APPENDIX A-1

CHEMICALS OF POTENTIAL INTEREST

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APPENDIX A-1

CHEMICALS OF POTENTIAL INTEREST

Table A-1 presents a comprehensive list of compounds typically found in
- hazardous waste; and
- hazardous waste combustion stack gas emissions.

Table A-1 identifies the Chemical Abstracts Service (CAS) number for each compound, and indicates whether a compound has been identified as a potential COPC by:
- U.S. EPA and state risk assessment reference documents;
- Emission test results that have identified the compound in the emissions from hazardous waste combustion facilities; or
- Other literature that suggests that the risks from the compound may be significant.

We provide Table A-1 to help you make sure that the trial/risk burn considers the full range of compounds potentially emitted from a combustor, and the appropriate analytical method. A risk assessment won't necessarily evaluate every metal and potential PIC listed in Table A-1. Once the trial/risk burn stack tests are completed, the risk assessment COPCs are selected from the stack test data, rather than Table A-1.

This discussion lists reference documents for each of the columns in Table A-1 and briefly describes the quality of data associated with these references. The evaluation of chemical toxicity is also discussed at the end of this section. This information is presented for informational purposes only.

A1.1 COLUMN 1: CHEMICAL ABSTRACTS SERVICE (CAS) NUMBER

The CAS number is a unique number assigned to each compound in the table.

A1.2 COLUMN 2: COMPOUND NAME

The most common compound name is listed. Where appropriate, common synonyms are also listed to help you identify particular compounds.

A1.3 COLUMN 3: COMPOUNDS LISTED IN 40 CFR PART 261 APPENDIX VII OR VIII

Appendix VII of Title 40 Code of Federal Regulations (40 CFR) Part 261 identifies compounds for which specific hazardous wastes, from specific and nonspecific sources, are listed (U.S. EPA 1995). Appendix VIII of 40 CFR Part 261 identifies acute hazardous wastes and toxic hazardous wastes associated with commercial chemical products, manufacturing chemical intermediates, and off-specification commercial chemical products (U.S. EPA 1995). This column lists hazardous waste codes for the associated compounds. We provide this list for reference purposes only, because it's commonly cited by other U.S. EPA combustion risk assessment documents as an original source of the product of incomplete combustion (PIC) lists. An explanation of the reasons for including a COPC on this list is beyond the scope of the HHRAP.

A1.4 COLUMN 4: CHEMICAL-SPECIFIC DATA AVAILABLE

This column lists those compounds for which the following are available (as presented in Appendix A-2): (1) chemical-specific physical and chemical information, and (2) chemical-specific fate-and-transport information.

A1.5 COLUMN 5: PICS RECOMMENDED BY U.S. EPA (1994a) FOR ALL HUMAN HEALTH RISK ASSESSMENTS (HHRA)

Compounds marked with an "X" in this column are identified by U.S. EPA (1994a) as PICs to be included in all HHRAs. U.S. EPA (1994a) does not describe the basis or references for including these PICs in all HHRAs. More information regarding these compounds is presented in Section 2.2 of the HHRAP.

A1.6 COLUMN 6: PICS IDENTIFIED IN COMBUSTION UNIT EMISSIONS (U.S. EPA 1993)

Compounds marked with an "X" in this column are identified in U.S. EPA (1993) as PICs. The source documents cited by U.S. EPA (1993) are described in the following subsections. These references have been cited by this and other Agency reference documents as "sources" of information regarding PIC emissions from hazardous waste combustors. U.S. EPA (1993) has, in turn, been cited by later guidance documents as a "source" of information regarding PIC emissions from hazardous waste combustors. However, as is indicated by the listing of the references from Dempsey and Oppelt (1993) (which is a summary of existing information), many of the reference documents appear to simply cite additional "sources" of information. We've not yet identified the original research and sampling data regarding PIC emissions but, based on a preliminary review of the information below, the sources of the "original" information cited by all of the most common reference documents may be limited and may have been published over 15 years ago.

A1.6.1 Demsey and Oppelt (1993)

The sections of Demsey and Oppelt (1993) regarding PICs from hazardous waste combustion facilities ("Combustion Byproduct Emissions" and "Table XVII: Organics that Could Potentially be Emitted from Devices Burning Hazardous Waste") cite the following references:

- U.S. EPA (1989b) didn't include a list of PICs from combustion sources. U.S. EPA (1989b) discussed ways of ensuring that PIC emissions don't pose an unacceptable risk to human health and the environment. Stack gas carbon monoxide (CO) concentration is a good indicator of combustion efficiency; therefore, controlling CO is a prudent and reasonable approach for minimizing the potential risk from PICs. The destruction and removal efficiency (DRE) standard of 40 CFR Part 264.242(a) limits stack emissions of principal organic hazardous constituents (POHCs) to 0.01 percent (or 0.0001 percent for dioxin-containing waste) of the quantity of POHC in the waste. This standard, however, does not impose a limit on PICs. Therefore, a limit of 100 parts per million by volume (ppmv) (Tier I) was imposed, below which PIC emissions do not pose unacceptable risks to human health. The proposed rule allows a waiver to the 100-ppmv CO limit, by (1) restricting total hydrocarbon (THC) emissions to 20 ppmv (Tier II), or (2) showing that THC emissions do not pose an unacceptable health risk by using prescribed risk assessment procedures.

The above limitations were also provided in the Federal Register, dated January 23, 1981 (U.S. EPA 1981) and April 27, 1990 (U.S. EPA 1990b)

C U.S. EPA (1981) doesn’t contain any information regarding PICs not contained in U.S. EPA (1989b). There is no discussion of “risk” in this document. Although the notice deals with permitting standards, there is no risk-based approach, and it appears to be an entirely technical discussion. Specifically, it deals with updated material for specific parts of 40 CFR.

- 40 CFR Part 122 (Incinerator Facility Permits)
- 40 CFR Part 264 (General Standards for Hazardous Waste Incineration)
- 40 CFR Part 265 (Interim Status Standards for Hazardous Waste Incineration)

Standards are technology-based, not risk-based.

C U.S. EPA (1990a) describes amendments to the hazardous waste incinerator regulations for the following purpose:

> Improve control of toxic metal emissions, HCl emissions, and residual organic emissions; amend the definitions of incinerators and industrial furnaces; propose definitions for plasma arc incinerators and infrared incinerators; propose to regulate carbon regeneration units as thermal treatment devices; and make a number of minor revisions to permitting procedures.

U.S. EPA (1990a) also states the following:

> The database on PIC emissions is limited therefore, the risk assessments may under-estimate risk. The assessments consider only the organic compounds that have been actually identified and quantified. Zero to 60 percent of total unburned hydrocarbon emissions have been chemically identified at any particular facility. Thus, the bulk of the hydrocarbon emissions have not been considered in those risk assessments. Although many of the unidentified, unquantified organic compounds may be non-toxic, some fraction of the organic emissions is undoubtedly toxic. . . .data on typical PIC emissions from hazardous waste combustion sources were compiled and assessed in recent EPA studies. These studies identified 37 individual compounds in the stack gas of the eight full-scale hazardous waste incinerators tested, out of which 17 were volatile compounds and 20 semivolatile compounds. Eight volatile compounds (benzene, toluene, chloroform, trichloroethylene, carbon tetrachloride, tetrachloroethylene, chlorobenzene, and methylene chloride), and one semivolatile compound (naphthalene) were identified most frequently in more than 50 percent of the tests. Some of these compounds are carcinogenic.

The sources for these statements appear to be Wallace et al. (1986) and Trenholm and Lee (1986).

Trenolm and Lee (1986), prepared by Andrew R. Trenholm of Midwest Research Institute and C.C. Lee at the U.S. EPA Hazardous Waste Engineering Research Laboratory, discussed that emissions from incinerators are only characterized for constituents listed in Appendix VIII. However, constituents not listed in Appendix VIII are also emitted from the stacks.

Data was obtained from HWERL-sponsored tests at eight hazardous waste incinerators, nine boilers that co-fired hazardous wastes, and five mineral processing kilns that fired hazardous wastes as fuel. In addition, SVOC emissions data for two municipal solid waste incinerators and seven coal-fired power plants were also reviewed. The common PICs are presented in the following table:

Volatile PICs Most Frequently Present in Stack Gases	
VOCs	**SVOCs**
Benzene	Naphthalene
Toluene	Phenol
Carbon Tetrachloride	Bis(2-ethylhexyl)phthalate
Chloroform	Diethylphthalate
Methylene Chloride	Butylbenzylphthalate
Trichloroethylene	Dibutylphathlate
Tetrachloroethylene	
1,1,1-Trichloroethane	
Chlorobenzene	

Tests were conducted for three incinerator runs to search for constituents not listed in Appendix VIII . These constituents include:

Non-Appendix VIII Constituents Present in Highest Concentrations in Stack Gases	
Acetone	Ethylbenzaldehyde
Ethylbenzene	Ethylbenzoic acid
Acetophenone	Ethylphenol
Benzaldehyde	Ethylphenyl-ethanone
Benzenedicarboxaldehyde	Ethynylbenzene
Benzoic acid	Phenylacetylene
Chlorocyclohexanol	1,1'-(1,4-phenylene)bisethanone
Cyclohexane	Phenylpropenol
Cyclohexanol	Propenylmethylbenzene
Cyclohexene	Tetramethyloxirane
Dioctyl adipate	Trimethylhexane
Ethenyl ethylbenzene	

Emission rates of compounds not in the waste feed were also provided.

- U.S. EPA (1985) didn't include a list of PICs from combustion sources. U.S. EPA (1985) discussed views and reviews by the Environmental Effects, Transport, and Fate Committee of the Science Advisory Board of issues related to the environmental impacts of the incineration of liquid hazardous wastes at sea and on land. Several issues were addressed, including issues concerning the combustion and incineration of hazardous waste. Major findings of the committee were as follows:

    - Fugitive emissions and spills may release as much or more material to the environment than the direct emissions from waste incineration processes.

    - Numerous PICs are formed during the combustion processes. However, only a fraction of them are identified or detected. It is possible that the aggregate of all compound emissions that are not categorized as other POHCs or PICs can be more toxic and pose greater risks than those listed. Although 99.99 percent DRE has been claimed, if the unburned or undetected hydrocarbon output is included, the DRE may actually be less than 99.99 percent. Therefore, the concept of destruction efficiency used by EPA was found to be incomplete and not useful for subsequent exposure assessments. All emissions and effluents must be identified and quantified, including their physical form and characteristics.

    - Local site-specific conditions must be used in characterizing exposure to receptors from waste incinerator emissions.

    - The evaluation of exposure durations and concentrations should be based on a detailed assessment of transport processes and the habits of the exposed organisms. The role of food chains needs particular attention.

    - At a minimum, the toxicities of representative emissions and effluents from incinerators should be tested on sensitive life stages of representative aquatic and terrestrial vertebrates, invertebrates, and plants of ecological importance.

- U.S. EPA (1990b) does not include a list of PICs from combustion sources. It was prepared by the PIC subcommittee of the Science Advisory Board to review the OSW proposal to control emissions of PICs from hazardous waste incinerators by instituting process controls that are based on CO and THC emission concentrations. U.S. EPA risk assessments indicate that emissions of PICs at currently measured levels are not likely to produce human effects. However, because the current DRE standard applies only to designated POHCs, 99.99 percent DRE does not preclude the possibility that emission of PICs could present significant human health risk. The following summarizes the major findings of the subcommittee review.

    - The concept of using CO and THC as guidance for incinerator operational control is reasonable.

    - At low CO levels, CO correlates well with THC; therefore, limiting CO in order to ensure high combustion efficiency and low THC levels is reasonable. At high CO concentrations, CO and THC do not correlate well; therefore, relying solely on the controlling of CO may not provide a reasonable control for THC. Continuous emissions monitoring of THC is preferred. Quantification of PICs alone is not practical with the sampling techniques that are available, primarily because PICs are normally emitted in the range of parts per billion (ppb) to parts per trillion (ppt).

  - A 100-ppmv limit for CO is reasonable. However, supporting documentation does not demonstrate that a CO concentration of 100 ppmv is better than 50 ppmv or 150 ppmv.
  - Continuous emissions monitoring of THC with a cold system appears to be practical for routine operations. However, a hot transfer line produces better analysis of THC concentrations and detection of a larger fraction of the THCs emitted.
  - The database characterizing PICs in emissions would not allow a correlation to be established with CO or THC levels for various combustion devices and conditions. Limited data introduces large uncertainties into U.S. EPA's risk assessment. Therefore, U.S. EPA's site-specific risk assessment process is limited in its usefulness in establishing acceptable THC levels. However, the risk assessment procedures are risk-based.

C U.S. EPA (1987) is a report prepared by Andrew R. Trenholm, Acurex Corporation, California, and staff members from the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. The paper discussed the lack of information on total emissions from combustion of hazardous wastes, particularly under conditions of less than optimal performance. The focus issue was whether additional constituents that are listed in Appendix VIII or not listed in Appendix VIII which were not identified in early tests might be emitted from hazardous waste combustion units. To address this issue and related issues, U.S. EPA initiated this project to qualitatively and quantitatively study the characteristics of all possible effluents, under steady-state and transient conditions. The following summarizes the major findings:

  - THC emissions detected as specific compounds ranged from 50 to 67 percent for five runs and were 91 percent for one run. The fraction of THC not detected is most likely explained by uncertainty in the measurements or other analytical problems.
  - Methane accounted for the largest fraction of THC.
  - Oxygenated aliphatic compounds made up the largest class of compounds among the SVOCs, both in total mass and number of compounds.
  - Transient upsets did not cause significant increases in the concentration of SVOCs or most VOCs. Three VOCs that were increased were methane, methylene chloride, and benzene.
  - Particulate and HCl emissions did not change between the steady-state and transient test runs.

C Duval and Rubey (1976) was prepared by D.S. Duval and W.A. Rubey of the University of Dayton Research Institute, Ohio. The objective of the study was to provide data from which requirements can be assigned for the thermal disposal of kepone. This report was primarily concerned with the high-temperature destruction of kepone, with DDT and Mirex used as comparative Analog. Laboratory tests were conducted to establish destruction temperature characteristics of the vaporized pesticides at preselected residence times. The following summarizes the major findings.

- Kepone was essentially destroyed at a 1-second residence time and a temperature range of 500°C to 700°C, depending on the pesticide.

- Major decomposition products detected were hexachlorocyclopentadiene and hexachlorobenzene for both kepone and Mirex. These products were formed in different thermal regions.

- The study demonstrated that the chemical nature of the effluent products depends on the temperature and residence time that the basic molecule experiences.

C Duval and Rubey (1977) discusses the experimental destruction temperature and residence time relationships for various PCB compounds and mixtures of PCBs. The document states that "upon thermal stressing in air, PCBs decompose to low-molecular-weight products." However, the document doesn't identify any of these low-molecular-weight products. In fact, the document states directly that the products weren't identified in the study. It further recommends that additional research be conducted on the "degradation products and effluents."

C Dellinger et al. (1984) was prepared by Barry Dellinger and others of the University of Dayton, Ohio. This paper presented the gas-phase thermal stability method under controlled laboratory conditions to rank the incinerability of compounds. The objective of this study was to determine the gas-phase thermal decomposition properties of 20 hazardous organic compounds.

The compounds were selected on the basis of (1) frequency of occurrence in hazardous waste samples, (2) apparent prevalence in stack effluents, and (3) representativeness of the spectrum of hazardous waste organic waste materials. The following summarizes the major findings.

- Gas-phase thermal stability method is a more effective means of ranking the incinerability of hazardous compounds in a waste.

- Numerous PICs were formed during the thermal decomposition of most of the compounds tested. However, PICs were not identified.

- Destruction efficiency of 99.99 percent is achieved at 2 seconds mean residence time in flowing air at 600°C to 950 °C.

- No single physical or chemical property describes the ranking scheme for incinerability.

C Dellinger et al. (1986) was prepared by Barry Dellinger, B. Douglas, L. Hall, John L. Graham, Sueann L. Mazer, and Wayne A. Rubey of the University of Dayton Research Institute, Dayton, Ohio, and Myron Malanchuk of U.S. EPA, Cincinnati, Ohio. The paper discussed the development of an incineration model based on laboratory studies conducted by using the nonflame mode of hazardous waste thermal decomposition. The results of these studies were compared to the flame-mode studies and field tests to evaluate the incineration model proposed. The model was based on the premise that incinerators do not operate continuously at optimum conditions. As a result, 1 percent or more of the feed and its flame treatment products must undergo further decomposition in the nonflame region to meet the DRE criterion of greater than 99.99 percent.

In the past, several methods were used to rank the incinerability of compounds. Nonflame studies, however, indicated that tests on compounds conducted at low oxygen concentrations provided a better correlation with field tests to determine the relative incinerability of compounds. Four experimental studies were conducted to develop and expand the database on POHCs and PICs.

Studies were conducted on individual compounds to evaluate degradation compounds and PICs from the original parent compound. The thermal degradation of 2,3',4,4',5-PCB was studied under four reaction atmospheres (at varying levels of oxygen) at a constant gas phase residence time of 2.0 seconds. Tests were conducted at temperatures ranging from 500ºC to 1,000ºC. Tests indicated that the yield of combustion products decreased with increased oxygen levels. Numerous major degradation products were identified from the thermal degradation of 2,3',4,4',5-PCB, including:

- Penta-, tetra-, and trichlorodibenzofurans
- Tetra- and trichlorobiphenyls
- Tri- and dichlorobenzene
- Tetra- and trichloronaphthalene
- Tri- and dichlorochlorophenylethlyene
- Tetrachlorobiphenylenes
- C_9H_8OCl
- $C_{10}H_3Cl_3$

Thermal decomposition of chloroform was studied. Numerous decomposition products were identified, including:

- CCl_4
- $C_2H_4Cl_2$
- C_2HCl_3
- C_2HCl_5
- C_2Cl_2
- C_2Cl_4
- C_3Cl_4
- C_4Cl_6

Thermal decomposition of polychlorinated phenols was studied in nitrogen (N_2) and oxygen atmospheres because of the potential formation of polychlorinated dibenzodioxins. Pentachlorophenol (PCP) thermal decomposition was studied. Numerous decomposition products of PCP were identified in N_2 and/or air atmospheres, including:

- Dichlorobutadiyne (in N_2)
- Tetrachloroethylene (in air)
- Tetrachloropropyne (in air)
- Trichlorofuran (in air)
- Tetrachlorofuran (in air)
- Trichlorobenzene (in N_2 and air)
- Tetrachlorobenzene (in N_2 and air)
- Pentachlorobenzene (in N_2 and air)
- Hexachlorobenzene (in N_2)

- Octachlorostyrene (in N_2)
- Hexachlorodihydronaphthalene (in N_2 and air)

The paper concluded that PICs in the air atmosphere may have formed directly from the parent material, whereas, in the nitrogen atmosphere, the principal PICs may have evolved from the thermal decomposition of other PICs.

