs	12,284	22,736	65,030	
Number of GW PWSs	10,980	20,380	59,440	
Number of SW PWSs	1,385	2,356	5,590	
Total Population	71,582,571	67,075,493	213,008,182	
Population of GW PWSs	40,399,177	24,960,222	85,681,696	
Population of SW PWSs	34,418,834	42,115,271	127,326,486	
			National Extrapolation⁴	
Occurrence by System			Round 1	Round 2
% PWSs with detections (> MRL)	0.350%	0.180%	228	117
Range of Cross-Section States	0 - 5.36%	0 - 3.36%	N/A	N/A
GW PWSs with detections	0.301%	0.132%	179	79
SW PWSs with detections	0.722%	0.594%	40	33
% PWSs > 1/2 Health Reference Level (HRL)	0.163%	0.079%	106	51
Range of Cross-Section States	0 - 5.36%	0 - 0.51%	N/A	N/A
GW PWSs > 1/2 Health Reference Level	0.118%	0.064%	70	38
SW PWSs > 1/2 Health Reference Level	0.505%	0.212%	28	12
% PWSs > Health Reference Level	0.114%	0.018%	74	11
Range of Cross-Section States	0 - 5.36%	0 - 0.24%	N/A	N/A
GW PWSs > Health Reference Level	0.064%	0.005%	38	3
SW PWSs > Health Reference Level	0.505%	0.127%	28	7
Occurrence by Population Served				
% PWS Population Served with detections	0.896%	2.360%	1,909,000	5,027,000
Range of Cross-Section States	0 - 11.38%	0 - 29.93%	N/A	N/A
GW PWS Population with detections	1.458%	0.186%	1,249,000	159,000
SW PWS Population with detections	0.153%	3.649%	194,000	4,646,000
% PWS Population Served > 1/2 Health Reference Level	0.569%	2.331%	1,213,000	4,965,000
Range of Cross-Section States	0 - 11.38%	0 - 29.92%	N/A	N/A
GW PWS Population > 1/2 Health Reference Level	0.978%	0.177%	838,000	152,000
SW PWS Population > 1/2 Health Reference Level	0.036%	3.607%	46,000	4,593,000
% PWS Population Served > Health Reference Level	0.367%	0.005%	781,000	10,000
Range of Cross-Section States	0 - 9.66%	0 - 0.02%	N/A	N/A
GW PWS Population > Health Reference Level	0.619%	0.011%	531,000	9,000
SW PWS Population > Health Reference Level	0.036%	0.001%	46,000	1,000

1. Summary Results based on data from 24-State Cross-Section, from URCIS, UCM (1987) Round 1.

2. Summary Results based on data from 20-State Cross-Section, from SDWIS/FED, UCM (1993) Round 2.

3. Total PWS and population numbers are from EPA March 2000 Water Industry Baseline Handbook.

4. National extrapolations are from the 24-State data and 20-State data using the Baseline Handbook system and population numbers.

- PWS = Public Water Systems; GW = Ground Water; SW = Surface Water; MRL = Minimum Reporting Level (for laboratory analyses);

- HRL = Health Reference Level, an estimated health effect level used for preliminary assessment for this review; N/A = Not Applicable

- The Health Reference Level used for hexachlorobutadiene is 0.9 µg/L. This is a draft value for working review only.

- Total Number of Samples = the total number of analytical records for hexachlorobutadiene.

- Median Concentration of Detections = the median analytical value of all the detections (analytical results greater than the MRL) (in µg/L).

- Total Number of PWSs = the total number of public water systems with records for hexachlorobutadiene.

- Total Population Served = the total population served by public water systems with records for hexachlorobutadiene.

- % PWS with detections, % PWS > 1/2 Health Reference Level, % PWS > Health Reference Level = percent of the total number of public water systems with at least one analytical result that exceeded the MRL, 1/2 Health Reference Level, Health Reference Level, respectively.

3.4 Conclusion

While there have not been detections of hexachlorobutadiene in ambient water reported in USGS NAWQA studies to date, it has been detected at a very low percentage of ATSDR HazDat sites and CERCLA NPL sites. Furthermore, releases have been reported through the Toxic Release Inventory.

Hexachlorobutadiene has also been detected in PWS samples collected under SDWA. Occurrence estimates are low for Round 1 and Round 2 UCM monitoring with only 0.13% and 0.05% of all samples showing detections, respectively. Significantly, the values for the 99th percentile and median concentrations of all samples are less than the Minimum Reporting Level. For Round 1 samples with detections, the median concentration is 0.25 µg/L and the 99th percentile concentration is 10 µg/L. Median and 99th percentile concentrations for Round 2 detections are 0.30 µg/L and 1.5 µg/L, respectively. Systems with detections only constitute 0.4% of Round 1 systems and 0.2% for Round 2. National estimates for the population served by PWSs with detections are also low, especially for detections greater than the Health Reference Level. For both rounds, these estimates are less than 0.5% of the national PWS population (Round 1: 754,537; Round 2: 9,721).

4.0 HEALTH EFFECTS

A description of the health effects and available dose-response information associated with exposure to hexachlorobutadiene (HCBd) is summarized below. A full description of the health effects and the dose-response information for threshold and non-threshold effects associated with exposure to hexachlorobutadiene are presented in Chapters 7 and 8 of the Health Effects Support Document for Hexachlorobutadiene (USEPA, 2003b).

4.1 Hazard Characterization and Mode of Action Implications

While available toxicological data indicate that HCBd has the potential to cause adverse health effects in animals, data on human health effects are limited to a few studies of occupational exposure to HCBd. These data, collected from inhalation exposure, are often confounded by simultaneous exposures to other chemicals in an occupational setting. Such equivocal data has made it difficult to establish a relationship between HCBd exposure and toxic/cytogenetic effects in human.