C Kramlich et al. (1984) doesn't include a list of PICs from combustion sources. It was prepared by J.C. Kramlich, W.R. Seeker, and M.P. Heap of Energy and Environmental Research Corporation, California; and C.C. Lee of the Industrial Waste Combustion Group, U.S. EPA. This paper presented a research program to study the flame-mode incineration of hazardous waste liquids in laboratory scale reactors. The objective of this study was to supply the flame-mode data used in evaluating the applicability of various approaches to ranking the ease of incinerability.

Five compounds were tested—chloroform, 1,1-dichloroethane, benzene, acrylonitrile, and chlorobenzene—because (1) their range of incinerabilities is broad, and (2) they are representative of liquid hazardous wastes. The following summarizes the findings.

- The flame section of the incinerator destroys greater than 99.995 percent of the wastes.

- The post-flame region destroys the remainder of the wastes.

- The destruction efficiency is reduced because of flame-related failures.

- Incinerability ranking depends on actual failure condition.

- No incinerability ranking system completely predicts the destruction efficiency of the compounds tested for all failure conditions.

C Trenholm and Hathaway (1984) was prepared by Andrew Trenholm and Roger Hathaway of Midwest Research Institute (MRI) in Missouri, and Don Oberacker, U.S. EPA, Cincinnati, Ohio. PICs were defined as any Appendix VIII hazardous organic constituent detected in the stack gas but not present in the waste feed at a concentration of 100 micrograms per gram or higher. Benzene and chloroform were the most commonly found PICs. PIC emissions were comparable to POHC emissions in concentration and total mass output. This document discussed PIC formation mechanisms and criteria for PIC formations.

MRI conducted a series of tests at eight operating hazardous waste incineration facilities and analyzed the collected samples for PICs. The tests were part of the technical support of U.S. EPA's preparation of a regulatory impact analysis for hazardous waste incinerators. Each incinerator had a liquid injection burner, and some facilities also included a rotary kiln or hearth. Three incinerators had no air pollution control devices. The remaining five had wet scrubbers for HCl control, and four of these had other particulate control devices. Twenty-nine compounds were classified as PICs from the eight incinerator tests and are presented in Table A1.6-1. In general, PIC concentrations were slightly higher than POHC concentrations, although this ratio varied from site to site. PIC output rate very rarely exceeded 0.01 percent of the POHC input rate. The document stated that the measurement of Appendix VIII compounds at low concentrations in the waste feed, auxiliary fuel, and inflow streams to control systems is often necessary to explain the presence of PICs.

TABLE A1.6-1
PICS IDENTIFIED BY TRENHOLM AND HATHAWAY (1984)

PICs Found In Stack Effluents			
PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Bromochloromethane	1	14	14
Bromodichloromethane	4	3	32
Bromoform	3	0.2	24
Bromomethane	1	1	1
Carbon disulfide	1	32	32
Chlorobenzene	3	1	10
Chloroform	5	1	1,330
Chloromethane	1	3	3
Chlorophenol, o-	1	22	22
Dibromochloromethane	4	1	12
Dichlorobenzene	1	4	4
Diethyl phthalate	1	7	7
Dimethylphenol, 2,4-	1	21	21
Fluoranthene	1	1	1
Hexachlorobenzene	1	7	7
Methyl ethyl ketone	1	3	3
Methylene chloride	2	2	27
Methylene bromide	1	18	18
Naphthalene	3	5	100
Nitrophenol, o-	2	2	50
Pentachlorophenol	1	6	6
Phenol	2	4	22
Pyrene	1	1	1
Tetrachloroethylene	3	0.1	2.5
Toluene	2	2	75
Trichlorobenzene	1	7	7
Trichloroethane, 1,1,1,-	3	0.1	1.5
Trichlorophenol, 2,4,6-	1	110	110

Notes:

ng/L = Nanograms per liter
PIC = Product of incomplete combustion

- Olexsey et al. (1985) was prepared by Robert A. Olexsey and others of the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. This document discussed PIC generation mechanisms and criteria for PIC formations. The paper provided data on emissions of PICs during full-scale tests conducted on incinerators and boilers burning hazardous waste (Trenholm et al. 1984; Castaldini et al. 1984). The documents referenced by this paper summarized a series of full-scale tests conducted on seven incinerators and five boilers conducted by U.S. EPA to support its regulatory development for incinerators and boilers. Commonly found PICs identified in these tests are presented in Tables A1.6-2 and A1.6-3.

TABLE A1.6-2
VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN BOILER EMISSIONS (OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	3	9.4	270
Chloroform	5	4.2	1,900
Chloromethane	4	4.6	410
Dichloroethane, 1,2-	3	1.3	1,200
Methylene chloride	4	83	2,000
Tetrachloroethylene	5	0.3	760
Trichloroethane, 1,1,1-	3	5.9	270

Notes:
ng/L = Nanograms per liter
PIC = Product of incomplete combustion

TABLE A1.6-3
VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN INCINERATOR EMISSIONS (OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Methylene chloride	2	2	27
Tetrachloroethylene	3	0.1	2.5
Toluene	2	2	75
Trichloroethane, 1,1,1-	3	0.1	1.5

Notes:
ng/L = Nanograms per liter
PIC = Product of incomplete combustion

- For incinerators, ratios of PIC emissions to POHC input ranged from 0.00007 to 0.0028 percent; and ratios of PIC emissions to POHC emissions ranged from 0.01 to 3.89. For boilers, ratios of PIC emissions to POHC input ranged from 0.0032 to 0.3987 percent, and ratios of PIC emissions to POHC emissions ranged from 5.44 to 22.5. These data indicated that PIC emissions were higher for boilers than for incinerators; that is, PIC emissions were reduced with increased POHC

DRE which is higher for incinerators. The document proposed seven methods to control PICs and recommended further research on PIC generation mechanisms and control technologies.

C Trenholm et al. (1992) was prepared by Andrew R. Trenholm and David W. Kapella of MRI in North Carolina and Gary D. Hinshaw of MRI in Missouri. The paper discusses the following issues regarding emissions from incinerators that burn hazardous waste:

- emissions of specific constituents presented in Appendix VIII,
- emissions of specific compounds or types of compounds, and
- data on the size and molecular weight of compounds emitted.

The following were among the major issues discussed.

- PICs were studied through U.S. EPA-sponsored tests at eight incinerators, nine industrial boilers, and five mineral processing kilns. The study was limited to compounds presented in Appendix VIII. In all, 52 organic compounds (32 VOCs and 20 SVOCs) were identified. The VOC concentrations were significantly higher than the SVOC concentrations. PICs listed in this paper included:
    - benzene,
    - toluene,
    - carbon tetrachloride,
    - trichloromethane,
    - dichloromethane,
    - trichloroethene,
    - tetrachloroethene,
    - 1,1,1-trichloroethane,
    - cholorobenzene,
    - naphthalene, and
    - phenol.

- From the U.S. EPA-sponsored tests, (1) volatile compounds listed in Appendix VIII identified were only a fraction—sometimes about one-half—of the total organic compounds identified, and (2) semivolatile compounds not listed in Appendix VIII identified were three to 30 times the quantity of organic compounds listed in Appendix VIII . Table A1.6-4 lists the compounds identified by the U.S. EPA-sponsored tests.

TABLE A1.6-4
MOST FREQUENTLY IDENTIFIED PICS
(TRENHOLM, KAPELLA, AND HINSHAW 1992)

Appendix VIII Volatile Organic Compounds	Appendix VIII Semivolatile Organic Compounds	Compounds Not Listed in Appendix VIII
Benzene	Bis(2-Ethylhexyl)phthalate	(1,4-Phenylene)bisethanone, 1,1'-
Carbon tetrachloride	Butylbenzylphthalate	Acetone
Chlorobenzene	Dibutylphtahlate	Acetophenone
Chloroform	Diethylphthalate	Benzaldehyde
Methylene chloride	Naphthalene	Benzenedicarboxaldehyde
Tetrachloroethylene	Phenol	Benzoic acid
Toluene		Chlorocyclohexanol
Trichloroethane, 1,1,1-		Cyclohexane
Trichloroethylene		Cyclohexanol
		Ethylbenzene
		Ethylbenzoic acid
		Ethylphenol
		Ethylphenyl-ethanone
		Ethynylbenzene
		Phenylpropenol
		Propenylmethylbenzene
		Tetramethyloxirane
		Trimethylhexane

- A study of hazardous waste incinerator stack effluent was conducted to characterize the types of compounds emitted. Twenty-nine compounds were identified at a concentration range of 0.1 to 980 nanograms per liter. Methane, chloromethane, and chloroform accounted for more than one-half of the total mass of VOCs detected. Other than methane, oxygenated aliphatic hydrocarbons formed the highest fraction of the total emissions.

- Based on the incinerator stack effluent study, it was found that as combustion conditions deteriorate, increases in mass emissions are first noted with VOCs. Emissions of these compounds, most notably C1 to C3 compounds, increase proportionately more than larger compounds. For larger compounds, available data indicate that emission increases are more likely to be aromatic compounds.

A1.6.3 CARB (1990b)

CARB prepared "Technical Support Document of Proposed Dioxins Control Measures for Medical Waste Incinerators" to meet the requirements of California Health and Safety Code Section 39666 that a needs report be prepared for proposed rules. The report presents a proposed airborne toxic control measure for dioxin emissions from medical waste-burning facilities. The report concentrates on dioxin, furan, and cadmium emissions, although other pollutants detected during the tests are listed. Table A1.6-5 lists these pollutants.

TABLE A1.6-5
COPCS IDENTIFIED BY CARB (1990b)

COPC		
Ammonia	Dibromoethane, 1,2-	Nickel
Arsenic	Dichloroethane	Nitrogen oxides
Benzene	Dichloromethane	PM
Bromodichloromethane	Dichloropropane, 1,2-	PAHs
Cadmium	Ethylbenzene	Sulfur dioxide
Carbon dioxide	Freon	Tetrachloroethene
Carbon monoxide	Hydrocarbon, total	Tetratrichloromethylene
Carbon tetrachloride	Hydrogen chloride	Toluene
Chlorobenzenes	Hydrogen fluoride	Tribromomethane
Chlorodibromomethane	Iron	Trichlorethane
Chloroform	Lead	Trichloroethane, 1,1,1-
Chlorophenols	Manganese	Trichloroethylene
Chromium, hexavalent	Mercury	Trichlorotrifluroethane
Chromium, total	Mesitylene	Vinyl chloride
Copper	Methyl isobutyl ketone	Xylenes
Cumene	Napthalene	Zinc

Notes:
PAH = Polynuclear aromatic hydrocarbons
PM = Particulate matter

A1.6.4 CARB (1991)

CARB prepared “Air Pollution Control at Resource Recovery Facilities 1991 Update” to update information presented in its 1984 report, entitled “Air Pollution Control at Resource Recovery Facilities.” Specifically, the document updates available guidelines concerning incinerator technology, emissions control technology, and emission limits for municipal waste, hospital waste, biomass, tire, manure, landfill and digester gas, and sewer sludge incinerators. The document states that its guidelines represent levels that have been achieved by existing facilities.

In addition, the document summarizes the ultimate analysis of waste types undergoing treatment in the facilities described above. An appendix summarizes stack gas analysis data for numerous operating facilities. Pollutants identified in the analyses are summarized in Table A1.6-6.

TABLE A1.6-6
STACK GAS ANALYSIS DATA (CARB 1991)

	Incinerator Type [a]						
Pollutant	**Municipal Waste (5)**	**Hospital Waste (7)**	**Biomass (4)**	**Manure (1)**	**Tire (1)**	**Landfill Gas (20)**	**Sewage Sludge and Digester Gas (5)**
Nitrogen oxides	U	U	U	U	U	U	U
Sulfur oxides	U	U	ND	U	U	U	U
Particulate matter	U	U	U	U	U	U	U
Carbon monoxide	U	U	U	U	U	U	U
Total hydrocarbons	U	U	U	U	U	U	U
Hydrogen chloride	U	U	NA	NA	U	NA	NA
Hydrogen fluoride	U	NA	NA	NA	NA	NA	NA
Amonnia	NA	NA	U	NA	U	NA	NA
Carbon dioxide	U	U	U	U	U	NA	U
Oxygen	U	U	U	U	U	NA	U
Arsenic	U	U	U	NA	U	U	U
Beryllium	U	NA	NA	NA	U	U [b]	U
Cadmium	U	U	U	NA	ND	U [b]	U
Chromium (total)	U	U	U	NA	U	U	U
Chromium (hexavalent)	ND	U	NA	NA	U	NA	NA
Copper	U	NA	NA	NA	NA	U	NA
Mercury	U	U	NA	NA	ND	U	U
Iron	NA	NA	U	NA	NA	NA	NA
Manganese	NA	NA	U	NA	NA	NA	NA
Nickel	U	U	U	NA	ND	U	U
Lead	U	U	U	NA	ND	U	U
Zinc	NA	NA	NA	NA	NA	U	NA
Polyaromatic hydrocarbons [b]	U	NA	U	NA	U	NA	NA
Polychlorinated biphenyls [b]	U	ND	U	NA	U	NA	NA
CP [b]	U	NA	U	NA	U	NA	NA
CB [b]	U	NA	U	NA	U	NA	NA
Benzene	U	U	U	NA	NA	NA	NA
Polychlorinated dibenzo(p) dioxins [b]	U	U	U	NA	U	NA	NA
Polychlorinated dibenzofurans [b]	U	U	U	NA	U	NA	NA
2,3,7,8-Tetrachloro dibenzo(p)dioxin equivalents [b]	U	U	U	NA	U	NA	U

Notes:

U = Detected in at least one emission test
ND = Not detected in any emission test
NA = No analysis

[a] Number in parentheses indicates the number of facilities for which data were tabulated.

[b] Isomers and/or homologues that were not detected were added to total values at one-half the detection limit; pollutant may not have actually been detected.

A1.6.5 U.S. EPA (1988)

This document, referenced by some documents as a 1989 document, was prepared in 1988.

U.S. EPA prepared "Hospital Waste Combustion Study: Data Gathering Phase" to assemble available information on hospital waste combustion so that U.S. EPA can evaluate whether airborne pollutant emissions from hospital waste combustion should be regulated. While preparing this document, U.S. EPA reviewed the pertinent literature to determine which studies would be helpful in completing the database on toxic emissions from medical waste incinerators. The report clearly addresses only those pollutants for which emissions data were found. The data reviewed were mostly for larger, controlled air incinerators; and the more commonly used retort incinerators were not evaluated.

The study identified several categories of pollutants that were measured in stack gases; these are discussed in the following paragraphs.

Where evaluated, acid gases were detected in stack gases. For example, HCl was detected in 24 of 28 tests; HCl concentration not recorded in the remaining four tests.

Particulate matter (PM) was detected in all stack tests for 30 facilities at concentrations ranging from 0.001 grains per dry standard cubic foot (gr/dscf), at a facility with PM add-on control devices, to 0.22 gr/dscf at facilities without such control devices.

Trace metals were detected in stack tests for three medical waste incineration facilities. Metals detected include arsenic, cadmium, chromium, iron, manganese, nickel, and lead. The document also states that fine-particle enrichment processes could lead to emissions of molybdenum, tin, selenium, vanadium, and zinc. However, test results for these trace metals are not presented.

With respect to organic emissions, dioxins and furans were detected in emissions from three facilities, both with and without pollution control devices. Other organic emissions detected in stack tests cited in this report include CO, THC, trichlorotrifluoroethane, tetrachloromethane, tetrachloroethene, and trichloroethylene.

In a stack testing conducted on three Canadian biomedical waste incinerators, PCBs and PAHs were either not detected (one facility) or not analyzed (two facilities).

A1.6.6 CARB (1996)

In May 1996, CARB prepared "Proposed Amendments to the Emission Inventory Criteria and Guidelines Report Published in Accordance with the Air Toxics 'Hot Spots' Information and Assessment Act of 1987." The purpose of the report is to present the basis of CARB's recommended amendments to the Air Toxics Hot Spots Program. The report states that California Health and Safety Code (HSC) 44321 requires CARB to compile the list of toxic substances that must be monitored from "designated reference lists of substances." Therefore, the document is not a primary source of toxics emission information. The primary sources of information are mandated by California HSC 44321, as follows:

- California HSC 44321(a): National Toxicology Program, International Agency for Research on Cancer

- California HSC 44321(b): Governor's List of Carcinogens and Reproductive Toxicants

- California HSC 44321(c): CARB
- California HSC 44321(d): Hazard Evaluation System and Information Service
- California HSC 44321(e): U.S. EPA
- California HSC 44321(f): California HSC

The lists of toxic substances presented in the document are not restricted to incinerator facilities, but apply to any facility discharging airborne pollutants to the atmosphere. The document also removes numerous substances, primarily medicinal compounds, from lists of toxic chemicals that must always be evaluated, and places them on lists of toxic compounds that require evaluation only if a facility manufactures that substance.

A1.7 COLUMN 7: U.S. EPA-RECOMMENDED AND POTENTIAL PICS (1994a; 1994b)

Compounds marked with an “X” in the appropriate cells are identified in U.S. EPA (1994a and 1994b). Based on information presented in U.S. EPA (1994b), these tables were developed from available U.S. EPA data and from lists of toxic compounds from various U.S. EPA programs. Because the source lists were not developed as lists of toxic PICs, U.S. EPA deleted compounds that were not appropriate (U.S. EPA 1994b). U.S. EPA acknowledged the importance of using focused studies to develop a PIC list that is (1) appropriately protective of the environment, and (2) not excessively burdensome on the regulated community. Nevertheless, Tables 1 and 2 in U.S. EPA (1994b) were compiled as draft lists for use during the interim period. Tables in U.S. EPA (1994b) were to be revised as additional PIC data were collected. U.S. EPA Permits and State Program Division is currently updating these tables; however, a target completion date is not available. Tables 1 and 2 are based on the following (U.S. EPA 1994b):

- Hazardous waste constituent list in 40 CFR Part 261, Appendix VIII
- hazardous air pollutants (HAP) list
- Office of Research and Development list of organic compounds found in combustion devices developed for U.S. EPA (1993)

The following compounds were deleted from this list:

- Pesticide compounds not likely to be a PIC
- Federal Drug Administration-regulated drugs
- Carcinogenic sugar substitutes
- Compounds without chemical-specific listings (for example, “coal tar”)
- Compounds without U.S. EPA-established sampling and analysis methods
- Metallic compounds (because of difficulty in analyzing the specific compounds; metals are still included in elemental totals)

- Compounds with low octanol-water partition coefficients and no inhalation toxicity data
- Compounds with low toxicity values
- Naturally-occurring plant toxins

Specific compounds were retained on Tables 1 and 2 on the following basis:

- Pesticides with a molecular structure simple enough to be of concern as a PIC
- Compounds with very high octanol-water partition coefficients

A1.8 COLUMN 8: PICS ACTUALLY DETECTED IN STACK EMISSIONS

Compounds marked by an “X” in the appropriate cells are PICs that have actually been detected in stack emissions. U.S. EPA compiled this list by evaluating the studies highlighted in Section A1.6.

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APPENDIX A-1

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APPENDIX A-2

CHEMICAL-SPECIFIC PARAMETER VALUES

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CONTENTS

LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS

$\mathbf{D}_{air}$ = Density of air (g/cm^3)
$\mathbf{D}_{forage}$ = Density of forage (g/cm^3)

Ba_{beef} = Biotransfer factor in beef
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
$Ba_{chicken}$ = Biotransfer factor in chicken
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{egg} = Biotransfer factor in eggs
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{milk} = Biotransfer factor in milk
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{pork} = Biotransfer factor in pork
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
BAF_{fish} = Bioaccumulation factor in fish
(mg COPC/kg FW tissue)/(mg COPC/L total water column)
OR (L water/kg FW tissue)
BCF_{fish} = Bioconcentration factor in fish (L/kg FW OR unitless)
Br_{ag} = Plant-soil bioconcentration factor in aboveground produce
(:g COPC/g DW plant)/(:g COPC/g DW soil)—unitless
$Br_{forage/silage}$ = Plant-soil bioconcentration factor in forage and silage
(:g COPC/g DW plant)/(:g COPC/g DW soil)—unitless
Br_{grain} = Plant-soil bioconcentration factor in grain
(:g COPC/g DW grain)/(:g COPC/g DW soil)—unitless
$\mathrm{Br}_{\mathrm{rootveg}}$ = Plant-soil bioconcentration factor for belowground produce
(:g COPC/g DW plant)/(:g COPC/g DW soil)—unitless
$BSAF_{fish}$ = Biota-sediment accumulation factor in fish
(mg COPC/kg lipid tissue)/(mg COPC/kg sediment)—unitless
B_{vol} = Volumetric air-to-leaf biotransfer factor in leaf
(:g COPC/L FW plant)/(:g COPC/L air)—unitless
Bv_{ag} = COPC air-to-plant biotransfer factor for aboveground produce
(:g COPC/g DW plant)/(:g COPC/g air)—unitless
$Bv_{forage/silage}$ = Air-to-plant biotransfer factor in forage and silage
(:g COPC/g DW plant)/(:g COPC/g air)—unitless

c = Junge constant = 1.7 x 10^{-04} (atm-cm)

D_a = Diffusivity of COPC in air (cm^2/s)
D_w = Diffusivity of COPC in water (cm^2/s)

$f_{oc,bs}$ = Fraction of organic carbon in bottom sediment (unitless)
$f_{oc,s}$ = Fraction of organic carbon in soil (unitless)
$f_{oc,sw}$ = Fraction of organic carbon in suspended sediment (unitless)
f_{water} = Fraction of COPC in water (unitless)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
Fw = Fraction of wet deposition that adheres to plant surfaces (unitless)

H = Henry’s law constant

Inhalation CSF = Inhalation cancer slope factor (mg/kg-day)$^{-1}$
Inhalation URF = Inhalation unit risk factor (μg/m^3)$^{-1}$

Kd_s = Soil-water partition coefficient (mL water/g soil OR cm^3 water/g soil)
Kd_{sw} = Suspended sediment-surface water partition coefficient
(L water/kg suspended sediment OR cm^3 water/g suspended sediment)
Kd_{bs} = Bed sediment-sediment pore water partition coefficient
(L water/kg bottom sediment OR cm^3 water/g bottom sediment)
K_{ow} = Octanol/water partitioning coefficient
(mg COPC/L octanol)/(mg COPC/L octanol)—unitless
K_{oc} = Soil organic carbon-water partition coefficient (mL water/g soil)
ksg = COPC soil loss constant due to biotic and abiotic degradation (yr^{-1})

MW = Molecular weight of COPC (g/mole)

p°_{L} = Liquid-phase vapor pressure of COPC (atm)
p°_{S} = Solid-phase vapor pressure of COPC (atm)

Oral CSF = Oral cancer slope factor (mg/kg-day)$^{-1}$

R = Universal gas constant (atm-m^3/mol-K)
RCF = Root concentration factor
(μg COPC/g DW plant)/(μg COPC/mL soil water)
RfC = Reference concentration (mg/m^3)
RfD = Reference dose (mg/kg/day)
Rp = Interception factor of edible portion of plant (unitless)

S = Solubility of COPC in water (mg COPC/L water)
ΔS_f = Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
S_T = Whitby’s average surface area of particulates (aerosols)
= 3.5 x 10^{-06} cm^2/cm^3 air for background plus local sources
= 1.1 x 10^{-05} cm^2/cm^3 air for urban sources

$t_{1/2}$ = Half-time of COPC in soil (days)
T_a = Ambient air temperature (K)
T_m = Melting point temperature (K)
TEF = Toxicity equivalency factor (unitless)

Vp = Vapor pressure of COPC (atm)

APPENDIX A-2

The following sections provide the general methodology and references we used to determine our recommended parameter values. You can find the recommended parameter values themselves in the HHRAP Companion Database (also known as the HHRAP database). In the HHRAP database we provide compound-specific values for

1. physical and chemical properties;
2. fate-and-transport parameters; and
3. Health benchmarks for chronic and acute exposure.

A2-1 GENERAL ANALYSIS AND METHODOLOGY

This section describes the general analysis and criteria we followed to determine our recommended contaminant-specific parameter values.

1. We compared parameter values among primary and available sources of applicable data, placing priority for selection on sources that are (1) U.S. EPA or State agency peer reviewed, (2) recent, (3) original sources of the values, and (4) generally accessible.

2. We further further researched and evaluated sources of parameter values, and to the extent possible, included observations affecting usability in parameter-specific discussions for each compound.

3. We selected only parameter values from sources that could be verified and cited.

4. We generally preferred source-recommended parameter values. As necessary, we determined parameter values using correlations or equations, using input parameter values provided in the HHRAP database.

5. When multiple parameter values were reported in a particular source (e.g., CHEMFATE), we selected the source-recommended value in most cases. If more than one parameter value is recommended by the source, then we selected the recommended value that falls closest to the average of the source-recommended values.

6. When reviewing and selecting parameter values from published literature or studies, we preferred using measured values over other types of data.

A2-2 PHYSICAL AND CHEMICAL PROPERTIES

A2-2.1 Molecular Weight (*MW*)

Molecular weight (*MW*) of a compound is defined as the sum of atomic weights of all atoms in the compound's molecule.

For most compounds (except PCDDs and PCDFs, and methyl mercury), we obtained *MW* values from one of the following sources, as cited:

- U.S. EPA. 2004b. *Superfund Chemical Data Matrix (SCDM).* OERR. Washington, D.C. January.

- Syracuse Research Corporation (SRC). 2003a. CHEMFATE Database. SRC. Syracuse, NY.

- Syracuse Research Corporation (SRC). 2003b. PHYSPROP Database. SRC. Syracuse, NY.

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- Recommended value reported in published literature. When multiple parameter values were reported in a particular source (e.g., database), we selected the recommended value in most cases.

PCDDs and PCDFs We obtained *MW* values for PCDDs and PCDFs from U.S. EPA (2000).

- U.S. EPA. 2000. *Exposure and Human Health Reassessment of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds.* Draft Final Report. Office of Research and Development. Washington, D.C. EPA/600/P-00/001 Bc. September.

Mercuric Compounds We obtained *MW* values for elemental mercury and mercuric chloride from the preferred sources listed above. We obtained the *MW* value for methyl mercury from U.S. EPA (1997b).

- U.S. EPA. 1997b. *Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment.* OAQPS and ORD. EPA-452/R-97-005. December.

A2-2.2 Melting Point Temperature (T_m)

Melting point temperature (T_m) is the temperature of the compound (in degrees Kelvin [K]) at which the solid state of the compound undergoes a phase change to a liquid phase. At ambient temperatures and at an atmospheric pressure of 1 atmosphere, compounds are generally in either a solid or liquid state.

For most compounds (except PCDDs and PCDFs), we obtained values for T_m from one of the following sources, as cited:

- U.S. EPA. 2004b. *Superfund Chemical Data Matrix (SCDM).* OERR. Washington, D.C. January.

- Syracuse Research Corporation (SRC). 2003a. CHEMFATE Database. SRC. Syracuse, NY.

- Syracuse Research Corporation (SRC). 2003b. PHYSPROP Database. SRC. Syracuse, NY.

- Lide, D.R. 2003. *CRC Handbook of Chemistry and Physics, 83rd Edition*. CRC Press. Boca Raton, Florida.
- O'Neil, M., and A. Smith. 2001. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals.* 13th Edition. Merck and Company, Inc. Rahway, New Jersey.
- Recommended value reported in published literature. When multiple parameter values were reported in a particular source (e.g., database), we selected the recommended value in most cases.

When a recommended range is provided instead of a singe numerical value, we selected the average of the range.

PCDDs and PCDFs We obtained T_m values for PCDDs and PCDFs from U.S. EPA (2000). U.S. EPA (2000) provides T_m values for PCDDs and PCDFs, and states that the values were obtained from various cited literature sources. We selected the midpoint of the range of values provided in U.S. EPA (2000).

Metals We obtained T_m values for metals, if available and except for mercury, from the preferred sources listed above.

Mercuric Compounds We obtained *Tm* values for elemental mercury and mercuric chloride from the list of preferred sources noted above. A *Tm* value for methyl mercury wasn't available in preferred sources or literature.

A2-2.3 Vapor Pressure (*Vp*)

The vapor pressure (*Vp*) of a substance is defined as the pressure in atmospheres exerted by the vapor (gas) of a compound when it is under equilibrium conditions. It provides a semi-quantitative rate at which it will volatilize from soil and/or water.

For most compounds (except PCDDs and PCDFs), we obtained values for *Vp* from the following preferred sources:

- U.S. EPA. 2004b. *Superfund Chemical Data Matrix (SCDM).* OERR. Washington, D.C. January.
- Syracuse Research Corporation (SRC). 2003a. CHEMFATE Database. SRC. Syracuse, NY.
- Syracuse Research Corporation (SRC). 2003b. PHYSPROP Database. SRC. Syracuse, NY.
- Lide, D.R. 2003. *CRC Handbook of Chemistry and Physics, 83rd Edition*. CRC Press. Boca Raton, Florida.
- O'Neil, M., and A. Smith. 2001. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals.* 13th Edition. Merck and Company, Inc. Rahway, New Jersey.

C Calculated using procedures set forth by:

> Lyman et al. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society. Washington, DC.

- Recommended value reported in published literature. When multiple parameter values were reported in a particular source (e.g., database), we selected the recommended value in most cases.

If a *Vp* value wasn't available in SCDM, then we obtained a vapor pressure value from CHEMFATE, PHYSPROP, CRC Handbook of Chemistry and Physics, or The Merck Index. If more than one value was recommended by the source, then we selected the recommended value that fell closest to the average of the recommended values. If a recommended value wasn't available, we selected a value measured at 25/C. If more than one value measured at 25/C was available, then we selected the value falling closest to the average of the available values. If no value was available at 25/C, then we followed the same method using values determined within the range of 20 to 30/C.

If no vapor pressure values were available in any of the preferred references, then we used the procedures described in Lyman et al. (1990) to calculate vapor pressure.

For nonmetallic substances, if vapor pressure wasn't available, we obtained a normal boiling point from the sources and used it to assign a default vapor pressure. If the boiling point is <25/C at 1 atmosphere (atm) , we selected a default vapor pressure of 760 Torr, and we assume the substance is a gas at 25/C. As with SCDM, if no vapor pressure is available for a substance and the normal boiling point is equal or greater than 25/C, we assume the substance is in a particulate form, rather than a gaseous form, and we assigned a vapor pressure of zero in order to calculate *Fv*. We made this assumption because the absence of a vapor pressure value often reflects an extremely low and difficult to measure (under standard conditions) value for nongaseous substances (U.S. EPA 2004b).

SCDM prefers CHEMFATE-recommended values over estimated or calculated values. If more than one recommended value is in CHEMFATE, SCDM selected the highest of the values. If a recommended value is not available, SCDM uses a value measured at 25/C. If more than one value measured at 25/C is available, SCDM uses the highest one. If no value is available at 25/C, values determined within the range of 20 to 30/C are used. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified in CHEMFATE for all vapor pressure measurements for a substance, SCDM uses the highest value. For values not available in CHEMFATE, SCDM followed a similar approach to that outlined above.

PCDDs and PCDFs We obtained *Vp* values for PCDDs and PCDFs from U.S. EPA (2000). Congener group average values were substituted for missing individual congener specific values.

Metals Except for mercury compounds, metals that do not have *Vp* values in the references above we assigned a *Vp* value of zero since they are assumed to be (1) nonvolatile at ambient temperatures, and (2) insoluble in water, except as certain weak acids.

Mercuric Compounds Mercury is a relatively volatile compound. We obtained the *Vp* value for elemental mercury from a preferred source listed above. We obtianed the *Vp* value for mercuric chloride from U.S. EPA (1997b). The *Vp* value for methyl mercury was not available in preferred sources or literature.

A2-2.4 Aqueous Solubility (*S*)

The aqueous solubility (*S*) of a compound is defined as the saturated concentration of the compound in water (mg COPC/L water) at a given temperature and pressure, usually at soil/water temperatures and atmospheric pressure (Montgomery and Welkom 1991).

For most compounds (except PCDDs and PCDFs and metals), we obtained values for *S* from the following preferred sources:

- U.S. EPA. 2004b. *Superfund Chemical Data Matrix (SCDM).* OERR. Washington, D.C. January.
- Syracuse Research Corporation (SRC). 2003a. CHEMFATE Database. SRC. Syracuse, NY.
- Syracuse Research Corporation (SRC). 2003b. PHYSPROP Database. SRC. Syracuse, NY.
- Dean, J.A. 2002. *Lange's Handbook of Chemistry.* 15th Edition. McGraw-Hill. New York.
- Calculated using procedures set forth by:

  Lyman et al. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society. Washington, DC.

- Recommended value reported in published literature. When multiple parameter values were reported in a particular source (e.g., database), we selected the recommended value in most cases.

If a *S* value wasn't available in SCDM, then we obtained solubility values from CHEMFATE, PHYSPROP, or Lange's Handbook of Chemistry. If more than one value was recommended by the source, then we selected the recommended value falling closest to the average of the recommended values. If a recommended value wasn't available, we selected a value measured at 25/C. If more than one value measured at 25/C is available, then we selected the value falling closest to the average of the available values. If no value was available at 25/C, we used the same method using values determined within the range of 20 to 30/C.

If no solubility values were available in any of the preferred references, we used the procedures described in Lyman et al. (1990) to calculate vapor pressure.

SCDM prefers CHEMFATE-recommended values over estimated or calculated values. If more than one recommended value is in CHEMFATE, SCDM selected the highest of the values. If a recommended value is not available, SCDM uses a value measured at 25/C. If more than one value measured at 25/C is available, SCDM uses the highest one. If no value is available at 25/C, values determined within the range of 20 to 30/C are used. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified in CHEMFATE for all vapor pressure measurements for a substance, SCDM uses the highest value. For values not available in CHEMFATE, SCDM followed a similar approach to that outlined above for determining values reported in Table A-1.

PCDDs and PCDFs We obtained *S* values for PCDDs and PCDFs from U.S. EPA (2000). Congener group average values were substituted for missing individual congener specific values.

Metals We obtained *S* values for metallic compounds, if available and except for mercury, from the preferred sources listed for organic and inorganic compounds.

Mercuric Compounds Mercury is a relatively volatile compound. We obtained *S* values for elemental mercury and mercuric chloride from the preferred sources listed above. Methyl mercury is stated in the Merck Index as being insoluble in water. Therefore, we assigned an *S* value of zero for methyl mercury.

A2-2.5 Fraction of Contaminant Air Concentration in the Vapor Phase (F_v)

Organics For most compounds (except metals and some mercury compounds), we calculated the fraction of contaminant air concentration in the vapor phase (F_v) using the following equation:

$$Fv = 1 - \frac{c\ S_T}{p^\circ_L + c\ S_T}$$

Equation A-2-1

C Junge, C. E. 1977. *Fate of Pollutants in the Air and Water Environments*, Part I; Suffet, I. H., Ed.; Wiley; New York. Pages 7-26.

If the contaminant is a liquid at ambient temperatures (that is, when p°_L is known), we used Equation A-2-1 to calculate F_v using the *Vp* value recommended for that contaminant in the HHRAP database. If the contaminant is a solid at ambient temperatures (that is, when p°_S is known), we used the following equation (Bidleman 1988) calculate p°_L from p°_S, for use in Equation A-2-1 (using *Vp* and T_m values presented for each contaminant in the HHRAP database):

$$\ln\left(\frac{p^\circ_L}{p^\circ_S}\right) = \frac{\Delta S_f}{R}\ \frac{(T_m - T)}{T}$$

Equation A-2-2

where

c = Junge constant = 1.7 x 10^{-04} (atm-cm)
p°_L = Liquid phase vapor pressure of compound (atm)
p°_s = Solid phase vapor pressure of compound (atm)
R = Universal ideal gas constant (atm-m^3/mole$^-$K)
)S_f = Entropy of fusion [)S_f/R = 6.79 (unitless)]
S_T = Whitby's average surface area of particulates (aerosols)
T_a = Ambient air temperature (K)—assumed to be 25°C or 298 K

C Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology*. Volume 22. Number 4. Pages 361-367.

According to Bidleman (1988), Equation A-2-1 assumes that the Junge constant (*c*) is constant for all compounds. However, *c* can depend on (1) the compound (sorbate) molecular weight, (2) the surface concentration for monolayer coverage, and (3) the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate.