Figure 3-3: States with PWSs with detections of hexachlorobutadiene (any PWSs with results greater than the Minimum Reporting Level [MRL]) for Round 1 (above) and Round 2 (below) cross-section States

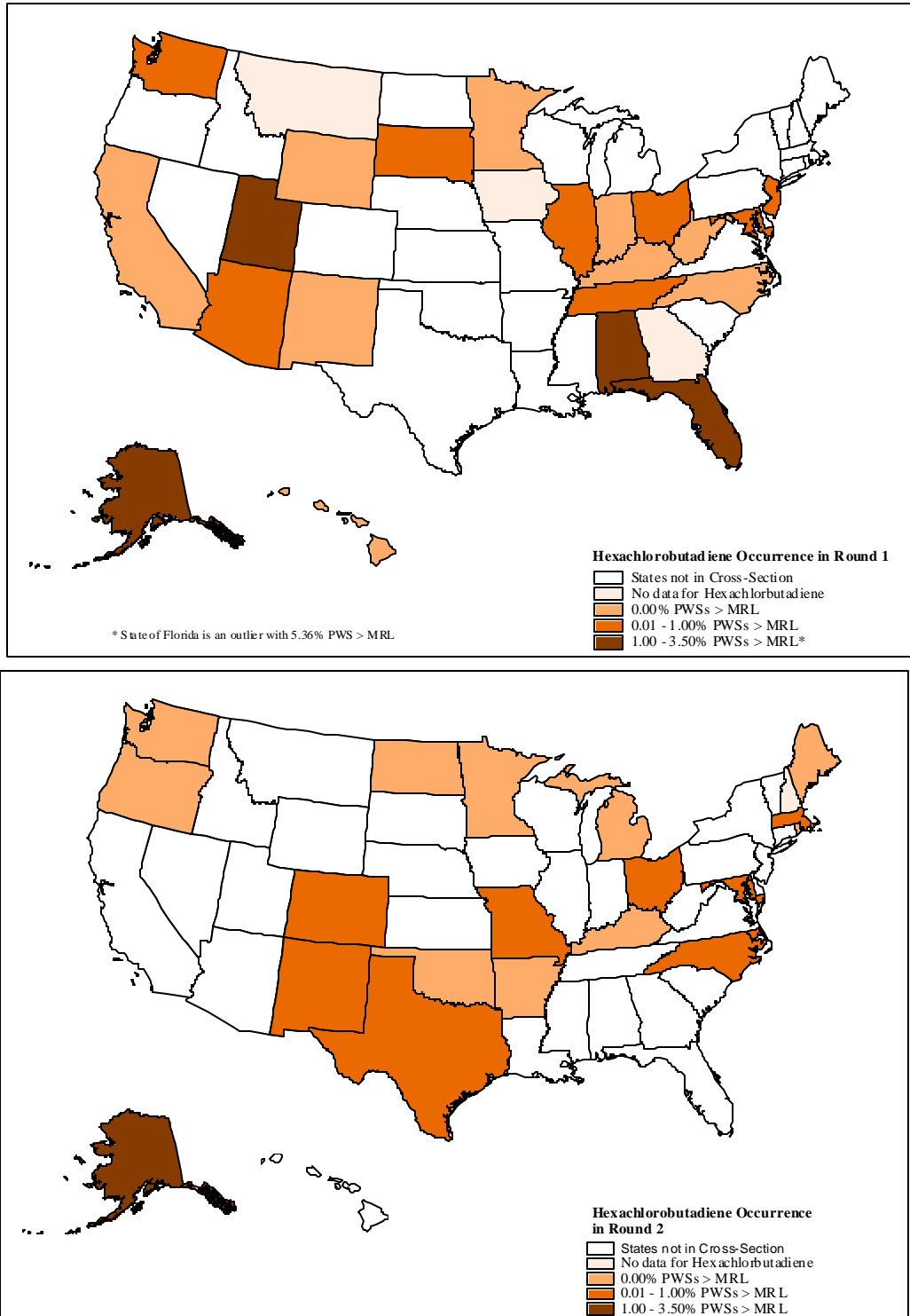
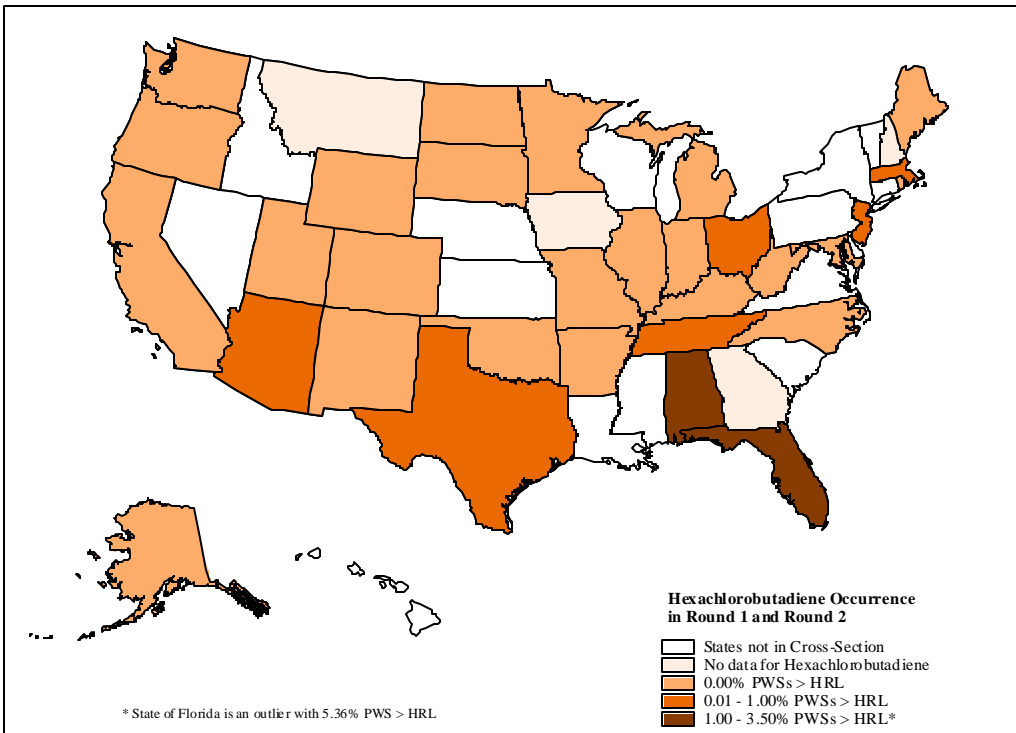
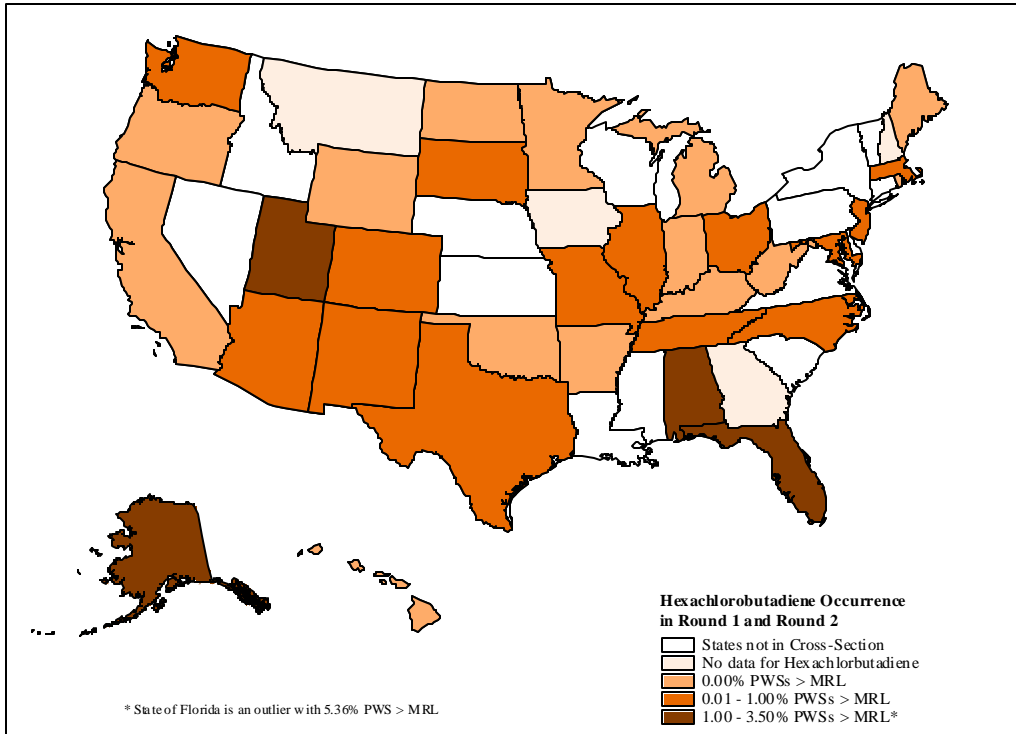