Metals As in U.S. EPA (1994b), we assumed all metals (except mercury) are present predominately in the particulate phase and not in the vapor phase ($Vp = 0$), and therefore, assigned F_v values of zero.

Mercuric Compounds Elemental mercury and mercuric chloride are relatively volatile and exist in the vapor phase (U.S. EPA 1997b). Therefore, we calculated the Fv value for elemental mercury using Equation A-2-1.

Based on discussions in U.S. EPA (1997b), we assigned mercuric chloride an Fv value of 0.85. Also, consistent with information provided in U.S. EPA (1997b), we assumed methyl mercury doesn't exist in the air phase and, therefore, assigned it an Fv of zero.

A2-2.6 Henry's Law Constant (*H*)

Henry's Law constant (*H*) is also referred to as the air-water partition coefficient, and is defined as the ratio of the partial pressure of a compound in air to the concentration of the compound in water at a given temperature under equilibrium conditions. Henry's Law constant values generally can be (1) calculated from the theoretical equation defining the constant, (2) measured, or (3) estimated from the compound structure.

For most compounds (excluding PCDDs and PCDFs), we obtained *H* values from the following preferred sources:

- U.S. EPA. 2004b. *Superfund Chemical Data Matrix (SCDM).* OERR. Washington, D.C. January.
- Syracuse Research Corporation (SRC). 2003a. CHEMFATE Database. SRC. Syracuse, NY.
- Syracuse Research Corporation (SRC). 2003b. PHYSPROP Database. SRC. Syracuse, NY.
- Calculated using procedures set forth by:

    Lyman et al. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society. Washington, DC.

$$H = \frac{Vp \cdot MW}{S} \qquad \text{Equation A-2-3}$$

where

H = Henry's Law constant (atm-m^3/mole)
Vp = Vapor pressure of COPC (atm)
S = Solubility of COPC in water (mg COPC/L water)

H values calculated with Equation A-2-3 used MW, S, and Vp values found in the HHRAP database.

PCDDs and PCDFs We obtained H values for PCDDs and PCDFs from U.S. EPA (2000). We substituted congener group average values for missing individual congener specific values.

Metals We obtained H values for metallic compounds, if available and except for mercury, from the preferred sources listed above. Metals that do not have H values in the references above we assigned a value of zero since the subject metals are assumed to be (1) nonvolatile at ambient temperatures, and (2) insoluble in water, except as certain weak acids.

Mercuric Compounds We obtained H values for elemental mercury, mercuric chloride, and methyl mercury from U.S. EPA (1997b).

A2-2.7 Diffusivity in Air (D_a) and Water (D_w)

Diffusivity or diffusion coefficients in air (D_a) and water (D_w) are used to calculate the liquid or gas phase transfer of a contaminant into a water body.

For most compounds (except PCDDs and PCDFs), we obtained diffusion coefficients in air (D_a) and water (D_w) values from the following preferred source:

- U.S. EPA. 2004c. *WATER9—Air Emissions Models Wastewater Treatment*. Version 2.0.0. OAQPS. Research Triangle Park. North Carolina. July 1.

If values weren't available in U.S. EPA (2004c), we calculated values using procedures set forth by:

- U.S. EPA. 1997b. *Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment.* OAQPS and ORD. EPA-452/R-97-005. December.

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}} \qquad \text{Equation A-2-4}$$

$$D_{w,i} = \frac{22 \times 10^{-5}}{(MW_i)^{2/3}} \qquad \text{Equation A-2-5}$$

D_w and D_a values calculated with Equations A-2-4 and A-2-5 used *MW* values recommended in the HHRAP database.

PCDDs and PCDFs We obtained Diffusivity values in air and water for 2,3,7,8-TCDD and 2,3,7,8-TCDF from U.S. EPA (2004c). For all other congeners of PCDDs and PCDFs, (1) we recommend a default *Dw* value of 8 x 10^{-06} cm^2/s, and (2) we estimated *Da* values from PCDD and PCDF values using the following equation recommended by U.S. EPA (2000) and obtained from Thibodeaux (1979):

$$\frac{D_x}{D_y} = \left(\frac{MW_y}{MW_x}\right)^{0.5} \qquad \text{Equation A-2-6}$$

where

$D_{x,y}$ = Diffusivities in air of compounds *x* and *y* (cm^2/s)
$MW_{x,y}$ = Molecular weights of compounds *x* and *y* (g/mol)

We calculated *Da* values for PCDD congeners using the *Da* value and *MW* for 2,3,7,8-TCDD. We calculated *Da* values for PCDF congeners using the *Da* value and *MW* for 2,3,7,8-TCDF. This approach is consistent with the methodology specified in U.S. EPA (2000). Values for diffusivity in water range from 1 x 10^{-06} to 1 x 10^{-05} cm^2/s; therefore, U.S. EPA (1995b) recommended a default value of 8 x 10^{-06} cm^2/s. Diffusivity values calculated using Equations A-2-4 and A-2-5 were within the range specified by U.S. EPA (1995b).

Metals We obtained dDiffusivity values for metallic compounds, if available and except for mercury, from the preferred sources listed for organic and inorganic compounds. If values for metals were not available in the preferred sources, we assigned a default value of zero since metals (except mercury and chromium) are generally considered (1) nonvolatile at ambient temperatures, and (2) insoluble in water, except as certain weak acids.

Mercuric Compounds We obtained the diffusivity value for elemental mercury from the WATER9 database (U.S. EPA 2004c). We calculated diffusivity values for mercuric chloride and methyl mercury using Equations A-4 and A-5.

A2-2.8 Octanol/Water Partitioning Coefficient (K_{ow})

The *n*-octanol/water partitioning coefficient (K_{ow}) is defined as the ratio of the solute concentration in the water-saturated *n*-octanol phase to the solute concentration in the *n*-octanol-saturated water phase (Montgomery and Welkom 1991).

For most compounds (except PCDDs and PCDFs, and mercuric chloride), we obtained K_{ow} values from the following preferred sources:

- U.S. EPA. 2004b. *Superfund Chemical Data Matrix (SCDM).* OERR. Washington, D.C. January.

- Syracuse Research Corporation (SRC). 2003a. CHEMFATE Database. SRC. Syracuse, NY.

- Syracuse Research Corporation (SRC). 2003b. PHYSPROP Database. SRC. Syracuse, NY.

- Lide, D.R. 2003. *CRC Handbook of Chemistry and Physics, 83rd Edition*. CRC Press. Boca Raton, Florida.

- Recommended value reported in published literature. When multiple parameter values were reported in a particular source (e.g., database), we selected the recommended value in most cases.

PCDDs and PCDFs We obtained K_{ow} values for the PCDDs and PCDFs from U.S. EPA (2000). Congener group average values were substituted for missing individual congener specific values.

Metals We obtained K_{ow} values for metals, if available and except for mercury, from the preferred sources listed above. K_{ow} values for metals not reported in the above sources we assumed to be zero. This assumption is based on the affinity of most metals to octanol approaches zero.

Mercuric Compounds We obtained the K_{ow} value for elemental mercury from the list of preferred sources above. The K_{ow} value for mercuric chloride comes from U.S. EPA (1997b). We couldn't find a K_{ow} value for methyl mercury.

A2-2.9 Soil Organic Carbon-Water Partition Coefficient (K_{oc})

The soil organic carbon-water partition coefficient (K_{oc}) or the organic carbon normalized soil sorption coefficient is defined as the ratio of adsorbed compound per unit weight of organic carbon to the aqueous solute concentration (Montgomery and Welkom 1991).

The partitioning of ionizing organic compounds can be significantly influenced by soil pH. Because of the soil mechanisms that are inherently involved, we discuss K_{oc} values for the ionizing organics and nonionizing organics separately.

A2-2.9.1 Ionizing Organic Compounds

Ionizing organic compounds include amines, carboxylic acids, and phenols. These compounds contain the functional groups that ionize under specific pH conditions, and include the following:

- Organic acids (2,4,6-trichlorophenol; pentachlorophenol; 2,3,4,5-tetrachlorophenol; 2,3,4,6-tetrachlorophenol; 2,4,5-trichlorophenol; 2,4-dichlorophenol; 2-chlorophenol; phenol; 2,4-dimethylphenol; 2-methylphenol; 2,4-dinitrophenol; and benzoic acid)

- Organic bases—n-nitroso-di-n-propylamine; n-nitrosodiphenylamine, and 4-chloroaniline)

We obtained K_{oc} values for ionizing organic compounds from the following:

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

The K_{oc} values for ionizing organic compounds provided by U.S. EPA (1996) were estimated on the basis of the degree of ionization and the relative proportions of neutral and ionized species. K_{oc} values for ionizing compounds can vary vastly, depending on the pH conditions in the environment. Therefore, for the aforementioned ionizing organic compounds, K_{oc} values in the HHRAP database are based on a pH value of 6.8 to correlate with typical environmental soils.

K_{oc} values were estimated on the basis of the assumption that the sorption of ionizing organic compounds is similar to hydrophobic organic sorption, because the soil organic carbon is the dominant sorbent. According to U.S. EPA (1996), for low pH conditions, these estimated values may overpredict sorption coefficients, because they ignore sorption to components other than organic carbon.

A2-2.9.2 Nonionizing Organic Compounds

Nonionizing organic compounds include volatile organics, chlorinated pesticides, polynuclear aromatic hydrocarbons (PAHs), and phthalates. We obtained K_{oc} values for nonionizing organic compounds from the following:

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

U.S. EPA (1996) calculated the geometric mean value from various measured values. For compounds for which K_{oc} values are not directly provided by U.S. EPA (1996), we calculated K_{oc} values using K_{ow} correlation equations provided in U.S. EPA (1996), as obtained from DiToro (1985). We used K_{ow} values recommended in the HHRAP database to calculate K_{oc} values.

For most semi-volatile nonionizing organic compounds -

$$\log K_{oc} = 0.00028 + (0.983 * \log K_{ow}) \qquad \text{Equation A-2-7}$$

- DiToro, D.M. 1985. "A Particle Interaction Model of Reversible Organic Chemical Sorption" *Chemosphere*. 14(10):1503-1538.

For the purposes of applying Equation A-2-7, we define semi-volatile compounds as having a Henry's Law Constant (*H*) value less than 10-3, consistent with general descriptions provided in Lyman et al. (1990).

For volatile nonionizing organics, chlorinated benzenes, and certain chlorinated pesticides -

$$\log K_{oc} = 0.0784 + (0.7919 * \log K_{ow}) \qquad r^2 = 0.97 \qquad \text{Equation A-2-8}$$

For the purposes of applying Equation A-2-8, we define volatile compounds as having a Henry's Law Constant (*H*) value greater than 10-3, consistent with general descriptions provided in Lyman et al. (1990).

PCDDs and PCDFs For PCDDs and PCDFs, we used the following correlation equation obtained from Karickhoff, et al. (1979), as cited by U.S. EPA (2000), , and K_{ow} values provided in the HHRAP database to calculate K_{oc} values.

$$\log K_{oc} = \log K_{ow} - 0.21 \qquad (n = 10,\ r^2 = 1.0) \qquad \text{Equation A-2-9}$$

C Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. "Sorption of Hydrophobic Pollutants on Natural Sediments." *Water Resources.* 13:241-248.

Metals We couldn't find K_{oc} values for metals within the preferred sources or available literature.

Mercuric Compounds We couldn't find K_{oc} values for mercury compounds within the preferred sources or available literature.

A2-2.10 Partitioning Coefficients for Soil-Water (Kd_s), Suspended Sediment-Surface Water (Kd_{sw}), and Bottom Sediment-Sediment Pore Water (Kd_{bs})

Partition coefficients (*Kd*) describe the partitioning of a compound between sorbing material, such as soil, soil pore-water, surface water, suspended solids, and bed sediments. For organic compounds, *Kd* is estimated to be a function of the organic-carbon partition coefficient and the fraction of organic carbon in the partitioning media. For metals, *Kd* is assumed to be independent of the organic carbon in the partitioning media and, therefore, partitioning is similar in all sorbing media.

The soil-water partition coefficient (Kd_s) describes the partitioning of a compound between soil pore-water and soil particles, and strongly influences the release and movement of a compound into the subsurface soils and underlying aquifer. The suspended sediment-surface water partition coefficient (Kd_{sw}) describes the partitioning of a compound between surface water and suspended solids or sediments. The bed sediment-sediment pore-water partition coefficient (Kd_{bs}) describes the partitioning of a compound between the bed sediments and bed sediment pore-water.

For most compounds (including PCDDs and PCDFs), we obtained Kd_s values from the following preferred sources:

C U.S. EPA. 2004b. *Superfund Chemical Data Matrix (SCDM).* OERR. Washington, D.C. January.

C U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides through Agriculture." Oak Ridge National Laboratory. Oak Ridge, Tennessee.

- RTI. 1996. *Chemical Properties for SCDM Development.* Prepared for U.S. EPA Office of Emergency and Remedial Response. Washington, DC.

- Calculated using procedures consistent with:

  U.S. EPA. 1993d. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

We assume that soil organic carbon is the dominant sorbing component in soils and sediments. Therefore, *Kd* values not directly available in the preferred sources were calculated using the following fraction organic carbon (f_{OC}) correlation equations provided in U.S. EPA (1993d):

$$Kd_s = f_{oc,s} \cdot K_{oc} \qquad \text{Equation A-2-10}$$

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \qquad \text{Equation A-2-11}$$

$$Kd_{bs} = f_{oc,bs} \cdot K_{oc} \qquad \text{Equation A-2-12}$$

- U.S. EPA. 1993d. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

U.S. EPA (1993d), based on literature searches, states that f_{OC} could range as follows:

- 0.002 to 0.024 in soils—for which a mid-range value of $f_{oc,s} = 0.01$ generally can be used.

- 0.05 to 0.1 in suspended sediments—for which a mid-range value of $f_{oc,sw} = 0.075$ generally can be used.

- 0.03 to 0.05 in bottom sediments—for which a mid-range value of $f_{oc,bs} = 0.04$ generally can be used.

We calculated *Kd* values using the K_{oc} values recommended in the HHRAP database, and mid-range f_{oc} values recommended by U.S. EPA (1993d).

Metals For metals (except mercury), *Kd* is governed by factors other than organic carbon, such as pH, redox, iron content, cation exchange capacity, and ion-chemistry. Therefore, *Kd* values for metals can't be calculated using the same correlation equations specified for organic compounds. We obtained *Kd* values, except lead and mercury, from the preferred sources listed above. SCDM obtained its values from U.S. EPA (1996), which provides values for *Kd* that are based on pH and are estimated using the MINTEQ2 geochemical speciation model. The MINTEQ2 model analyses were conducted under a variety of geochemical conditions and metal concentrations. The MINTEQ2 pH-dependent *Kd* values were estimated by holding constant the iron oxide at a medium value and the f_{oc} at 0.002.

Because organic carbon does not play a major role in partitioning for the metals, U.S. EPA (1994b) assumed that the partitioning is the same, regardless of the soil, suspended sediment, or bottom sediment phase. Therefore, we assumed that the values for partitioning coefficients Kd_s, Kd_{sw}, and Kd_{bs} for the metals are the same.

We obtained the *Kd* value for lead from the following:

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture." Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Mercuric Compounds We obtained Kd_s, Kd_{sw}, and Kd_{bs} values for mercury , mercuric chloride, and methyl mercury from U.S. EPA (1997b).

A2-2.11 Soil Loss Constant Due to Degradation (*ksg*)

Soil loss constant due to degradation (*ksg*) reflects loss of a compound from the soil by processes other than leaching. Degradation rates in the soil media include biotic and abiotic mechanisms of transformation. Abiotic degradation includes photolysis, hydrolysis, and redox reactions. Hydrolysis and redox reactions can be significant abiotic mechanisms in soil (U.S. EPA 1990).

Lyman et al. (1990) states that degradation rates can be assumed to follow first order kinetics in a homogenous media. Therefore, the half-life ($t_{½}$) of compounds can be related to the degradation rate constant (*ksg*) as follows:

$$ksg = \frac{0.693}{t_{½}} \qquad \text{Equation A-2-13}$$

Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil. Therefore, if the $t_{½}$ for all of the mechanisms of transformation are known, the degradation rate can be calculated using Equation A-2-13. However, literature sources don't generally provide sufficient data for all such mechanisms, especially for soil.

For most compounds (except PCDDs and PCDFs, PCBs, metals, and mercury), we calculated *ksg* values using half-life soil values obtained from the following preferred sources:

- Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., and Michalenko, E.M. 1991. *Handbook of Environmental Degradation Rates.* Lewis Publishers. Chelsea, Michigan.

- Recommended value reported in published sources or literature other than the preferred sources listed above. When multiple parameter values were reported in a particular source (e.g., database), we selected the recommended value in most cases.

Half-life values provided in Howard et al. (1991) indicate the disappearance of a substance in ground water or soil; with the principal degradation mechanisms being biodegradation and hydrolysis. Values reported were highly variable because of the different methods used for measurements, in addition to the various controlling factors that could affect them. Therefore, Howard et al. (1991) provided a range of half-life values found in the literature, usually for the fastest reaction mechanism. We used high-end half-life values to calculate *ksg* values.

For half-life values obtained from literature sources, if more than one value was recommended by the source, then we selected the value falling closest to the average of the recommended values. This value was used to calculate the *ksg* value recommended in the HHRAP database. If no recommended values were available, we used a value measured at 25/C. If more than one value measured at 25/C was available, then we used the value falling closest to the average of the available values to calculate the *ksg* value recommended in the HHRAP database. If no value was available at 25/C, we used values determined within the range of 20 to 30/C following the same method.

For contaminants with no reported soil degradation rates, we recommend a default value of zero.

PCDDs, PCDFs, and PCBs For PCDDs, PCDFs, and PCBs, we obtained *ksg* values from U.S. EPA (2000); which discussed experimental studies that were conducted on PCDDs and PCDFs degradation mechanisms. U.S. EPA (2000) stated that based on available studies, it appears reasonable to assign a uniform rate of degradation for all PCDD/F congeners, and PCBs. The specific degradation rate provided by U.S. EPA (2000) was 0.0277 yr^{-1}, which translates to a half-life of 25 years.

Metals For the metals, literature states that the metals are transformed, but not degraded, by such mechanisms; therefore, we assume *ksg* values are zero for metals with no reported half-life values in soil.

Mercuric Compounds For mercury, mercuric chloride, and methylmercury, U.S. EPA (1997b) recommended *ksg* values of zero.