Figure 3-4: Cross-section States (Round 1 and Round 2 combined) with PWSs with detections of hexachlorobutadiene (above) and concentrations greater than the Health Reference Level (below)



Animals studies demonstrate selective effects of HCBd on the proximal tubule of the kidney. For example, renal toxicity has been observed in rodents following single acute exposures of 100–200 mg HCBd/kg and short-term exposures to 3 mg/kg-day and above. Furthermore, subchronic and chronic studies on rodents have indicated renal damage at a lowest observed adverse effect level (LOAEL) of 2 mg/kg-day. Progressive effects over time from HCBd exposure include kidney weight changes, increased urinary excretion of coproporphyrin, and increased renal tubular epithelial hyperplasia.

Developmental effects and neurotoxicity have been observed in studies that used higher HCBd doses than in the previous studies (Harleman and Seinen, 1979; Badaeva et al., 1985). In addition, pups with lower birth weights and reduced growth have been reported after administering maternal dosages of 8.1-15 mg/kg-day to rats (Harleman and Seinen, 1979).

Results from mutagenicity studies with HCBd are ambiguous. Some studies have shown HCBd and its degradates to be mutagenic in specific chemical environments (Vamvakas et al., 1988; Reichert et al., 1984). HCBd metabolites have been shown to bind to mitochondrial DNA *in vivo* in mice, and induce DNA repair in cultured porcine kidney cell, suggesting genotoxic potential (Schrenk and Dekant, 1989; Vamvakas et al., 1989). However, no human studies of HCBd carcinogenicity have been reported and only one animal study has been performed (Kociba et al., 1977). In this study, neoplastic changes were observed in the liver at the highest dose (which exceeded the maximum tolerated dose [MTD]). The dosage necessary to cause these significant adverse effects suggests that tumor formation may be secondary to cytotoxicity.

In order to evaluate the hazard posed by HCBd, the threat to humans must be extrapolated from data on rodents, raising the issue of applicability. Nephrotoxicity caused by HCBd is dependent on a multistep bioactivation mechanism involving both kidney and liver enzymes. *In vitro* studies with human renal cytosol and cultured human proximal tubule cells suggest that humans have the potential to form HCBd-glutathione conjugates and to metabolize HCBd cysteine conjugates to toxic metabolites. However, the rate of metabolism, particularly for the reaction catalyzed by β -lyase, appears to be much lower for humans than for rodents (Lock, 1994; Lash et al., 1990).

4.2 Dose-Response Characterization and Implications in Risk Assessment

Noncancer effects

Renal effects in rodents, resulting from short-term exposure to HCBd, appear to have LOAELs of 5–20 mg/kg-day, depending on the following factors: rodent species/strain, length of exposure, and method of administration. For female Sprague-Dawley rats administered HCBd for 3 weeks, no effect was observed after 3 mg/kg-day oral dose, reduced body weight gain and food consumption after a 10 mg/kg-day dose, and renal tubular degeneration, necrosis and regeneration were observed at a 30 mg/kg-day dose (Kociba et al., 1971; Schwetz et al., 1977). Male Sprague-Dawley rats exposed to HCBd via ingestion for 3 weeks identified a LOAEL of 20 mg/kg-day and a no observed adverse

effect level (NOAEL) of 0.2 mg/kg-day for kidney damage and increased relative kidney weight (Stott et al., 1981). In a four-week oral study with Wistar rats, a LOAEL of 8 mg/kg-day and a NOAEL of 2.25 mg/kg-day were identified for decreased body weight gain and renal tubular effects (Jonker et al., 1993). A 2-week feeding study in Wistar rats identified a LOAEL of 4.6 mg/kg-day (the lowest dose tested) for renal tubular epithelial cell degeneration (Harleman and Seinen, 1979). Lastly, in a 2-week oral exposure study on B6C3F₁ mice, a LOAEL of 3–5 mg/kg-day (the lowest dose tested) was reported for renal tubular necrosis (NTP, 1991).

In a subchronic 13-week oral exposure study of HCBd in B6C3F₁ mice, a NOAEL of 1.5 mg/kg-day was identified for male mice based on renal tubular cell regeneration (NTP, 1991). In females, 1 of 10 mice in the lowest dose group (0.2 mg/kg-day) was affected with tubular regeneration. The authors of this study concluded that insufficient data existed to identify a NOAEL for the female mice (NTP, 1991). Others (USEPA, 1998b; WHO, 1994) have also concluded that this observed effect is not statistically significant. As a result, 0.2 mg/kg-day may be considered close to the NOAEL for renal injury in female mice.

In a lifetime oral exposure study on HCBd (Kociba et al., 1977), a NOAEL of 0.2 mg/kg-day and a LOAEL of 2 mg/kg-day in rats was identified, based on an increase in renal tubular epithelial cell hyperplasia/regeneration and an altered renal function (increased urinary coproporphyrin excretion). The significance of this NOAEL value from a chronic study is that it is identical to the value identified from the 13-week NTP study on female mice (NTP, 1991), suggesting that female mice may be more sensitive than rats to HCBd.

The EPA's Reference Dose (RfD) for HCBd is 2×10^{-4} mg/kg-day (1998b). The RfD is an estimate of a daily exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious effects over a lifetime. The RfD is derived from a NOAEL of 0.2 mg/kg-day for renal tubular epithelial cell hyperplasia/regeneration from the Kociba et al. (1977) and NTP (1991) studies. A composite uncertainty factor of 1,000 was used in the derivation of the RfD to account for extrapolation from animals to humans (factor of 10); protection of sensitive subpopulations (factor of 10); use of a NOAEL that may be closer to a LOAEL (factor of 3); and database deficiency (factor of 3) due to lack of a 2-generation reproductive study.

Cancer effects

The single lifetime exposure study in rats is also a valuable source of data on tumor formation (Kociba et al., 1977). Only at the highest dose of 20 mg/kg-day (which exceeded the level at which significant non-carcinogenic effects were seen, i.e. mortality, renal toxicity, and body weight depression) were tumors observed in both sexes. No tumors were observed in the group administered the second highest dose of 2 mg/kg-day. Also, no definitive shape from the dose-response curve could be determined from this data set.

Data from Kociba et al. (1977) indicate that the tumor dose response curves are strongly non-linear and that renal tumors are only observed at HCBd doses that cause toxicity. HCBd appears to

be carcinogenic only at cytotoxic dose. Under EPA's 1986 Guidelines for Carcinogen Risk Assessment, HCBd is classified as a Group C, possible human carcinogen (USEPA, 1986). EPA's draft Ambient Water Quality Criteria for HCBd recommends using a non-linear approach for dose-response extrapolation, since the non-linear margin of exposure approach may be more appropriate for assessing the dose-response of HCBd (USEPA, 1998b).

4.3 Relative Source Contribution

Relative source contribution analysis compares the magnitude of exposure expected via drinking water to the magnitude of exposure from intake of HCBd in other media, such as food, air, and soil. To perform this analysis, intake of HCBd from drinking water must be estimated. Occurrence data for HCBd in water and other media are presented in Chapter 3 of this document.

The 99th percentile concentration for all samples (i.e., those with detectable and nondetectable levels of HCBd) from Round 1 and Round 2 PWS sampling is below the MRL. As a convention, a value of half the MRL is often used as an estimate of the concentration of a contaminant in samples/systems whose results are less than the MRL. However, for Round 1 and Round 2, States have reported a wide range of values for the MRLs. Therefore, a single estimate of the MRL for HCBd is unavailable.

The median concentration (0.3 µg/L) for HCBd in samples with detectable levels is used to estimate intake from drinking water. The exposure estimate for an average individual is determined by multiplying the drinking water concentration by daily water intake (2 liters/day) and dividing by average adult body weight (70 kg). The estimated exposure to HCBd from drinking water for an average person is 8.6×10^{-6} mg/kg-day. For children, assuming a daily water intake of 1 liter/day and body weight of 10 kg, the exposure estimate is 3.0×10^{-5} mg/kg-day.

The estimated food:drinking water exposure ratio is 0.02 for an adult and 0.008 for a child. The estimated air:drinking water exposure is 14 for an adult and 21 for a child. Collectively, these data indicate that intake from drinking water is low when compared to intake from air, though when compared to possible intake from food.

4.4 Sensitive Populations

The primary target organ for HCBd is the kidney. Existing nephropathy or age-related kidney degeneration has been observed to increase the risk of renal injury in humans. Therefore, sensitive populations for HCBd exposure may include people with pre-existing kidney or liver damage, or the elderly. Furthermore, although it is unlikely that human newborns would be acutely exposed to significant doses of HCBd, acute exposures for young rats and mice have shown to cause toxicity at lower doses than for adults (Hook et al., 1983; Lock et al., 1984).

Calculation of medium-specific exposure ratios indicates that HCBD intake from air is about 14 – 20 fold greater than intake from water. As a result, regulation of HCBD in drinking water may not significantly reduce the risk to adverse effects from HCBD for sensitive populations.

4.5 Exposure and Risk Information

Approximately 2 – 5 million people are served by systems with detections of HCBd. When average daily intakes from drinking water are compared with intakes from air, drinking water accounts for a relatively small proportion of total HCBd intake. Relative intake rates from food may be higher, while intakes from soil are unknown. On the basis of these observations, the impact of regulating HCBd concentrations in drinking water on health risk reduction is likely to be small.