A2-2.12 BIOCONCENTRATION AND BIOTRANSFER FACTORS FOR PLANTS

A2-2.12.1 Root Concentration Factor (*RCF*)

The root concentration factor (*RCF*) is used to calculate the belowground transfer of contaminants from soil to a root vegetable. The *RCF* was developed based on experiments conducted by Briggs et al. (1982) which measured uptake of compounds into barley roots from growth solution.

For compounds with log K_{ow} values of 2.0 and higher, we used the following correlation equation to obtain *RCF* values:

$$\log(RCF) = 0.77 \log K_{ow} - 1.52 \qquad (n = 7,\ r = 0.981) \qquad \text{Equation A-2-14}$$

For compounds with log K_{ow} values less than 2.0, we used the following correlation equation to obtain *RCF* values:

$$\log(RCF - 0.82) = 0.77 \log K_{ow} - 1.52 \qquad \text{Equation A-2-15}$$

We obtained these equations from the following document:

- Briggs, G.G., R.H. Bromilow, and A.A. Evans, 1982. "Relationships Between Lipophilicity and Root Uptake and Translocation of Non-ionized Chemicals by Barley." *Pesticide Science*. Volume 13. Pages 495-504.

These equations estimate a *RCF* value in fresh weight (FW) units, which was then converted to dry weight (DW) units using a moisture content of 87 percent in root vegetables (U.S. EPA 1997c; Pennington 1994).

Briggs et al. (1982) derived the correlation equations above from studies using 18 compounds with log K_{ow} values ranging from -0.57 to 4.6. In addition, a validation exercise, in which predictions of dioxin-like compounds (log Kow values from 6.0 to 8.2) in carrots were compared with observations, shows this factor to adequately perform for this class of compounds (Muller et al. 1994). Therefore, *RCF* values for compounds with outlying log K_{ow} values have been capped in line with the test data used to formulate the correlation equation. We assigned compounds with log K_{ow} values less than -0.57 an *RCF* value corresponding to a log K_{ow} value of -0.57. At the high end of the range, we assigned compounds with log K_{ow} values greater than 8.2 (considering the validation studies using dioxin-like compounds) an *RCF* value corresponding to a log K_{ow} value of 8.2.

As in previous U.S. EPA guidance (U.S. EPA 1994a), we recommend using Equation A-2-14 in calculating exposure to dioxin-like compounds. We used K_{ow} values available in the HHRAP database to calculate each *RCF* value.

Metals For metals, no referenced *RCF* values were available in published literature. However, plant-soil biotransfer factors for root vegetables ($Br_{rootveg}$) were available in the literature and, therefore, *RCF* values, normally used to calculate $Br_{rootveg}$ values, aren't needed for the metals.

Mercuric Compounds No *RCF* values were available in the literature for mercury, mercuric chloride, and methyl mercury. However, plant-soil biotransfer factors for root vegetables ($Br_{rootveg}$) were available in U.S. EPA (1997b) and, therefore, *RCF* values, normally used to calculate $Br_{rootveg}$ values, aren't needed for the mercuric compounds.

A2-2.12.2 Plant-Soil BCFs in Root Vegetables ($Br_{rootveg}$)

The plant-soil bioconcentration factor for compounds in root vegetables ($Br_{rootveg}$) accounts for uptake from soil to the belowground root vegetables or produce.

For most compounds, we used the following equation from U.S. EPA (1995b) to calculate values for $Br_{rootveg}$ on a dry weight basis:

$$Br_{rootveg} = \frac{RCF}{Kd_s} \qquad \text{Equation A-2-16}$$

We calculated $Br_{rootveg}$ values using the *RCF* and Kd_s values listed in the HHRAP database.

<u>Metals</u> We obtained the $Br_{rootveg}$ values for metals (except nickel, cadmium, selenium, and arsenic) from Baes et al. (1984). *Br* values in Baes et al. (1984) are dry weight values provided for nonvegetative (reproductive) growth, such as tubers.

For nickel, cadmium, selenium, and arsenic, *we obtained* $Br_{rootveg}$ values from the following document:

C U.S. EPA. 1992b. *Technical Support Document for the Land Application of Sewage Sludge. Volumes I and II.* EPA 822/R-93-001a. Office of Water. Washington, D.C.

For nickel, cadmium, selenium, and arsenic—$Br_{root\ veg}$ values were calculated by multiplying the uptake slope factors [(:g COPC/g DW plant)/(kg COPC applied/hectare)] for root vegetables by a conversion factor of $2x10^9$ g/hectare soil. In deriving the conversion factor, U.S. EPA (1992b) assumed a soil average dry bulk density of 1.33 g/cm^3 and a soil incorporation depth of 15 cm.

<u>Mercuric Componds</u> We obtained $Br_{rootveg}$ values for mercuric chloride and methyl mercury from U.S. EPA (1997b) on a dry weight basis. The HHRAP methodolgy assumes elemental mercury doesn't deposit onto soils, and therefore there's no plant uptake through the soil. Therefore, a $Br_{rootveg}$ value for elemental mercury isn't applicable.

A2-2.12.3 Plant-Soil BCFs for Aboveground Produce (Br_{ag}) and Forage (Br_{forage})

The plant-soil bioconcentration factor (*Br*) for aboveground produce accounts for the uptake from soil and the subsequent transport of contaminants through the roots to the aboveground plant parts. As addressed in U.S. EPA (1995b), the *Br* value for most compounds is a function of water solubility, which is inversely proportional to K_{ow}. The *Br* value for metals is a function of the bioavailability of the metals in soil.

For all compounds, including PCDDs and PCDFs, (1) the subscript "*ag*" represents aboveground produce which applies to exposed fruits and vegetables, and protected fruits and vegetables, and (2) the subscript "*forage*" represents forage, but the values also apply to silage and grain. For metals, (1) aboveground fruits (both exposed and protected) are represented by $Br_{ag\ (fruit)}$; (2) aboveground vegetables (both exposed and protected) are represented by $Br_{ag(veg)}$, (3) forage is represented by Br_{forage}, but the values also apply to silage, and (4) grains are represented by Br_{grain}.

For most compounds, we used the following correlation equations to calculate values for Br_{ag} and Br_{forage} on a dry weight basis:

$$\log Br_{ag} = 1.588 - 0.578\ (\log K_{ow}) \qquad (n = 29,\ r = 0.73)$$ Equation A-2-17

$$\log Br_{forage} = 1.588 - 0.578\ (\log K_{ow}) \qquad (n = 29,\ r = 0.73)$$ Equation A-2-18

We obtained these correlation equations from;

C Travis, C.C. and A.D. Arms. 1988. Bioconcentration of Organics in Beef, Milk, and Vegetation. *Environmental Science and Technology*. 22:271-274.

Travis and Arms (1988) developed a correlation equation for vegetation that doesn't distinguish between aboveground produce and forage or silage or grain. Due to lack of literature data, we used the Travis and Arms (1988) correlation equation to calculate *Br* values for both aboveground produce and forage.

The above correlation equations for *Br* values were derived from experiments conducted on compound classes such as DDT, pesticides, PCDDs, PCDFs, and PCBs, representing compounds with log K_{ow} values ranging from 1.15 to 9.35. Therefore, *Br* values for compounds with outlying log K_{ow} values have been capped in line with the test data used to formulate the correlation equation. Compounds with log K_{ow} values less than 1.15 we assigned a *Br* value corresponding to a log K_{ow} value of 1.15. At the high end of the range, compounds with log K_{ow} values greater than 9.35 we assigned a *Br* value corresponding to a log K_{ow} value of 9.35. We used the log K_{ow} values listed in the HHRAP database to calculate each *Br* value.

Metals For metals, we derived *Br* values from uptake slope factors provided in the following document:

C U.S. EPA. 1992b. *Technical Support Document for the Land Application of Sewage Sludge*. Volumes I and II. EPA 822/R-93-001a. Office of Water. Washington, DC.

Uptake slopes provided in U.S. EPA (1992b) are the ratio of contaminant concentration in dry weight plant tissue to the mass of contaminant applied per hectare soil. These uptake slopes were multiplied by 2×10^9 g/hectare soil to convert to *Br* values. The conversion factor was derived using the U.S. EPA (1992b) assumed soil bulk density of 1.33 g/cm^3, and an incorporation depth of 15 cm.

For other metals, we obtained *Br* values from Baes et al. (1984). Baes et al. (1984) described biotransfer factors (on a dry weight basis) from plant-soil uptake for (1) vegetative growth (leaves and stems) "Bv"; and (2) nonvegetative or reproductive growth (fruits, seeds, and tubers) "Br". Note that *Bv* is defined as the air-to-plant biotransfer factor.

We used the following methodology to derive *Br* values on a dry weight basis:

a. For nickel, cadmium, selenium, zinc, and arsenic, $Br_{ag\ (fruit)}$ values were calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil (uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for garden fruits). All other metals were obtained by selecting "Br" values for nonvegetative growth (reproductive) provided in Baes et al. (1984).

b. For nickel, cadmium, selenium, zinc, and arsenic, $Br_{ag\ (veg)}$ values were calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2 x10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b). For other metals, "Br" values for nonvegetative (reproductive) growth and "Bv" values for vegetative growth—obtained from Baes et al. (1984)—were weighted as 75% (reproductive) and 25% vegetative. The resulting values were adopted as $Br_{ag\ (veg)}$ values.

c. For nickel, cadmium, selenium, zinc, and arsenic, Br_{forage} values were calculated by multiplying the uptake slope factors with a conversion factor of 2x10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables. For other metals, Br_{forage} values were obtained from Baes et al. (1984). "Bv" values for vegetative growth (such as leaves and stems) in Baes et al. (1984) were used for Br_{forage}.

d. For nickel, cadmium, selenium, zinc, and arsenic, Br_{grain} values were calculated by multiplying the uptake slope factors with a conversion factor of 2 x10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals. For other metals, Br_{grain} value was obtained from Baes et al. (1984). "Br" values for nonvegetative growth as recommended by Baes et al. (1984) were used for Br_{grain}.

e. Consumption rates used to obtain the weighted average Br_{ag} value for aboveground produce are as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.

Mercuric Compounds We obtained Br_{ag} values for mercuric chloride and methyl mercury as described above. We obtained Br_{forage} values on a dry weight basis for mercuric chloride and methyl mercury from U.S. EPA (1997b). The HHRAP methodology assumes that elemental mercury doesn't deposit onto soils. Therefore, it's assumed that there's no plant uptake through the soil.

A2-2.12.4 Air-to-Plant BTFs for Aboveground Produce (Bv_{ag}) and Forage (Bv_{forage})

The air-to-plant biotransfer factor (*Bv*) is defined as the ratio of contaminant concentration in aboveground plant parts to the contaminant concentration in air. We calculated *Bv* values only for aboveground exposed produce (both fruits and vegetables). We assume that aboveground protected produce (both fruits and vegetables) and belowground produce are protected from air-to-plant transfer. According to U.S. EPA (1995b), root vegetables are assumed to be also protected from air-to-plant transfer.

For most compounds (excluding PCDDs and PCDFs), we calculated the air-to-plant biotransfer factor for aboveground produce (Bv_{ag}) and forage (Bv_{forage}) using correlation equations derived for azalea leaves in the following documents:

- Bacci E., D. Calamari, C. Gaggi, and M. Vighi. 1990. "Bioconcentration of Organic Chemical Vapors in Plant Leaves: Experimental Measurements and Correlation." *Environmental Science and Technology*. Volume 24. Number 6. Pages 885-889.

- Bacci E., M. Cerejeira, C. Gaggi, G. Chemello, D. Calamari, and M. Vighi. 1992. "Chlorinated Dioxins: Volatilization from Soils and Bioconcentration in Plant Leaves." *Bulletin of Environmental Contamination and Toxicology*. Volume 48. Pages 401-408.

Bacci et al. (1992) developed a correlation equation using data collected for the uptake of 1,2,3,4-tetrachlorodibenzo-p-dioxin (TCDD) in azalea leaves, and data obtained from Bacci et al. (1990). The Bv obtained was then evaluated for 14 organic compounds to develop a correlation equation with K_{ow} and H. Bacci et al. (1992) derived the following equations without distinguishing between forage and aboveground produce:

$$\log B_{vol} = 1.065 \log K_{ow} - \log\left(\frac{H}{RT}\right) - 1.654 \qquad (r = 0.957)$$ Equation A-2-19

$$Bv = \frac{\rho_{air} \cdot B_{vol}}{(1 - f_{water}) \cdot \rho_{forage}}$$ Equation A-2-20

where

B_{vol} = Volumetric air-to-plant biotransfer factor (fresh-weight basis)
Bv = Mass-based air-to-plant biotransfer factor (dry-weight basis)
ρ_{air} = 1.19 g/L (Weast 1981)
ρ_{forage} = 770 g/L (Macrady and Maggard 1993)
f_{water} = 0.85 (fraction of forage that is water—Macrady and Maggard [1993])

We calculated Bv vlaues using Equations A-2-19 and A-2-20, and the values for H and K_{ow} listed in the HHRAP database; based on a T of 25°C or 298.1 K. We adopted the resulting Bv values for both forage (Bv_{forage}) and aboveground produce (Bv_{ag}). Please note the following uncertainty associated with these variables:

- For organics (except PCDDs and PCDFs), U.S. EPA (1993d) recommended reducing Bv values by a factor of 10 before use. This was based on the work conducted by U.S. EPA (1993d) for U.S. EPA (1994a) as an interim correction factor. Welsch-Pausch et al (1995) conducted experiments to determine concentrations of PCDDs and PCDFs in air and resulting biotransfer to welsh ray grass. This was documented in the following:

    - Welsch-Pausch, K.M. McLachlan, and G. Umlauf. 1995. "Determination of the Principal Pathways of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans to Lolium Multiflorum (Welsh Ray Grass)". *Environmental Science and Technology*. 29: 1090-1098.

A follow-up study based on Welsch-Pausch et al. (1995) was conducted by Lorber (1995) (see discussion below for PCDDs and PCDFs). In a following publication, Lorber (1997) concluded that the Bacci factor reduced by a factor of 100 was close in line with observations made by him through various studies, including the Welsch-Pausch et al. (1995) experiments. Therefore, we calculated *Bv* values using the Bacci et al. (1992) correlation equations and then reduced by a factor of 100 for all organics, excluding PCDDs and PCDFs.

PCDDs and PCDFs For PCDDs and PCDFs, we obtained *Bv* values, on a dry weight basis, from the following:

- Lorber, M. and P. Pinsky. 1999. "An Evaluation of Three Empirical Air-to-Leaf Models for Polychlorinated Dibenzo-p-Dioxins and Dibenzofurans". National Center for Environmental Assessment (NCEA). U.S. EPA. Washington D.C. Accepted for publication in *Chemosphere*.

U.S. EPA (1993d) stated that, for dioxin-like compounds, using the Bacci et al. (1992) equations may overpredict *Bv* values by a factor of 40. This was because the Bacci et al. (1990) and Bacci et al. (1992) experiments did not take photodegradation effects into account. Therefore, U.S. EPA (1993d) recommended that *Bv* values calculated using Equations A-2-19 and A-2-20 be reduced by a factor of 40 for dioxin-like compounds.

However, according to Lorber (1995), the Bacci algorithm divided by 40 may not be appropriate because

- the physical and chemical properties of dioxin congeners are generally outside the range of the 14 organic compounds used by Bacci (1990), and
- the factor of 40 derived from one experiment on 2,3,7,8-TCDD may not apply to all dioxin congeners.

Welsch-Pausch et al. (1995) conducted experiments to obtain data on uptake of PCDDs and PCDFs from air to *Lolium Multiflorum* (Welsh Ray grass). The data includes grass concentrations and air concentrations for dioxin congener groups, but not the invidual congeners. Lorber (1995) used data from Welsch-Pausch et al.(1995) to develop an air-to-leaf transfer factor for each dioxin-congener group. *Bv* values developed by Lorber (1995) were about an order of magnitude less than values calculated using the Bacci et al. (1990) and (1992) correlation equations. Lorber (1995) speculated that this difference could be attributed to several factors including experimental design, climate, and lipid content of plant species used.

We obtained the *Br* values for PCDDs and PCDFs listed in the HHRAP database from the experimentally derived values of Lorber (1995). However, Lorber (1995) stated that these values should be considered carefully by users of this methodology because of the inherent uncertainties associated with the data.

Metals For metals, we found no literature sources for the *Bv* values. U.S. EPA (1995b) quoted from the following document, that metals were assumed not to experience air to leaf transfer:

- Belcher, G.D., and C.C. Travis. 1989. "Modeling Support for the RURA and Municipal Waste Combustion Projects: Final Report on Sensitivity and Uncertainty Analysis for the Terrestrial Food Chain Model." Interagency Agreement No. 1824-A020-A1. Office of Risk Analysis, Health and Safety Research Division. Oak Ridge National Laboratory. Oak Ridge, Tennessee. October.

As with the above cited references, we assumed *Bv* values for metals (excluding elemental mercury) are zero.

Mercury The HHRAP assumes that mercury emissions consist of both the elemental and divalent forms. However, only small amounts of elemental mercury is assumed to be deposited based on its behavior in the atmosphere. Elemental mercury either dissipates into the global cycle or is converted to the divalent form. The HHRAP assumes methyl mercury doesn't exist in air emissions or in the air phase. Additional basis for the assumption regarding mercury transfer from air to plants includes

- elemental mercury reaching or depositing onto the plant surfaces is negligible, and
- biotransfer of methyl mercury from air is zero.

This is based on assumptions made regarding speciation and fate and transport of mercury from emissions. Therefore, we assume the *Bv* values for elemental and methyl mercury are zero. The *Bv* value for mercuric chloride (dry weight basis) comes from U.S. EPA (1997b).

If field data suggests otherwise, *Bv* values (1) provided in U.S. EPA (1997b) for methyl mercury can be used, and (2) need to be determined for elemental mercury. Please note that uptake of mercury from air into the aboveground plant tissue is primarily in the divalent form. We assume that a part of the divalent form of mercury is converted to methyl mercury once in the plant tissue.

A2-2.13 BIOTRANSFER FACTORS FOR ANIMALS

The biotransfer factor for animals (*Ba*) is the ratio of contaminant concentration in fresh weight animal tissue to the daily intake of contaminant by the animal.