National population estimates for HCBd exposure were derived using summary statistics for Round 1 and Round 2 PWS cross-sectional data and population data from the *Water Industry Baseline Handbook* (USEPA, 2000e). An estimated 1.9 to 5 million people are served by public water supplies that have detected HCBd. Of this population, approximately 1.2 million people could be exposed to over one-half of the health reference level (HRL), based on data from Round 1 sampling, while about 5 million people could be exposed at one-half the HRL, based on Round 2 sampling. Based on the data from Round 1 sampling, about 781,000 individuals were exposed to concentrations at or above the HRL. Based on Round 2 sampling results, an estimated 10,000 persons could be exposed at or above the HRL. The Round 2 based estimate is probably a better estimate of possible exposure since the database is more recent, and more representative of the cross-section population served by ground water.

4.6 Conclusion

In conclusion, while there is evidence that HCBd may have adverse health effects in animals at moderate-to-high doses, available data on human subjects are limited and ambiguous. Nevertheless, using a conservative health reference level, national exposure data indicate that it is unlikely that HCBd will occur at frequencies that are of public health concern. It is therefore unlikely that regulation represents a meaningful opportunity for health risk reduction in persons served by public water systems. All CCL regulatory determinations and further analysis are formally presented in the *Federal Register* Notices (USEPA, 2002a; 67 FR 38222; and USEPA, 2003a; 68 FR 42898).

5.0 TECHNOLOGY ASSESSMENT

If a determination has been made to regulate a contaminant, SDWA requires development of proposed regulations within 2 years of making the decision. It is critical to have suitable monitoring methods and treatment technologies to support regulation development according to the schedules defined in the SDWA.

5.1 Analytical Methods

The availability of analytical methods does not influence EPA's determination of whether or not a CCL contaminant *should* be regulated. However, before EPA actually regulates a contaminant and establishes a Maximum Contaminant Level (MCL), there must be an analytical method suitable for

routine monitoring. Therefore, EPA needs to have approved methods available for any CCL regulatory determination contaminant before it is regulated with an NPDWR. These methods must be suitable for compliance monitoring and should be cost effective, rapid, and easy to use.

Hexachlorobutadiene is an unregulated contaminant for which monitoring was required under the Unregulated Contaminant Monitoring Program (USEPA, 1987; 52 FR 25690). It already has well-documented analytical methods developed specifically for low-level drinking water analyses.

For hexachlorobutadiene, there are two analytical methods available. EPA Method 524.2 is a well established, and sensitive, purge and trap gas chromatographic mass spectrometry (MS) method with a detection limit of 0.11 µg/L. EPA Method 502.2, a purge and trap method using conventional gas chromatography detectors (PID and ELCD in series), has a method detection limit (MDL) of 0.06 µg/L.

5.2 Treatment Technology

Treatment technologies also do not influence the determination of whether or not a contaminant should be regulated. But before a contaminant can be regulated with an NPDWR, treatment technologies must be readily available. EPA's Office of Research and Development (ORD) has researched treatment technologies for all of the organic compounds listed as regulatory determination priorities on the CCL, including hexachlorobutadiene. The two appropriate technologies reviewed were granular activated carbon (GAC) and air stripping.

Granular activated carbon treatment removes contaminants via the physical and chemical process of sorption, by which the contaminants attach to the carbon surface as water passes through the carbon bed. Activated carbon has a large sorption capacity for many water impurities including synthetic organic contaminants, taste and odor causing compounds, and some species of mercury (USEPA, 1998a). Adsorption capacity is typically represented by the Freundlich isotherm constants, with higher Freundlich K values indicating greater sorption potential.

Air stripping involves the continuous contact of air with the water being treated, allowing volatile dissolved contaminants to transfer from the source water to the air. After contact, the "contaminated air" is swept from the system, taking the contaminant out of contact with the treated water. The driving force for the water-to-air transfer of the volatile contaminants is the contaminant's concentration gradient between the water and air. The Henry's Law constant is a commonly used indicator of the tendency of a contaminant to partition from water to air. A larger Henry's constant indicates a greater equilibrium of the contaminant in the air. Thus, contaminants having larger Henry's constants are more easily removed by air stripping.

Predictive computer modeling and specific chemical characteristics were used to determine the isotherm constants needed to evaluate the two treatment technologies. The rule of thumb used for SDWA compounds, learned through the development of cost-and-technology documents to support other drinking water regulations, is that GAC is considered to be cost-effective if the contaminant has a

Freundlich (K) value above 200 (Speth and Adams, 1993). For air stripping, a compound with a Henry's constant above dibromochloropropane (0.005) or ethylene dibromide (0.037) is considered strippable at a reasonable cost.

Hexachlorobutadiene has a predicted Freundlich (K) value of 154,000 and a predicted Henry's Law constant of 1.1. Therefore, both GAC and air stripping are applicable treatment technologies.

6.0 SUMMARY AND CONCLUSIONS - DETERMINATION OUTCOME

Three statutory criteria are used to guide the determination of whether regulation of a CCL contaminant is warranted: 1) the contaminant may adversely affect the health of persons; 2) the contaminant is known or is likely to occur in public water systems with a frequency, and at levels, of public health concern; and 3) regulation of the contaminant presents a meaningful opportunity for health risk reduction for persons served by public water systems. As required by SDWA, a decision to regulate a contaminant commits the EPA to propose a Maximum Contaminant Level Goal (MCLG) and promulgate a National Primary Drinking Water Regulation (NPDWR) for the contaminant. A decision not to regulate a contaminant is considered a final Agency action and is subject to judicial review. The Agency can choose to publish a Health Advisory (a nonregulatory action) or other guidance for any contaminant on the CCL that does not meet the criteria for regulation.

While available toxicological data indicate that HCBD has the potential to cause adverse health effects in animals, data on human health effects are limited to a few studies of occupational exposure to HCBD. Data collected from inhalation exposure are often confounded by simultaneous exposures to other chemicals in an occupational setting. Such equivocal data has made it difficult to establish a relationship between HCBD exposure and toxic/cytogenetic effects in human.