A2-2.13.1 BTFs for Beef (Ba_{beef}) and Milk (Ba_{milk})

The main route of human exposure to many highly lipophilic compounds is through ingestion of contaminated agricultural products such as beef and milk (McLachlan 1993). The transfer of contaminants from environmental media (e.g., air, soil, water) and food (e.g. grain, silage) into livestock products (e.g., beef, milk) has historically been either determined by direct measurement of contaminants in livestock products, or predicted using regression models.

Organic Compounds

When empirical data are lacking for biotransfer of organc chemicals, one of the most widely used approaches to predict contaminant transfer from environmental media and food to beef tissue and milk are the regression models developed by Travis and Arms (1988), which relate chemical octanol-water partition coefficient (K_{ow}) to biotransfer into beef and milk. These regressions, however, are hampered by the limited log K_{ow} range and questions surrounding the validity of the underlying biotransfer data set. In response, EPA developed a new methodology for predicting beef and milk biotransfer factors (See report entitled: "Methodology for Predicting Cattle Biotransfer Factors" (RTI 2005) for complete documentation of the approach).

Using EPA's updated methodology, we predicted biotransfer factors for organic chemicals with the following single equation:

$$\log Ba_{fat} = -0.099\ (\log K_{ow})^2 + 1.07\ \log K_{ow} - 3.56 \qquad (n = 305,\ r^2 = 0.8259)$$

Equation A-2-21

where

Ba_{fat} = Biotransfer factor ([mg /kg Fat]/[mg/day])
K_{ow} = Octanol-water partition coefficient (unitless).

Values for Ba_{fat} were adjusted to account for the assumed fat content of milk and beef as shown below:

$$Ba_{milk} = 10^{\log Ba_{fat}} \times 0.04 \qquad \text{Equation A-2-22}$$

$$Ba_{beef} = 10^{\log Ba_{fat}} \times 0.19 \qquad \text{Equation A-2-23}$$

The log K_{ow}'s of the chemicals used to derive the equation ranged from -0.67 to 8.2. Therefore we used equation A-2-21 for organic chemicals having a log Kow between -0.67 and 8.2. Compounds with log K_{ow} values less than -0.67 were assigned Ba_{beef} and Ba_{milk} values corresponding to a log K_{ow} value of -0.67. At the high end of the range, compounds with log K_{ow} values greater than 8.2 were assigned Ba_{beef} and Ba_{milk} values corresponding to a log K_{ow} value of 8.2. We used the K_{ow} values in the HHRAP database to calculate Ba_{beef} and Ba_{milk} values.

Highly Metabolized Organic Compounds

As discussed in RTI (2005), Equation A-2-21 might overestimate biotransfer of highly metabolized chemicals, producing an upper bound estimate for these chemicals. Of those chemicals relevant to the HHRAP (and therefore included in the HHRAP companion database), Phthalates and PAHs fall within this group (see HHRAP Chapter 2 for more information on the phthalate and PAH chemical categories).

One way to account for this potential overestimation is to rely upon a metabolism factor to improve model predictions. For example, EPA developed a metabolism factor of 0.01 (i.e., 99% of the chemical ingested is metabolized) for bis-ethylhexyl phthalate (BEHP, See Chapter 2). When this factor is applied to the biotransfer factors predicted using the regression equation recommended above for BEHP, the biotransfer factors are reduced by two orders of magnitude. These metabolism-adjusted predicted biotransfer factors are close in magnitude to the empirically derived biotransfer factors found in the literature, which supports using this metabolism factor. Unfortunately, EPA has not developed metabolism factors for other organic chemicals, due to limited availability of empirically derived data (see Chapter 2).

For those highly metabolized chemicals that don't have metabolism factors, we still consider it reasonable to use estimated Ba values for the following reasons:

- Few chemicals have had all their degradation products identified;
- If identified, the degradation products may in fact be as toxic as, or even more toxic than, the parent compound (the degradation products of PAHs, for example, are toxic). Unless data demonstrates that all degradation products are nontoxic (as is the case for BEHP), the only way to address toxic degradation products in the HHRAP is to include their mass in the mass of the parent chemical; and

- the metabolic degradation products may themselves be persistent. For example, DDT is metabolized to DDD and DDE, which remain persistent.

It should also be noted that not all chemicals are metabolized at the same rate and may remain in animal tissue as the parent compound through establishment of steady state concentrations. In fact, many of the chemicals in the biotransfer data set that are well predicted by Equation A-2-21 are metabolized to other compounds. DDT is metabolized to DDE, and lindane (used to derive the regression, but not in the HHRAP) is metabolized to many different compounds. For DDT and lindane, biotransfer factors are well predicted using Equation A-2-21. Thus, just because a chemical undergoes biotransformation to other compounds, doesn't necessarily mean Equation A-2-21over-estimates its biotransfer.

Lacking sufficient data to identify all degradation products, characterize all degradation products as nontoxic, and ensure that all potentially toxic degradation products are less persistent than the parent chemical, we consider it reasonably protective to use the Ba_{beef} and Ba_{milk} values for the parent chemical as predicted, without adjustment. If a highly metabolized chemical is found to drive the risk assessment, then we recommend re-evaluating the appropriateness of the Ba_{beef} and Ba_{milk} values.

Ionizing Organic Compounds

To improve BTF estimates for organic acids, we used the first-order dissociation constant (pKa) to account for chemical ionization. For these chemicals, K_{ow} is a weighted value calculated based on the fraction of the chemical in the neutral form such that:

$$K_{ow} = K_{ow}n \times (FracNeutral) + K_{ow}i \times (1 - FracNeutral) \qquad \text{Equation A-2-24}$$

where

$K_{ow}n$ = partition coefficient for the neutral species (unitless),
$K_{ow}i$ = partition coefficient for the ionized species (mol/L),
FracNeutral = fraction of neutral species present for organic acids (unitless).

Accounting for the fraction of ionizable organics in the neutral form is important because K_{ow} can vary considerably depending on pH. The cow's small intestine, where chemicals can be absorbed, has a near neutral pH (Umphrey and Staples, 1992). Thus, the neutral fraction is determined using a pH equal to 7 in the following equation (Lee et al., 1990):

$$FracNeutral = \frac{[HA]}{[HA] - [A-]} = \left(1 + 10 pH - pKa\right) \qquad \text{Equation A-2-25}$$

where

[HA] = equilibrium concentration of organic acid (mol/L),
[A-] = equilibrium concentration of anion (mol/L), and
pKa = acid dissociation constant (unitless).

If a value for log $K_{ow}i$ wasn't available, we estimated log $K_{ow}i$ assuming a ratio of log $K_{ow}i$ to log $K_{ow}n$ of 0.015. This ratio is a conservative value developed by EPA to apply to organic acids without data for log $K_{ow}i$ (U.S. EPA, 1996).

Metals

We obtained Ba_{beef} and Ba_{milk} values for metals (except cadmium, mercury, selenium, and zinc), on a fresh weight basis, from Baes et al. (1984). For cadmium, selenium, and zinc, U.S. EPA (1995a) cited *Ba* values derived by dividing uptake slopes [(g COPC/kg DW tissue)/(g COPC/kg DW feed)], obtained from U.S. EPA (1992b), by a daily consumption rate of 20 kg DW per day for beef and dairy cattle.

We obtained our recommended values from Baes et al. (1984) for all metals except cadmium, selenium, and zinc. We calculated *Ba* values for cadmium, selenium, and zinc using uptake slope factors and consumption rates provided in U.S. EPA (1992b) and U.S. EPA (1995a), converting the result to a fresh weight basis by assuming a moisture content of 87 percent in milk and 70 percent in beef. Moisture content in beef and milk were obtained from the following:

C U.S. EPA. 1997c. *Exposure Factors Handbook*. "Food Ingestion Factors". Volume II. EPA/600/P-95/002Fb. August.

C Pennington, J.A.T. 1994. *Food Value of Portions Commonly Used*. Sixteenth Edition. J.B. Lippincott Company, Philadelphia.

We provide the calculated fresh weight Ba_{beef} *and* Ba_{milk} values in the HHRAP database.

Mercuric Compounds

The HHRAP assumes that elemental mercury neither deposits onto soils nor transfers to aboveground plant parts. Therefore, there's no transfer of elemental mercury into animal tissue. Therefore, we recommend *Ba* values of zero for elemental mercury. This based on assumptions made regarding speciation and fate and transport of mercury from emission sources.

If field data suggests otherwise, Ba_{beef} and Ba_{milk} values for elemental mercury can be derived from the uptake slope factors provided in U.S. EPA (1992b) and U.S. EPA (1995a); using the same consumption rates discussed earlier for metals like cadmium, selenium, and zinc.

We derived the Ba_{beef} and Ba_{milk} values listed in the HHRAP database for mercuric chloride and methyl mercury from data in U.S. EPA (1997b). U.S. EPA (1997b) provided Ba_{beef} and Ba_{milk} values for mercury, but did not specify for which form of mercury. As in U.S. EPA (1997b), we assume mercury speciates into 87 percent divalent mercury and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the Ba_{beef} and Ba_{milk} values provided in U.S. EPA (1997b) were for total mercury in animal tissue, the biotransfer factors in U.S. EPA (1997b) can be apportioned in the fractions assumed to be found in animal tissue. Therefore, we based the values reported in the HHRAP database on the following:

C We converted the default Ba_{milk} value of 0.02 day/kg DW for mercury to a fresh weight basis assuming a 87 percent moisture content in milk (U.S. EPA 1997c; and Pennington 1994). We multiplied the resulting Ba_{milk} (fresh weight) value by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

C We converted the default Ba_{beef} value of 0.02 day/kg DW for mercury to a fresh weight basis assuming a 70 percent moisture content in beef (U.S. EPA 1997c; and Pennington 1994). We multiplied the resulting Ba_{beef} (fresh weight) value by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

A2-2.13.2 Biotransfer Factors for Pork (Ba_{pork})

For most compounds we derived Ba_{pork} values using the same method used to estimate Ba_{beef} values (see Section A2-2.13.1 above for a detailed description of the method & its limitations), modifying to reflect an assumed fat content of pork of 23%. Specifically, we used equation A-2-21 to generate Ba_{fat} values, which were then adjusted to account for the assumed fat content of pork as shown below:

$$Ba_{pork} = 10^{\log Ba_{fat}} \times 0.23 \qquad \text{Equation A-2-26}$$

The log K_{ow}'s of the chemicals used to derive the equation ranged from -0.67 to 8.2. Therefore we used equation A-2-21 for organic chemicals having a log Kow between -0.67 and 8.2. Compounds with log K_{ow} values less than -0.67 were assigned Ba_{pork} values corresponding to a log K_{ow} value of -0.67. At the high end of the range, compounds with log K_{ow} values greater than 8.2 were assigned Ba_{pork} values corresponding to a log K_{ow} value of 8.2. We used the K_{ow} values in the HHRAP database to calculate Ba_{pork} values.

This calculation is limited by the assumptions that:

- contaminants bioconcentrate in the fat tissues; and

- effects from differences in metabolism, digestive system, and feeding characteristics between beef cattle and pigs are minimal.

Metals For metals (except cadmium, selenium, and zinc), no data was available in the literature to calculate Ba_{pork} values.

For cadmium, selenium, and zinc, U.S. EPA (1995b) reported *Ba* values derived by dividing uptake slopes [(g COPC/kg DW tissue)/(g COPC/kg DW feed)], obtained from U.S. EPA (1992b), by a daily consumption rate of 4.7 kg DW per day for pigs provided in U.S. EPA (1995a). The dry weight Ba_{pork} values (for cadmium, selenium, and zinc) were converted to a fresh weight basis assuming a moisture content of 70 percent in pork (U.S. EPA 1997c; and Pennington 1994).

Mercuric Compounds The HHRAP assumes that elemental mercury neither deposits onto soils nor transfers to the aboveground plant parts; therefore, there's no transfer of elemental mercury into the animal tissue. Therefore, we recommend *Ba* values of zero for elemental mercury. This is based on the assumptions made regarding speciation and fate and transport of mercury from emissions.

If field data suggests otherwise, Ba_{pork} values for elemental mercury can be derived from the uptake slope factors provided in U.S. EPA (1992b) and U.S. EPA (1995a), using the same consumption rates discussed earlier for metals like cadmium, selenium, and zinc.

We derived Ba_{pork} values for mercuric chloride and methyl mercury from data in U.S. EPA (1997b). U.S. EPA (1997b) provided Ba_{pork} values for mercury, but did not specify for which form of mercury. As in U.S. EPA (1997b), the HHRAP assumes that mercury speciates into 87 percent divalent mercury and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the Ba_{pork} values provided in U.S. EPA (1997b) were for total mercury in animal tissue, biotransfer factors in U.S. EPA (1997b) can be apportioned in the fractions it is assumed to be found in animal tissue.

Therefore, we converted the U.S. EPA (1997b) Ba_{pork} value of 0.00013 day/kg DW for mercury to a fresh weight basis assuming a 70 percent moisture content in pork (U.S. EPA 1997c; and Pennington 1994).

We multiplied the resulting Ba_{pork} (fresh weight) value by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

A2-2.13.3 BTFs for Chicken ($Ba_{chicken}$) and Poultry Eggs (Ba_{egg})

Biotransfer factors for chicken ($Ba_{chicken}$) and poultry eggs (Ba_{egg}) are expressed as the ratio of the contaminant concentration in the fresh weight tissue to the contaminant intake from the feed. Biotransfer factors are calculated from bioconcentration factors for chicken and poultry eggs. BCFs are expressed as the ratio of the contaminant concentration in the fresh weight tissue to the contaminant concentration in dry weight soil.

For most compounds we derived Ba_{pork} values using the same method used to estimate Ba_{beef} values (see Section A2-2.13.1 above for a detailed description of the method & its limitations), modifying to reflect an assumed fat content of chicken of 14%, and eggs of 8%. Specifically, we used equation A-2-21 to generate Ba_{fat} values, which were then adjusted to account for the assumed fat content of chicken and eggs as shown below:

$$Ba_{chicken} = 10^{\log Ba_{fat}} \times 0.14 \qquad \text{Equation A-2-27}$$

$$Ba_{egg} = 10^{\log Ba_{fat}} \times 0.08 \qquad \text{Equation A-2-28}$$

The log K_{ow}'s of the chemicals used to derive the equations ranged from -0.67 to 8.2. Therefore we used equation A-2-21 for organic chemicals having a log Kow between -0.67 and 8.2. Compounds with log K_{ow} values less than -0.67 were assigned $Ba_{chicken}$ and Ba_{egg} values corresponding to a log K_{ow} value of -0.67. At the high end of the range, compounds with log K_{ow} values greater than 8.2 were assigned $Ba_{chicken}$ and Ba_{egg} values corresponding to a log K_{ow} value of 8.2. We used the logK_{ow} values in the HHRAP database to calculate $Ba_{chicken}$ and Ba_{egg} values.

These calculations are limited by the assumptions that:

- contaminants bioconcentrate in the fat tissues; and
- effects from differences in metabolism, digestive system, or feeding characteristics between beef cattle and chickens are minimal.

Please note that the scenario of principal concern for chicken and egg contamination is for home grown chickens. The raising of home grown chickens would be characteristic of free range and semi-free range housing conditions where poultry do come in contact with soil, and possibly vegetation, insects, and benthic organisms. The applicability of this scenario to commercial poultry operations characterized by housing conditions that do not provide chickens access to soil would need to be assessed on a case-by-case basis.

Metals $Ba_{chicken}$ and Ba_{egg} values for all metals except cadmium, selenium, and zinc, weren't available in the literature. For cadmium, selenium, and zinc, U.S. EPA (1995a) cited *Ba* values that were derived by dividing uptake slopes [(g COPC/kg DW tissue)/(g COPC/kg DW feed)], obtained from U.S. EPA (1992b), by a daily consumption rate of 0.2 kilograms DW per day by chicken. To obtain values listed in the HHRAP database, we converted the dry weight *Ba* value to a fresh weight value by assuming a moisture content of 75 percent in eggs and chicken (U.S. EPA 1997c; and Pennington 1994).

Mercury The HHRAP assumes that elemental mercury neither deposits onto soils nor transfers to the aboveground plant parts or grains. Therefore, there's no transfer of elemental mercury into animal tissue. Therefore, we recommend *Ba* values of zero for elemental mercury. This is based on the assumptions made regarding speciation and fate and transport of mercury from emission sources.

If field data suggests otherwise, $Ba_{chicken}$ and Ba_{egg} values for elemental mercury can be derived from the uptake slope factors provided in U.S. EPA (1992b) and U.S. EPA (1995a), using the same consumption rates discussed earlier for metals like cadmium, selenium, and zinc.

We derived $Ba_{chicken}$ and Ba_{egg} values for mercuric chloride and methyl mercury from data in U.S. EPA (1997b). U.S. EPA (1997b) provided $Ba_{chicken}$ and Ba_{egg} values for mercury, but did not specify for which form of mercury. As in U.S. EPA (1997b), the HHRAP assumes mercury speciates into 87 percent divalent mercury and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the $Ba_{chicken}$ and Ba_{egg} values provided in U.S. EPA (1997b) were for total mercury in animal tissue, then biotransfer factors in U.S. EPA (1997b) can be apportioned in the fractions it is assumed to be found in animal tissue.

Therefore, we based the values reported in the HHRAP database on the following:

- We converted the U.S. EPA (1997b) $Ba_{chicken}$ value of 0.11 day/kg DW for mercury to a fresh weight basis assuming a 75 percent moisture content in chicken (U.S. EPA 1997c; and Pennington 1994). We multiplied the resulting $Ba_{chicken}$ (fresh weight) value by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

- We converted the U.S. EPA (1997b) Ba_{egg} value of 0.11 day/kg DW for mercury to a fresh weight basis assuming a 75 percent moisture content in eggs (U.S. EPA 1997c; and Pennington 1994). We multiplied the resulting Ba_{egg} (fresh weight) value by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

A2-2.13.4 Bioconcentration and Bioaccumulation Factors for Fish

Bioconcentration and bioaccumulation factors for fish are used for various compounds, depending on the K_{ow} value of the compound. We recommend using bioconcentration factors for fish (BCF_{fish}) for compounds (except PCDDs, PCDFs, and PCBs) with a log K_{ow} value less than 4.0; and for metals (except lead and mercury). We recommend using bioaccumulation factors for fish (BAF_{fish}) for compounds (except PCDDs, PCDFs, and PCBs) with a log K_{ow} value greater than 4.0, lead, and mercuric compounds. We recommend also using biota-sediment accumulation factors for fish ($BSAF_{fish}$) for PCDDs, PCDFs, and PCBs.

A2-2.13.4.1 Bioconcentration Factors for Fish (BCF_{fish})

BCF_{fish} is the ratio of the contaminant concentration in fish to the contaminant concentration in the water column where the fish is exposed. It accounts for uptake of contaminants by fish from water passing across the gills. We derived *BCF* values for fish for all organic compounds with a log K_{ow} of less than 4.0 (cutoff value with BAF_{fish}) and for all metals, except lead and mercury, as cited in U.S. EPA (1995b). This implies that the concentration of contaminant in the fish is only due to water intake by the fish, and compounds with a log K_{ow} of less than 4.0 are assumed not to significantly bioaccumulate.

It is generally assumed that field measured BCFs are based on total (dissolved and suspended) water column concentrations, and laboratory measured BCFs are based on dissolved water column concentrations. This distinction is important for compounds with a log K_{ow} of greater than or equal to 4.0, because significant amounts of a contaminant can partition into the suspended sediment organic carbon (or particulate phase) of the water column. For compounds with a log K_{ow} of less than 4.0, most of the contaminant is associated with the dissolved phase of the water column and negligible amounts of the contaminant is associated with the suspended sediment phase in the water column. Therefore, for compounds with a log K_{ow} of less than 4.0, BCF values based on dissolved contaminant water concentrations in the water column are essentially the same as BCF values based on total (dissolved + suspended) contaminant water concentrations in the water column.

Our recommended BCF values don't recognize differences in total versus dissolved water concentrations when calculating fish concentrations from BCF_{fish} values for compounds with a log K_{ow} of less than 4.0. Since, dissolved water concentrations is the major contributing factor from compounds with a log K_{ow} of less than 4.0, all BCF_{fish} values (regardless of whether they were derived using total or dissolved water concentrations) can be multiplied by the contaminant concentration in the dissolved water column (C_{dw}) to calculate fish concentrations. This assumption is necessary because (1) literature data is often unclear if the water concentrations are dissolved or total concentrations, and (2) most of the literature reviewed indicated that laboratory experiments were conducted using filtered or distilled water; or the experiments were conducted using fresh water, but were filtered before analyses for water concentrations.

For most compounds, we calculated *BCF* values using best fit log K_{ow} correlation equations derived by Meylan et al. (1999):

C Meylan, W., P.H. Howard, R.S. Boethling, D. Aronson, H. Printup, and S. Gouchie. 1999. "Improved Method for Estimating Bioconcentration/Bioaccumulation Factor from Octanol/Water Partition Coefficient". *Environmental Toxicology and Chemistry*. 18(4):664-672.

Meylan et al. (1999) collected information on measured BCF and other key experimental details for 694 chemicals. Log *BCF* was then regressed against log K_{ow} , and chemicals with significant deviations from the line of best fit were analyzed by chemical structure. The resulting algorithm classifies a substance as either nonionic or ionic, the latter group including carboxylic acids, sulfonic acids and their salts, and quaternary N compounds. Log *BCF* for nonionics was estimated from log K_{ow} and a series of correction factors if applicable; different equations apply for log K_{ow} 1.0 to 7.0 and >7.0 (Meylan et al. 1999). These equations are as follows:

For log K_{ow} < 1 :

$$\log BCF = 0.50$$

Equation A-2-27

For log K_{ow} 1 to 7:

$$\log BCF = 0.77 \log K_{ow} - 0.70 + \Sigma \; Correction \; Factors$$

Equation A-2-28

For log K_{ow} > 7:

$$\log BCF = -1.37 \log K_{ow} + 14.4 + \Sigma \; Correction \; Factors$$

Equation A-2-29

For log K_{ow} >10.5:

$$\log BCF = 0.50$$

Equation A-2-30

For ionic compounds (carboxylic acids, sulfonic acids and salts, compounds with N of +5 valence), were categorized by log K_{ow}, and a log *BCF* in the range 0.5 to 1.75 was assigned as follows:

For log K_{ow} < 5 : $\log BCF = 0.50$ Equation A-2-31

For log K_{ow} 5 to 6: $\log BCF = 0.75$ Equation A-2-32

For log K_{ow} 6 to 7: $\log BCF = 1.75$ Equation A-2-33

For log K_{ow} 7 to 9: $\log BCF = 1.00$ Equation A-2-34

For log K_{ow} > 9: $\log BCF = 0.50$ Equation A-2-35

We assume that BCF_{fish} values calculated using the above correlation equations were (1) based on dissolved water concentrations, and (2) not lipid-normalized.

<u>Metals</u> We obtained measured BCF_{fish} values for metals (except lead and mercury) from various literature studies, as cited in U.S. EPA (1999a). Values not available in U.S. EPA (1999a) we estimated using the correlation equations above. BCF_{fish} values obtained from U.S. EPA (1999a) were characterized as follows:

- Field-measured or laboratory-measured values from various experimental studies were evaluated by U.S. EPA (1999a). This information is summarized in the following document:

  > U.S. EPA. 1999a. *Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities.* Peer Review Draft. August.

  Field-measured data is only (1) available for a limited number of compounds, and (2) based on a single study. In such cases, the field-measured value or the geometric mean of field-measured values were compared with the geometric mean of laboratory-measured values, and the higher one used. A detailed discussion on sources of *BCF* values and methodology followed were provided in Appendix C of U.S. EPA (1999a).

Measured values from various experimental studies were evaluated by U.S. EPA (1999a). Detailed discussion and sources of measured values were provided in U.S. EPA (1999a). For lead and some mercury compounds, a *BAF* was determined to be more applicable than a *BCF*, since those compounds tends to bioaccumulate.

<u>Mercury</u> As in U.S. EPA (1997b), elemental mercury isn't expected to deposit significantly onto soils and surface water. Therefore, it's assumed that there is no transfer of elemental mercury into fish. Fish are assumed to be exposed only to the divalent and organic forms of mercury that exist in the water and soil/sediment media. However, as with the conservative approach adopted by previous guidance documents, all of mercury in the fish is assumed to exist or be converted to the methyl mercury (organic) form after uptake into the fish tissue. Therefore, *BCF* and *BAF* values are not considered applicable for divalent mercury (mercuric chloride). For methyl mercury, a *BAF* was determined to be more applicable than a *BCF*, since mercury tends to bioaccumulate.

A2-2.13.4.2 Bioaccumulation Factors for Fish (BAF_{fish})

BAF_{fish} is the ratio of the contaminant concentration in fish to the contaminant concentration in the water body where the fish are exposed. The BAF_{fish} accounts for uptake of contaminants by fish from water and sediments passing across the gills, and from consumption of various foods including plankton, daphnids, and other fish.

For compounds with a log K_{ow} of greater than or equal to 4.0, contaminants can significantly partition into the suspended sediment organic carbon (or particulate phase) of the water column. Therefore, *BAF* values should generally be based on total (dissolved and suspended) water column concentrations. *BAF* values for fish reported in the HHRAP database were used for organic compounds (except PCBs, PCDDs, and PCDFs) with a log K_{ow} greater than 4.0, lead and some mercuric compounds.

In general we assumed that:

- Field-measured BAFs were based on total (dissolved and suspended) water column concentrations;
- Laboratory-measured BCFs, and therefore the BAFs predicted from them, were based on dissolved water column concentrations; and
- BCFs estimated using correlation Equations A-2-24 through A-2-32, and therefore the BAFs predicted from them, were based on dissolved water column concentrations.

In addition, we assumed that field-measured BCFs for compounds with a log K_{ow} greater than 4.0 were equal to BAFs, because the tissue concentrations are a result of uptake of water (dissolved and suspended), sediment, and various trophic level food.

For most organic compounds (except PCBs, PCDDs and PCDFs) with a log K_{ow} greater than 4.0, the FCM, which accounts for accumulation through the food chain in addition to water, becomes greater than 1. Therefore, a BAF_{fish}, which takes the food chain into consideration, is more appropriate than a BCF_{fish} (U.S. EPA 1995c; 1998). As in U.S. EPA (1995c; 1998), we assumed that *BAF* values for inorganic chemicals equal *BCFs* (i.e., the *FCM* is 1.0), unless chemical specific biomagnification data support using a *FCM* other than 1.0.

For consistency, we adjusted all field-measured BAF (or BCF) values using the methodology suggested in U.S. EPA (1998), to include only the dissolved water column fractions; (i.e., the BAFs based on total water concentrations were converted to BAFs based on dissolved water concentrations). This was done so that all BAF_{fish} values (based on dissolved water concentrations) can be multiplied by the contaminant concentration in the dissolved water column (C_{dw}) to calculate fish concentrations.

We used the following equation cited in U.S. EPA (1998) to convert the *BAF* based on total water concentrations to a *BAF* based on dissolved water concentrations:

$$f_{fd} = \frac{1}{1 + \frac{(DOC)\ (K_{ow})}{10} + (POC)\ (K_{ow})} \qquad \text{Equation A-2-36}$$

where

f_{fd} = fraction of COPC that is freely dissolved in water
DOC = concentration of dissolved organic carbon, kg organic carbon / L water
POC = concentration of particulate organic carbon, kg organic carbon / L water

Since, the Gobas (1993) model was derived from a study conducted at Lake Ontario, DOC and POC values for Lake Ontario were used. Values cited in U.S. EPA (1998) were:

DOC = 2×10^{-6} kg/L
POC = 7.5×10^{-9} kg/L

A *BAF* based on dissolved water concentrations can be calculated from a *BAF* based on total water concentrations as follows:

$$BAF\ (dissolved) = \frac{BAF\ (total)}{f_{fd}} - 1 \qquad \text{Equation A-2-37}$$

Metals (lead) For lead, the food-chain multiplier becomes greater than 1; therefore, a BAF is more appropriate. We obtained the BAF_{fish} value reported in the HHRAP database for lead as a geometric mean from various literature sources described in U.S. EPA (1999a). Since we recommend assuming that metals are insoluble under neutral conditions, the dissolved and total water concentrations are almost equal. However, for consistency, we adjusted the BAF_{fish} value for lead for dissolved fractions.

Mercuric Compounds As in U.S. EPA (1997b), we don't expect elemental mercury to deposit significantly onto soils and surface water. Therefore, there it is assumed that there is no transfer of elemental mercury into fish. Fish are assumed to be exposed only to the divalent and organic forms of mercury that exists in the water and soil/sediment media. However, consistent with the conservative approach adopted by previous guidance documents, all of mercury in the fish is assumed to exist or be converted to the methyl mercury (organic) form after uptake into the fish tissue. Therefore, we obtained the BAF_{fish} value for methyl mercury from U.S. EPA (1997b) for a trophic level 4 fish.

A2-2.13.4.3 Biota-Sediment Accumulation Factor for Fish ($BSAF_{fish}$)

PCDDs, PCDFs, and PCBs $BSAF_{fish}$ accounts for the transfer of contaminants from the bottom sediment to the lipid in fish. U.S. EPA (2000) and (1993d) recommended using $BSAF_{fish}$ values for dioxin-like compounds, including PCBs, because of their lipophilic nature. U.S. EPA (1995b) also stated that $BSAF_{fish}$ values (1) were used for 2,3,7,8-TCDD and PCBs to estimate protective sediment concentrations instead of surface water concentrations, and (2) were a more reliable measure of bioaccumulation potential because of the analytical difficulties in measuring dissolved concentrations in surface water. Therefore, for PCDDs, PCDFs, and PCBs, The HHRAP database includes $BSAF_{fish}$ values instead of BAFs for fish. We obtained the $BSAF_{fish}$ values from U.S. EPA (2000).

U.S. EPA (2000) provided exposure scenarios for conducting site-specific assessments to dioxin-like compounds. For each scenario, U.S. EPA (2000) recommended the use of the following $BSAF_{fish}$ values based on the amount of chlorination of the PCDD or PCDF:

C For TetraCDDs and TetraCDFs, $BSAF_{fish} = 9.0 \times 10^{-02}$

C For PentaCDDs and PentaCDFs, $BSAF_{fish} = 9.0 \times 10^{-02}$

C For HexaCDDs and HexaCDFs, $BSAF_{fish} = 4.0 \text{ x } 10^{-02}$

C For HeptaCDDs and HeptaCDFs, $BSAF_{fish} = 5.0 \text{ x } 10^{-03}$

C For OctaCDDs and OctaCDFs, $BSAF_{fish} = 1.0 \text{ x } 10^{-04}$

Homologue group $BSAF_{fish}$ values obtained from U.S. EPA (2000) were either measured or estimated values that were based on a whole fish lipid content of 7 percent and an organic carbon content of 3 percent.

A2-3 TOXICITY BENCHMARKS

The following sections discuss carcinogenic and noncarcinogenic toxicity benchmarks of compounds. The toxicity information provided in the HHRAP is for informational purposes to help permitting authorities explain the basis for selecting contaminants of concern. Since toxicity benchmarks and slope factors may change as additional toxicity research is conducted, we highly recommend consulting with the most current versions of the sources listed below before completing a risk assessment, to ensure that the toxicity data used in the risk assessment is based upon the most current Agency consensus.

A2-3.1 Prioritization of Data Sources for Chronic Toxicity Benchmarks

In December 2003, the Office of Superfund Remediation and Technology Innovation distributed OSWER Directive 9285.7-53, (U.S. EPA 2004a) updating the hierachy of sources of human health toxicity values originally distributed in Risk Assessment Guidance for Superfund Volume I, Part A, Human Health Evaluation Manual (RAGS) (U.S. EPA 1989). We recommend using the same heirarchy of sources for acquiring human health toxicity data to be used in performing risk assessments of hazardous waste combustion facilities.

We gathered the following parameter values for the database:

- Chronic Oral Toxicity Benchmarks:
  - Oral Reference Doses (*RfD*s) for effects other than cancer (non-cancer)
  - Oral Cancer Slope Factors (*CSF*s) for cancer

- Chronic Inhalation Toxicity Benchmarks:
  - Inhalation Reference Concentrations (*RfC*s) for effects other than cancer (non-cancer)
  - Unit Risk Factors (*URF*s) for cancer

As with other Agency applications (i.e., U.S. EPA Superfund, Resource Conservation and Recovery Act [RCRA] , and Air Toxics), toxicity benchmarks available in the U.S. EPA Integrated Risk Information System (IRIS) (U.S. EPA 2005) were given first priority. For contaminants lacking current IRIS assessments, we obtained toxicity benchmark values from one of the following data sources:

- Provisional Peer-Reviewed Toxicity Values (PPRTVs)

- Other Peer Reviewed Values:

- California Environmental Protection Agency (CalEPA) chronic Reference Exposure Levels (RELs) and Unit Risk Estimate (UREs)

- U.S. Agency for Toxic Substances and Disease Registry (ATSDR) chronic Minimum Risk Levels (MRLs)

- U.S. EPA. 1997a. Health Effects Assessment Summary Tables (HEAST) and older health effects assessment documents not incorporated into HEAST - U.S. EPA Office of Research and Development (ORD)-National Center for Environmental Assessment (EPA-NCEA)

Dose-response assessments that have achieved full intra-agency consensus are incorporated in IRIS, which is regularly updated and available on-line (U.S. EPA 2005). As of 1996, benchmark values placed on IRIS have undergone external peer review and Agency consensus review. Both the U.S. EPA Superfund and RCRA programs accept the primacy of human health toxicity values contained in U.S. EPA's IRIS. The primacy of IRIS toxicity values is also identified in Risk Assessment Guidance for Superfund (RAGS) hierarchy (U.S. EPA 1989).

A Provisional Peer-Reviewed Toxicity Value (PPRTV) is a toxicity value derived for use in the U.S. EPA Superfund Program when such value is not available in U.S. EPA's IRIS (PPRTVs currently represent the second tier of human health toxicity values for the U.S. EPA Superfund and RCRA hazardous waste programs). PPRTVs are derived after a review of the relevant scientific literature using the methods, sources of data, and guidance for value derivation used by the U.S. EPA IRIS Program. All provisional toxicity values receive internal review by two EPA scientists and external peer review by at least two scientific experts. A third scientific review is performed if there is a conflict between the two original external reviewers. PPRTVs differ in part from IRIS values in that PPRTVs do not receive the multi-program consensus review provided for IRIS values. This is because IRIS values are generally intended to be used in all U.S. EPA programs, while PPRTVs are developed specifically for the Superfund Program. In general, the need for a PPRTV is eliminated once an analogous IRIS value becomes available. Once IRIS values become available, PPRTVs are generally removed from the PPRTV database.

U.S. EPA ORD is concerned that PPRTV's may be seen (and used) as equivalent to IRIS values, and has restricted ***direct*** access to the PPRTV values database to only EPA employees. EPA employees can access the PPRTV database directly via the EPA intranet web site. All others wishing to gain access to PPRTV values need to register as approved users.

If you are on an approved or registered user list, and contact the EPA Center which derives PPRTVs they would email PPRTV assessments you request to you. Plus, if you are on this list, they would periodically email you a list of what contaminants are in the PPRTV database. If you think that you would like to be on this list, please contact a risk assessor or toxicologist in an EPA Superfund or hazardous waste program in the EPA Regional Office containing sites you are working on or expect to work on. You may also apply to be put on the list by sending an email, with "PPRTV Approved User Application" in the subject line, to HHRAPFeedback@EPA.GOV. Please include the following information in the body of the email:

- Your name
- Your affiliation (e.g. company or regulatory agency you work for, or civic/public organization, or other entity interested in a risk assessment using PPRTVs)
- Email address (if it's different than the address form which you send the application)

As described on the U.S. EPA ORD Air Toxics web site (http://www.epa.gov/ttn/atw), the California Environmental Protection Agency (CalEPA) Office of Environmental Health Hazard Assessment has developed dose-response assessments for many substances, based both on carcinogenicity and health effects other than cancer. The process for developing these assessments is similar to that used by U.S. EPA to develop IRIS values and incorporates significant external scientific peer review. The non-cancer information includes available inhalation health risk guidance values expressed as chronic inhalation and oral reference exposure levels (RELs). CalEPA defines the REL as a concentration level at (or below) which no health effects are anticipated, a concept that is substantially similar to U.S. EPA's non-cancer dose-response assessment perspective. The HHRAP database shows the chronic REL when no IRIS RfC/RfD or PPRTV exists.

CalEPA's quantitative dose-response information on carcinogenicity by inhalation exposure is expressed in terms of the URE, defined similarly to EPA's URE. The HHRAP database shows specific CalEPA UREs where no IRIS or PPRTV values exist. CalEPA's dose response assessments for carcinogens and noncarcinogens are available on-line.