Evidence indicates that renal damage may be caused by acute, subchronic, or chronic HCBD oral exposures in rodents. A few animal studies have also reported liver effects and neurotoxicity. Review of animal dose-response data suggests that subchronic and chronic LOAEL values for HCBD toxicity are generally at 2 mg/kg-day and above. The EPA has classified HCBD as a Group C, possible human carcinogen (USEPA, 1986) and set the reference dose for HCBD at 2×10^{-4} mg/kg-day (1998a).

HCBD in the United States is generated as a waste by-product from the chlorination of hydrocarbons. Monitoring data indicate that HCBD is infrequently detected in public water supplies, however, when it is detected, HCBD rarely exceeds the HRL or a value of one-half the HRL. The physiochemical properties of the contaminant and the available data for environmental fate indicate that HCBD in surface water is likely to be rapidly degraded by biotic and abiotic process, although it has the potential for bioaccumulation.

USGS NAWQA studies to date have not reported detections of HCBD in ambient water, although HCBD has been reported through the Toxic Release Inventory. The contaminant has also been

detected at a very low percentage of ATSDR HazDat and CERCLA NPL sites. Detection of HCBd in PWS samples collected under SDWA indicate low occurrence estimates for Round 1 and Round 2 monitoring, with only 0.13% and 0.05%, respectively, of all samples showing detections. Significantly, the values for the 99th percentile and median concentrations of all samples are less than the Minimum Reporting Level. For Round 1 samples with detections, the median concentration is 0.25 µg/L and the 99th percentile concentration is 10 µg/L. Median and 99th percentile concentrations for Round 2 detections are 0.30 µg/L and 1.5 µg/L, respectively. Systems with detections only constitute 0.4% of Round 1 systems and 0.2% for Round 2. National estimates for the population served by PWSs with detections are also low, especially for detections greater than the Health Reference Level of 0.9 µg/L. For both rounds, the estimates are less than 0.5% of the national PWS population.

Approximately 2–5 million people are served by systems with detections of HCBd. When average daily intakes from drinking water are compared with intakes from air, drinking water accounts for a relatively small proportion of total HCBd intake. Relative intake rates from food may be higher, while intakes from soil are unknown.

EPA considers exposure to both the general population and sensitive populations, including the fetus, infant, and children, in making its regulatory determination. Existing nephropathy or age-related kidney degeneration has been observed to increase the risk of renal injury in humans. Therefore, sensitive populations for HCBd exposure may include people with pre-existing kidney or liver damage, or the elderly. An extra factor of ten is included in the health reference level to add protection for sensitive subpopulations.

In conclusion, while there is evidence that HCBd is capable of causing adverse health effects in humans, it is unlikely to occur with a frequency, or at levels, of public health concern. Monitoring data indicate that hexachlorobutadiene is infrequently detected in public water supplies; when HCBd is detected, it very rarely exceeds the HRL or a value of one-half the HRL. Therefore regulation of hexachlorobutadiene is unlikely to represent a meaningful opportunity for health risk reduction. All CCL regulatory determinations and further analysis are formally presented in the *Federal Register* Notices (USEPA, 2002a; 67 FR 38222; and USEPA, 2003a; 68 FR 42898).

This page intentionally left blank.

REFERENCES

- Agency for Toxic Substances and Disease Registry (ATSDR). 1994. *Toxicological Profile for Hexachlorobutadiene*. TP-93/08. U.S. Department of Health and Human Services, Public Health Service. 135 pp. and appendices.
- ATSDR. 1995. *ToxFAQ for Hexachlorobutadiene*. Atlanta, GA: Agency for Toxic Substances and Disease Registry. Available on the Internet at <http://www.atsdr.cdc.gov/tfacts42.html> Last modified September, 1995.
- ATSDR. 2000. *Hazardous Substance Release and Health Effects Database*. Available on the Internet at: <http://www.atsdr.cdc.gov/hazdat.htm> Last modified August 19, 2000.
- Badaeva, L.N., L.M. Ovsyannikova and N.I. Kiseleva. 1985. [Manifestation of Neurotoxic Effect of Chloroorganic Pesticide Hexachlorobutadiene During Postnatal Period of Ontogenesis in Rats]. *Arch. Anat. Gistol. Embriol.* 89:44-49 (original in Russian; as cited in WHO, 1994).
- Cadmus. 2000. *Methods for Estimating Contaminant Occurrence and Exposure in Public Drinking Water Systems in Support of CCL Determinations*. Draft report to EPA, Washington, D.C., by Cadmus Group, Waltham, MA, July 25, 2000.
- Harleman, J.H. and W. Seinen. 1979. Short-Term Toxicity and Reproduction Studies in Rats with Hexachloro-(1,3)-butadiene. *Toxicol. Appl. Pharmacol.* 47:1-14.
- Hook, J.B., J. Ishmael and E.A. Lock. 1983. Nephrotoxicity of Hexachloro-1,3-butadiene in the Rat: the Effect of Age, Sex, and Strain. *Toxicol. Appl. Pharmacol.* 67:122-131.
- Howard, Philip H. 1989. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals: Volume 1: Large Production and Priority Pollutants*. Chelsea, MI: Lewis Publishers, Inc. 574 pp.
- Jonker, D., R.A. Woutersen, P.J. van Bladeren, et al. 1993b. Subacute (4-wk) Oral Toxicity of a Combination of Four Nephrotoxins in Rats: Comparison with the Toxicity of the Individual Compounds. *Food Chem. Toxicol.* 31:125-136.
- Kociba, R.J., D.G. Keyes, G.C. Jersey, et al. 1977. Results of a 2-Year Chronic Toxicity Study with Hexachlorobutadiene in rats. *Am. Ind. Hyg. Assoc. J.* 38:589-602.
- Kolpin, D.W., J.E. Barbash, and R.J. Gilliom. 2000. Pesticides in Ground Water of the United States, 1992-1996. *Ground Water.* 38(6):858-863.