As with U.S. EPA ORD Air Toxics, ATSDR chronic MRL values were listed in the HHRAP database for assessing noncancer effects. As described on the U.S. EPA ORD Air Toxics web site (http://www.epa.gov/ttn/atw), U.S. Agency for Toxic Substances and Disease Registry (ATSDR) develops and publishes Minimum Risk Levels (MRLs) for many toxic substances. The MRL is defined as an estimate of daily human exposure to a substance that is likely to be without an appreciable risk of adverse effects (other than cancer) over a specified duration of exposure. MRLs can be derived for chronic exposures by the inhalation and oral routes. ATSDR describes MRLs as substance-specific estimates to be used by health assessors to select environmental contaminants for further evaluation. MRLs are presented with only 1 significant figure and are considered to be levels below which contaminants are unlikely to pose a health threat. Exposures above an MRL do not necessarily represent a threat, and MRLs are therefore not intended for use as predictors of adverse health effects or for setting cleanup levels. ATSDR publishes MRLs as part of pollutant-specific toxicological profile documents, and also in a regularly updated on-line table.

Health Effects Assessment Summary Tables (HEAST) (U.S. EPA. 1997a) consist of dose-response assessments for some substances that were prepared by the EPA Office of Research and Development (ORD), but not submitted for internal U.S. EPA consensus. For some substances, older health effects assessment documents omitted from HEAST also exist and are generally cited in Table A-1 as ORD-National Center for Environmental Assessment (EPA-NCEA) values. In 1989 and for several years thereafter, HEAST was updated on a quarterly basis. HEAST is no longer updated with new values, but existing values are deleted as revised values become available on IRIS.

A2-3.2 Explanation of Calculated Toxicity Benchmark Values

In the assessment of risk from contaminants, EPA-derived or reviewed toxicity benchmarks values are recommended. However, for numerous compounds, a complete set of inhalation and oral EPA-derived toxicity benchmarks are not available. In such cases, toxicity benchmark values were calculated based on available EPA-derived benchmarks values. For instance, if the oral *RfD* (mg/kg/day) was available and the inhalation *RfC* (mg/m^3) was not; the *RfC* was calculated by dividing the *RfD* by an average human inhalation rate of 20 m^3/day and multiplying by the average human body weight of 70 kg. This conversion is based on a route-to-route extrapolation, which assumes that the toxicity of the given chemical is equivalent over all routes of exposure.

Although conversion based on a route-to-route extrapolation of oral dose-response or inhalation information is not optimal risk assessment practice, the alternative would be to omit these substances altogether from any quantitative risk estimate, and thereby, providing a de facto false negative result of potential risk for the considered route or pathway. Therefore, using route-to-route extrapolation of oral dose-response or inhalation information when applying the HHRAP is preferable when no toxicological benchmark value is available in the peer reviewed data sources listed. However, assumptions and uncertainties involved when using toxicity benchmarks calculated based on route-to-route extrapolation should limit their use to screening-level or priority type risk assessments.

The following methodology was used to calculate missing toxicity benchmark values using available benchmarks that are based on route-to-route extrapolation:

1) *Oral RfD*s presented in the peer reviewed sources cited above were used if available. Missing *Oral RfD*s were calculated from the *RfC* assuming route-to-route extrapolation using the following equation:

$$Oral\ RfD = \frac{RfC \cdot 20\ m^3/d}{70\ kg\ BW}$$ Equation A-2-38

*RfC*s presented in the peer reviewed sources cited above were used when available. If *RfC*s were not available they were calculated from the *RfD* assuming route-to-route extrapolation and using the inverse of the equation above.

2) For *Inhalation URF*s, values were obtained from the peer reviewed sources cited above. If the *Inhalation URF*s were not available they were calculated from *Oral CSF*, using the following equation:

$$Inhal.\ URF = \frac{Oral\ CSF \cdot 20\ m^3/d}{70\ kg \times 1000\ \mu g/mg}$$ Equation A-2-39

*Oral CSF*s presented in the peer reviewed sources cited above were used when available. Missing *Oral CSFs* were calculated from *Inhalation URF* values assuming route-to-route extrapolation and using the inverse of the equation above.

A2-3.3 Uncertainties Involved when using Toxicity Benchmarks Calculated based on Route-to-Route Extrapolation

The conversion based on a route-to-route extrapolation, which assumes that the toxicity of the given chemical is equivalent over all routes of exposure, does introduce uncertainty into the assessment. By using this method, it is assumed that the qualitative data supporting the benchmark value for a certain route also applies to the route in question. For example, if an *RfD* is available and the *RfC* is calculated from that value, the assumption is made that the toxicity seen following oral exposure will be equivalent to toxicity following inhalation exposure. This assumption could overestimate or underestimate the toxicity of the given chemical following inhalation exposure.

Additional information regarding what to consider in the evaluation of route-to-route extrapolations can be found in the U.S. EPA (1994c) document *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry*.

A2-3.4 Prioritization of Data Sources for Acute Toxicity Benchmarks

Acute inhalation exposure guidelines and criteria are (1) designed to protect a variety of exposure groups including occupational workers, military personnel, and the general public, (2) based on varying exposure durations up to 24 hours in length, and (3) intended to protect against a variety of toxicity endpoints ranging from discomfort or mild adverse health effects to serious, debilitating, and potentially life-threatening effects, up to and including death.

Because of the daily operations of most emission sources and the potential for upset conditions to sometimes occur during operations, acute values developed to include intermittent exposures were considered more appropriate and more protective than values which are based on the strict assumption that acute exposures will be one-time only. Therefore, we recommend the Acute Reference Exposure Levels (Acute REL) developed by Cal/EPA, as the first choice for acute inhalation values (Cal/EPA 1999). Additional acute reference values which also do not exclude intermittent exposures are anticipated to be available from the EPA Office of Research and Development. When available, we recommend using those values (referred to as Acute Reference Concentrations [A-RfCs]) as the first choice, with the Cal/EPA acute RELs second in the hierarchy. Please note that the values we recommend using from all of the sources are based on one-hour exposures.

1. **Cal/EPA Acute RELs** – an acute REL represents the concentration in air at or below which no adverse health effects are anticipated in the general population, including sensitive individuals, for a specified exposure period (Cal/EPA 1999)
2. **Acute inhalation exposure guidelines (AEGL-1)** – an AEGL-1 value represents “the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.” (NAC 2002)

3. **Level 1 emergency planning guidelines (ERPG-1)** – an ERPG-1 value represents “the maximum concentration in air below which it is believed nearly all individuals could be exposed for up to one hour without experiencing other than mild transient adverse health effects or perceiving a clearly defined objectionable odor.” (AIHA 2004; SCAPA 2004)

4. **Temporary emergency exposure limits (TEEL-1)** – a TEEL-1 value represents “the maximum concentration in air below which it is believed nearly all individuals could be exposed without experiencing other than mild transient adverse health effects or perceiving a clearly defined odor.” (SCAPA 2004)

It should be noted that the TEEL-1 values (SCAPA 2004) are calculated based on an assumed exposure period of 15-minutes. To evaluate risks due to acute exposure based on the highest 1-hour average air concentrations, the TEEL-1 values were extrapolated from a 15-minute to a 1-hour exposure basis using a modification to Haber’s Rule developed by ten Berge (1986) and used by Cal/EPA to develop acute RELs (Cal/EPA 1999), as shown below.

$$C^n \times T = K$$ Equation A-2-40

where

C = Concentration (mg/m^3)
n = Constant greater than zero (unitless)
T = Time of exposure (hour)
K = Constant level or severity of response (unitless)

Where available, chemical-specific values for the parameter *n* as selected and recommended by Cal/EPA's Office of Environmental Health Hazard Assessment (OEHHA) based on the work of ten Berge (1986) and the open literature were used to make the extrapolations (Cal/EPA 1999). For chemicals for which a chemical-specific value of n was not available, extrapolations were made using a value of n = 1, as recommended by OEHHA, because the extrapolations were all based on an initial exposure period (15-minutes) of less than 1 hour duration (Cal/EPA 1999).

Use of the modified form of Haber's Rule allows contributions by both concentration and time to the overall severity of effect to be considered. However, the extrapolated air concentrations are to be interpreted carefully, and should not be interpreted to be absolutes. For example, chemical-specific values of the exponent n are sometimes based on a relatively limited set of dose-response data. Also, the majority of extrapolated TEEL-1 values were calculated using default exponent values and, therefore, are likely to be even less certain than exponent values based on limited data sets.

The hierarchy is presented in order of preference, from 1 (most preferred) to 4 (least preferred). If no acute REL value is available for a given contaminant, one can work down the list in order. If no AEGL-1 value is available, but an AEGL-2 value is available, the AEGL-2 can be selected as the AIEC only if it is a more protective value (lower in concentration) than an ERPG-1 or a TEEL-1 value if either of these values is available.

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CHEMICALS OF POTENTIAL CONCERN INCLUDED IN THE COMPANION DATABASE

CAS#	Compound
83-32-9	Acenaphthene
75-07-0	Acetaldehyde
67-64-1	Acetone
75-05-8	Acetonitrile
98-86-2	Acetophenone
107-02-8	Acrolein
107-13-1	Acrylonitrile
309-00-2	Aldrin
62-53-3	Aniline
120-12-7	Anthracene
7440-36-0	Antimony compounds
12674-11-2	Aroclor 1016
11097-69-1	Aroclor 1254
7440-38-2	Arsenic Compounds
1912-24-9	Atrazine
7440-39-3	Barium
100-52-7	Benzaldehyde
71-43-2	Benzene
56-55-3	Benzo(a)anthracene
50-32-8	Benzo(a)pyrene
205-99-2	Benzo(b)fluoranthene
207-08-9	Benzo(k)fluoranthene
65-85-0	Benzoic acid
100-47-0	Benzonitrile
100-51-6	Benzyl alcohol
100-44-7	Benzyl chloride
7440-41-7	Beryllium compounds
319-84-6	BHC, alpha- (alpha-Hexachlorocyclohexane)
319-85-7	BHC, beta- (beta-Hexachlorocyclohexane)
111-44-4	Bis(2-chlorethyl)ether
75-27-4	Bromodichloromethane
75-25-2	Bromoform (Tribromomethane)
101-55-3	Bromophenyl-phenylether, 4-
7440-43-9	Cadmium compounds
75-15-0	Carbon disulfide
56-23-5	Carbon tetrachloride
57-74-9	Chlordane
7782-50-5	Chlorine
59-50-7	Chloro-3-methylphenol, 4-
106-47-8	Chloroaniline, p-
108-90-7	Chlorobenzene
510-15-6	Chlorobenzilate
75-45-6	Chlorodifluoromethane
75-00-3	Chloroethane
67-66-3	Chloroform (Trichloromethane)
39638-32-9	Chloroisopropyl ether, bis-1,2-
91-58-7	Chloronaphthalene,2-
95-57-8	Chlorophenol, 2-
7005-72-3	Chlorophenyl-phenylether, 4-
2921-88-2	Chlorpyrifos
7440-47-3	Chromium compounds
18540-29-9	Chromium, hexavalent
218-01-9	Chrysene
108-39-4	Cresol, m- (3-Methylphenol)
95-48-7	Cresol, o-
106-44-5	Cresol, p-
98-82-8	Cumene (Isopropylbenzene)
57-12-5	Cyanide Compounds
72-54-8	DDD, 4,4'-
72-55-9	DDE, 4,4'-
50-29-3	DDT, 4-4'-
333-41-5	Diazinon
53-70-3	Dibenz(a,h)anthracene
96-12-8	Dibromo-3-chloropropane, 1,2-
124-48-1	Dibromochloromethane
95-50-1	Dichlorobenzene, 1,2-
541-73-1	Dichlorobenzene, 1,3-
106-46-7	Dichlorobenzene,1,4-
91-94-1	Dichlorobenzidine, 3,3'-
75-71-8	Dichlorodifluoromethane
75-34-3	Dichloroethane 1,1-
107-06-2	Dichloroethane, 1,2- (Ethylene Dichloride)
75-35-4	Dichloroethylene 1,1-
156-59-2	Dichloroethylene, cis-1,2-
156-60-5	Dichloroethylene-1,2 (trans)
120-83-2	Dichlorophenol, 2,4-
78-87-5	Dichloropropane, 1,2-
542-75-6	Dichloropropene, 1,3-
62-73-7	Dichlorvos
60-57-1	Dieldrin
84-66-2	Diethyl phthalate
131-11-3	Dimethyl phthalate
105-67-9	Dimethylphenol, 2,4-
119-90-4	Dimethyoxybenzidine, 3,3'-

CHEMICALS OF POTENTIAL CONCERN INCLUDED IN THE COMPANION DATABASE

CAS#	Compound
84-74-2	Di-n-butyl phthalate
99-65-0	Dinitrobenzene, 1,3-
51-28-5	Dinitrophenol, 2,4-
121-14-2	Dinitrotoluene, 2,4-
606-20-2	Dinitrotoluene, 2,6-
117-84-0	Di-n-octylphthalate
123-91-1	Dioxane, 1,4-
646-06-0	DIOXOLANE,1,3-
122-66-7	Diphenylhydrazine,1,2-
298-04-4	Disulfoton
115-29-7	Endosulfan I
72-20-8	Endrin
106-89-8	Epichlorohydrin (1-Chloro-2,3- epoxypropane)
97-63-2	Ethyl methacrylate
62-50-0	Ethyl methanesulfonate
100-41-4	Ethylbenzene
106-93-4	Ethylene Dibromide
75-21-8	Ethylene oxide
117-81-7	Ethylhexyl phthalate, bis-2-
206-44-0	Fluoranthene
86-73-7	Fluorene
50-00-0	Formaldehyde
64-18-6	Formic acid
35822-46-9	HeptaCDD, 1,2,3,4,6,7,8-
67562-39-4	HeptaCDF, 1,2,3,4,6,7,8-
55673-89-7	HeptaCDF, 1,2,3,4,7,8,9-
76-44-8	Heptachlor
1024-57-3	Heptachlor epoxide
39227-28-6	HexaCDD, 1,2,3,4,7,8-
57653-85-7	HexaCDD, 1,2,3,6,7,8-
19408-74-3	HexaCDD, 1,2,3,7,8,9-
70648-26-9	HexaCDF, 1,2,3,4,7,8-
57117-44-9	HexaCDF, 1,2,3,6,7,8-
72918-21-9	HexaCDF, 1,2,3,7,8,9-
60851-34-5	HexaCDF, 2,3,4,6,7,8-
87-68-3	Hexachloro-1,3-butadiene (Perchlorobutadiene)
118-74-1	Hexachlorobenzene
77-47-4	Hexachlorocyclopentadiene
67-72-1	Hexachloroethane (Perchloroethane)
70-30-4	Hexachlorophene
7647-01-0	Hydrogen chloride (Hydrochloric acid)
193-39-5	Indeno(1,2,3-cd) pyrene
78-59-1	Isophorone
7439-92-1	Lead compounds
121-75-5	Malathion
7487-94-7	Mercuric chloride
7439-97-6	Mercury (elemental)
126-98-7	Methacrylonitrile
67-56-1	Methanol
72-43-5	Methoxychlor
79-20-9	Methyl acetate
74-83-9	Methyl bromide (Bromomethane)
74-87-3	Methyl chloride (Chloromethane)
78-93-3	Methyl ethyl ketone (2-Butanone)
108-10-1	Methyl isobutyl ketone
22967-92-6	Methyl mercury
298-00-0	Methyl parathion
74-95-3	Methylene bromide
75-09-2	Methylene chloride
91-20-3	Naphthalene
7440-02-0	Nickel
88-74-4	Nitroaniline, 2-
99-09-2	Nitroaniline, 3-
100-01-6	Nitroaniline, 4-
98-95-3	Nitrobenzene
88-75-5	Nitrophenol, 2-
100-02-7	Nitrophenol, 4-
924-16-3	Nitroso-di-n-butylamine, n-
86-30-6	Nitrosodiphenylamine, n-
621-64-7	Nitrosodipropylamine, n-
3268-87-9	OctaCDD, 1,2,3,4,6,7,8,9-
39001-02-0	OctaCDF, 1,2,3,4,6,7,8,9-
40321-76-4	PentaCDD, 1,2,3,7,8-

CHEMICALS OF POTENTIAL CONCERN INCLUDED IN THE COMPANION DATABASE

CAS#	Compound
57117-41-6	PentaCDF, 1,2,3,7,8-
57117-31-4	PentaCDF, 2,3,4,7,8-
608-93-5	Pentachlorobenzene
82-68-8	Pentachloronitrobenzene (PCNB)
87-86-5	Pentachlorophenol
85-01-8	Phenanthrene
108-95-2	Phenol
298-02-2	Phorate
85-44-9	Phthalic anhydride (1,2-Benzene dicarboxylic anhydride)
23950-58-5	Pronamide
129-00-0	Pyrene
110-86-1	Pyridine
299-84-3	Ronnel
94-59-7	Safrole
7782-49-2	Selenium
7440-22-4	Silver
57-24-9	Strychnine
100-42-5	Styrene
1746-01-6	TetraCDD, 2,3,7,8-
51207-31-9	TetraCDF, 2,3,7,8-
95-94-3	Tetrachlorobenzene, 1,2,4,5-
630-20-6	Tetrachloroethane, 1,1,1,2-
79-34-5	Tetrachloroethane, 1,1,2,2-
127-18-4	Tetrachloroethylene (Perchloroethylene)
58-90-2	Tetrachlorophenol, 2,3,4,6-
109-99-9	Tetrahydrofuran
7440-28-0	Thallium (l)
108-88-3	Toluene
95-53-4	Toluidine, o-
87-61-6	Trichlorobenzene, 1,2,3-
120-82-1	Trichlorobenzene, 1,2,4-
71-55-6	Trichloroethane, 1,1,1-
79-00-5	Trichloroethane, 1,1,2-
79-01-6	Trichloroethylene
75-69-4	Trichlorofluoromethane (Freon 11)
95-95-4	Trichlorophenol, 2,4,5-
88-06-2	Trichlorophenol, 2,4,6-
96-18-4	Trichloropropane, 1,2,3-
108-67-8	Trimethylbenzene, 1,3,5-
99-35-4	Trinitrobenzene, 1,3,5 (sym-)
118-96-7	Trinitrotoluene, 2,4,6-
108-05-4	Vinyl acetate
75-01-4	Vinyl chloride
108-38-3	Xylene, m-
95-47-6	Xylene, o-
106-42-3	Xylene, p-
7440-66-6	Zinc