- Lapham, Wayne W., Kathleen M. Neitzert, Michael J. Moran, and John S. Zogorski. 1997. USGS Compiles Data Set for National Assessment of VOCs in Ground Water. *G. Water Mon. Remed.* 17(4):147-157.
- Larson, S.J., R.J. Gilliom, and P.D. Capel. 1999. *Pesticides in Streams of the United States--Initial Results from the National Water-Quality Assessment Program*. US Geological Survey Water-Resources Investigations Report 98-4222. 92 pp. Available on the Internet at: <http://water.wr.usgs.gov/pnsp/rep/wrir984222/>
- Lash, L.H., R.M. Nelson, R.A. Dyke, et al. 1990. Purification and Characterization of Human Kidney Cytosolic Conjugate Beta-Lyase Activity. *Drug Metab. Dispos.* 18:50-54.
- Leahy, P.P., and T.H. Thompson. 1994. *The National Water-Quality Assessment Program*. US Geological Survey Open-File Report 94-70. 4 pp. Available on the Internet at: <http://water.usgs.gov/nawqa/NAWQA.OFR94-70.html> Last updated August 23, 2000.
- Lock, E.A., J. Ishmael and J.B. Hook. 1984. Nephrotoxicity of hexachloro-1,3-butadiene in the Mouse: The Effect of Age, Sex, Strain, Monooxygenase Modifiers, and the Role of Glutathione. *Toxicol. Appl. Pharmacol.* 72:484-494.
- Lock, E.A. 1994. The Role of Mechanistic Studies in Understanding Target Organ Toxicity. *Arch. Toxicol.* 16(Suppl.):151-160.
- Lopes, Thomas J. and Shannon G. Dionne. 1998. *A Review of Semivolatile and Volatile Organic Compounds in Highway Runoff and Urban Stormwater*. US Geological Survey Open-File Report 98-409. 67 pp.
- National Toxicology Program (NTP). 1991. Toxicity Studies of Hexachloro-1,3-Butadiene in B6C3F₁ Mice (feed studies). National Toxicology Program US Department of Health and Human Services, Public Health Service, National Institute of Health, Research Triangle Park, NC. NIH Publication No. 91-3120.
- Reichert, D., T. Neudecker and S. Schutz. 1984. Mutagenicity of Hexachlorobutadiene, Perchlorobutenoic Acid and Perchlorobutenoic Acid Chloride. *Mutat. Res.* 137:89-93.
- Schrenk, D. and W. Dekant. 1989. Covalent Binding of Hexachlorobutadiene Metabolites to Renal and Hepatic DNA. *Carcinogenesis* 10:1139-1141.
- Schwetz, B.A., F.A. Smith and C.G. Humiston. 1977. Results of a Reproduction Study in Rats Fed Diets Containing Hexachlorobutadiene. *Toxicol. Appl. Pharmacol.* 42:387-398.

- Speth, T.F. and J.Q. Adams. 1993. GAC and Air-Stripping Design Support for the Safe Drinking Water Act. In: *Strategies and Technologies for Meeting SDWA Requirements*. Eds. R. Clark and R.S. Summers. Lancaster, PA: Technomic Publ. Co.
- Squillace, Paul J., Michael J. Moran, Wayne W. Lapham, Curtis V. Price, Rick M. Clawges, and John S. Zogorski. 1999. Volatile Organic Compounds in Untreated Ambient Groundwater of the United States, 1985-1995. *Env. Sci. and Tech.* 33(23):4176-4187.
- Stott, W.T., J.F. Quast and P.G. Watanabe. 1981. Differentiation of the Mechanisms of Oncogenicity of 1,4-Dioxane and 1,3-Hexachlorobutadiene in the Rat. *Toxicol. Appl. Pharmacol.* 60:287-300.
- US Environmental Protection Agency (USEPA). 1986. Guidelines for Carcinogen Risk Assessment. *Federal Register* 51, no. 185: 33992.
- USEPA. 1987. National Primary Drinking Water Regulations-Synthetic Organic Chemicals; Monitoring for Unregulated Contaminants; Final Rule. *Federal Register* 52, no. 130 (8 July): 25690.
- USEPA. 1989. *Hexachlorobutadiene: Drinking Water Health Advisory*. Washington, DC: Office of the Assistant Administrator for Water. 23 pp.
- USEPA. 1991. National Primary Drinking Water Regulations - Synthetic Organic Chemicals and inorganic Chemicals; Monitoring for Unregulated Contaminants; National Primary Drinking Water Regulations Implementation; National Secondary Drinking Water Regulations; Final Rule. *Federal Register* 56, no. 20 (30 January): 3526.
- USEPA. 1992. Drinking Water; National Primary Drinking Water Regulations – Synthetic Organic Chemicals and Inorganic Chemicals; National Primary Drinking Water Regulations Implementation. *Federal Register* 57, no. 138 (17 July): 31776.
- USEPA. 1996. *Emergency Planning and Community Right-to-Know Section 313, List of Toxic Chemicals*. Washington, D.C.: USEPA. Available on the Internet at: <http://www.epa.gov/tri/chemls2.pdf>. Last modified March 23, 2000. Link to site at: <http://www.epa.gov/tri/chemical.htm>
- USEPA. 1998a. Announcement of the Drinking Water Contaminant Candidate List; Notice. *Federal Register* 63, no. 40 (2 March):10273.
- USEPA. 1998b. Ambient Water Quality Criteria for the Protection of Human Health: Hexachlorobutadiene (Draft). Washington, D.C.: Office of Water. EPA Report 822-R-98-004.
- USEPA. 1999a. Suspension of Unregulated Contaminant Monitoring Requirements for Small Public Water Systems; Final Rule and Proposed Rule. *Federal Register* 64, no. 5 (8 January): 1494.

- USEPA. 1999b. Revisions to the Unregulated Contaminant Monitoring Regulation for Public Water Systems; Final Rule. *Federal Register* 64, no. 180 (17 September): 50556.
- USEPA. 1999c. *Superfund Hazardous Waste Site Basic Query Form*. Washington, D.C.: USEPA. Available on the Internet at: <http://www.epa.gov/superfund/sites/query/basic.htm> Last modified December 1, 1999.
- USEPA. 1999d. *A Review of Contaminant Occurrence in Public Water Systems*. EPA Report 816-R-99-006. Office of Water. 78 pp.
- USEPA. 2000a. *TRI Explorer: Are Year-to-Year Changes Comparable?* Washington, D.C.: USEPA. Available on the Internet at: www.epa.gov/triexplorer/years.htm Last modified May 5, 2000.
- USEPA. 2000b. *TRI Explorer: Trends*. Washington, D.C.: USEPA. Available on the Internet at: <http://www.epa.gov/triexplorer/trends.htm>. Last modified May 5, 2000.
- USEPA. 2000c. *The Toxic Release Inventory (TRI) and Factors to Consider when Using TRI Data*. Washington, D.C.: USEPA. Available on the Internet at: <http://www.epa.gov/tri/tri98/98over.pdf>. Last modified August 11, 2000. Link to site at: <http://www.epa.gov/tri/tri98>
- USEPA. 2000d. *What is the Toxic Release Inventory?* Washington, D.C.: USEPA. Available on the Internet at: <http://www.epa.gov/tri/general.htm> Last modified February 28, 2000.
- USEPA. 2000e. *Water Industry Baseline Handbook*. Second Edition (Draft). Washington, D.C.: US Environmental Protection Agency.
- USEPA. 2001a. *Analysis of National Occurrence of the 1998 Contaminant Candidate List Regulatory Determination Priority Contaminants in Public Water Systems*. Office of Water. EPA report 815-D-01-002. 77 pp.
- USEPA. 2001b. *Occurrence of Unregulated Contaminants in Public Water Systems: An Initial Assessment*. Office of Water. EPA report 815-P-00-001. Office of Water. 50 pp.
- USEPA. 2002a. Announcement of Preliminary Regulatory Determinations for Priority Contaminants on the Drinking Water Contaminant Candidate List. *Federal Register* 67, no. 106 (3 June): 38222.
- USEPA. 2002b. *Occurrence Estimation Methodology and Occurrence Findings Report for the Six-Year Review of Existing National Primary Drinking Water Regulations*. EPA Report/815-R-03-006, Office of Water. June 2003.

USEPA. 2003a. Announcement of Regulatory Determinations for Priority Contaminants on the Drinking Water Contaminant Candidate List; Notice. *Federal Register* 68, no. 138 (18 July): 42898.

USEPA. 2003b. *Health Effects Support Document for Hexachlorobutadiene*. Office of Water. EPA Report 822-R-03-002. February 2003. 135pp.

Vamvakas, S., F.J. Kordowich, W. Dekant, et al. 1988. Mutagenicity of Hexachloro-1,3-butadiene and its S Conjugates in the Ames Test -- Role of Activation by the Mercapturic Acid Pathway in its Nephrocarcinogenicity. *Carcinogenesis*. 9:907-910.

Vamvakas, S., W. Dekant and D. Henschler. 1989. Genotoxicity of Haloalkene and Haloalkane Glutathione S-Conjugates in Porcine Kidney Cells. *Toxicol. In Vitro*. 3:151-156.

WHO. 1994. *Environmental Health Criteria 156, Hexachlorobutadiene*. Geneva: World Health Organization, International Programme on Chemical Safety.

This page intentionally left blank.

APPENDIX A: Abbreviations and Acronyms

ACGIH	- American Conference of Governmental Industrial Hygienists
ATSDR	- Agency for Toxic Substances and Disease Registry
CAS	- Chemical Abstract Service
CCL	- Contaminant Candidate List
CERCLA	- Comprehensive Environmental Response, Compensation & Liability Act
CMR	- Chemical Monitoring Reform
CWS	- community water system
DBCP	- dibromochloropropane
ELCD	- electrolytic conductivity detector
EPA	- Environmental Protection Agency
EPCRA	- Emergency Planning and Community Right-to-Know Act
FR	- federal register
GAC	- granular activated carbon (treatment technology for organic compounds)
GC	- gas chromatography (a laboratory method)
g/mol	- grams per mole
GW	- ground water
HA	- Health Advisory
HAL	- Health Advisory level
HCBD	- hexachlorobutadiene
HRL	- Health Reference Level
IOC	- inorganic compound
IRIS	- Integrated Risk Information System
LOAEL	- lowest observed adverse effect level
MCL	- maximum contaminant level
MCLG	- maximum contaminant level goal
MDL	- method detection limit
mg/L	- milligrams per liter
MRL	- minimum reporting level
MS	- mass spectrometry (a laboratory method)
MTD	- maximum tolerated dose
NAWQA	- National Water Quality Assessment Program
NCOD	- National Drinking Water Contaminant Occurrence Database
NDWAC	- National Drinking Water Advisory Council
NIOSH	- National Institute for Occupational Safety and Health
NIRS	- National Inorganic and Radionuclide Survey
NOAEL	- no-observed adverse effect level
NPDWR	- National Primary Drinking Water Regulation
NPL	- National Priorities List
NPS	- National Pesticide Survey
NTNCWS	- non-transient non-community water system
OGWDW	- Office of Ground Water and Drinking Water

ORD	- Office of Research and Development
PGWD	- Pesticides in Ground Water Database
PID	- photoionization detector
ppm	- part per million
PWS	- public water system
RCRA	- Resource Conservation and Recovery Act
RfD	- Reference Dose
SARA	- Superfund Amendments and Reauthorization Act
SDWA	- Safe Drinking Water Act
SDWIS	- Safe Drinking Water Information System
SDWIS/FED	- Federal Safe Drinking Water Information System
SOC	- synthetic organic compound
SW	- surface water
TRI	- Toxic Release Inventory
UCM	- Unregulated Contaminant Monitoring
UCMR	- Unregulated Contaminant Monitoring Regulation/Rule
URCIS	- Unregulated Contaminant Monitoring Information System
USEPA	- United States Environmental Protection Agency
USGS	- United States Geological Survey
VOC	- volatile organic compound
µg/L	- micrograms per liter
µg/kg	- micrograms per kilogram
>MCL	- percentage of systems with exceedances
>MRL	- percentage of systems with detections