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User's Manual for the Database of Sources of Environmental Releases of Dioxin-Like Compounds in the United States: Reference Years 1987 and 1995

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1. INTRODUCTION

The National Database of Sources of Environmental Releases of Dioxin-like Compounds in the United States has been developed by EPA's Office of Research and Development (ORD) to be a repository of congener-specific chlorinated dibenzo-p-dioxin/dibenzofuran (CDD/CDF) emission data extracted from original test reports. The database was designed to accommodate facility-based emission data, as well as non-facility based sources (e.g., mobile sources such as automobiles, and area sources such as residential wood combustion). Test reports from various State agencies, trade associations, EPA program offices, and EPA regulatory dockets were consolidated and assimilated into the database. Most of the emission data in Version 3.0 of the database concern releases to air because few data are currently available on releases to other media.

The database contains information that can be analyzed to track emissions of CDD/CDF over time, compare homologue and congener profiles between and among source categories, and develop source-specific emission factors that can then be used to develop emission estimates. In a separate report (Volume 1, *Sources of Dioxin-Like Compounds in the United States*) (U.S. EPA, 2001), ORD has used the database to develop a national inventory of annual releases from a variety of sources for two reference years: 1987 and 1995. EPA selected 1987 primarily because, prior to this time, little empirical data existed for making source specific emission estimates. The year 1987 also corresponds roughly with the time when significant advances occurred in emissions measurement techniques and in the development of high resolution mass spectrometry and gas chromatography necessary for analytical laboratories to achieve low level detection of CDD and CDF congeners in environmental samples. Soon after this time, a number of facilities began upgrades specifically intended to reduce CDD/CDF emissions. Consequently, 1987 is also the latest time representative of the emissions occurring before widespread installation of dioxin-specific emission controls.

EPA selected 1995 as the latest time period that could practically be addressed consistent with the time table for producing the rest of the document. The data collected in the companion document to this document on CDD/CDF and dioxin-like PCB levels in environmental media and food were used to characterize conditions in the mid-1990s. So the emissions data and media/food data in these two volumes are presented on a roughly consistent basis. Since 1995, EPA has promulgated regulations limiting CDD/CDF emissions for a number of the source categories that contribute to the inventory including municipal waste combustors, medical waste incinerators, hazardous waste incinerators, cement kilns burning hazardous waste, and pulp and paper facilities using chlorine bleached processes. Consequently, the estimate of releases in

the 1995 inventory should not be assumed to accurately represent post-1995 releases. EPA intends to periodically revise this inventory.

The remainder of this document is divided into four sections. Instructions for using the database are discussed in Section 2. The structure of the database and the flow of information into and out of the database are described in Section 3. Assumptions made to standardize the data are described in Section 4 and sample calculations are provided in Section 5. Section 5 also describes the process used in U.S. EPA (2001) to develop nationwide annual CDD/CDF TEQ emission estimates based, to a large extent, on emission factors calculated using this database.

The *National Database* was created using Microsoft Excel 97[©] (hereafter, Excel 97[©]) in the manner of linked "workbooks." Certain calculations and manipulations of data performed in Excel[©] may be lost if the database is converted for use with other software; therefore, any recalculations for the data in the *National Database* should be performed using Excel[©]. The Excel[©] workbooks should be compatible with the MacPower version of Excel.

Because the database is stored on a CD-ROM, a CD player is required for use. Although there do not appear to be any memory constraints in using the CD-ROM, a computer with a 486 or Pentium processor and an adequate amount of RAM should be used.

2. USING THE DATABASE

Version 1.2 of the *National Database* was created in Excel 97[©]. This version of the database contains an interface that allows the user to link summary and individual facility files from an introductory screen (i.e. the main table) via the "hyperlink" function provided by Excel 97[©]. The user must first select which TEQ version of the Database to use (i.e., "I-TEFs" or "WHO98TEFs").

Version 3.0 of the *National Database* features a user-friendly interface (Figure 1), which has been designed to help users quickly locate information in the Database. Search capabilities have also been included in the Database to allow the user to locate facility emissions based on an EPA Identification Number, the State, the Facility's Name, or the Facility's Combustion Category.

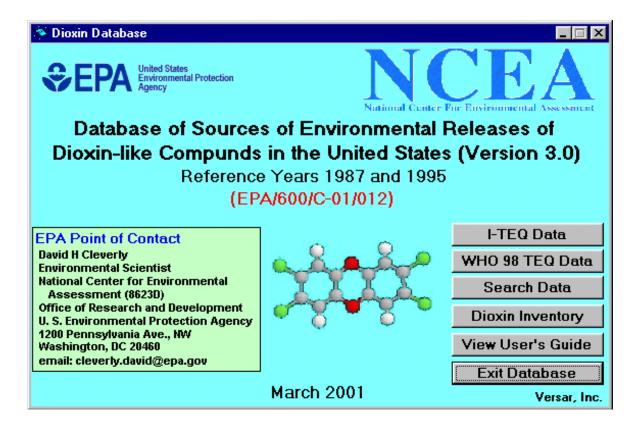


Figure 1. National Database Introductory Screen

2.1 GETTING STARTED

The *National Database* should automatically start upon placing the CD into the CD-ROM drive. However, if the introductory screen does not appear after a few seconds, use the following steps to start the database:

- Open Windows Explorer.
- Select the drive which represents the CD-ROM and open the introductory screen by clicking **DioxinDb**, the file name of the dioxin database executable file.

Note: The DioxinDb program will only work for Windows-based computers. Computers with other operating systems should proceed to Section 3.1 for a discussion of the CD's directory structure.

The introductory screen for the *National Database* allows the user to select from the I-TEQ data, the WHO 98 TEQ data, or to search for data in the database. The introductory screen also allows the user to view the User's Guide and the Dioxin Inventory of I-TEQ_{DF} and TEQ_{DF}-WHO₉₈ releases for 1995 and 1987, both PDF files. Selecting the **I-TEQ Data** button or the WHO 98 TEQ Data button will open the appropriate Source Category Interface. The Source

Category Interfaces are Excel 97[©] files which allow the user to view data based on the combustion source category. For more information on these interfaces, please refer to Section 2.2.

To search the *National Database* for data from a particular facility, the user should select the **Search Data** button. Upon pressing this button the Search Dioxin Database screen should appear (Figure 2). The user can search for data based on an EPA Identification number, a State of interest, a Facility's Name, or by Combustion Category.

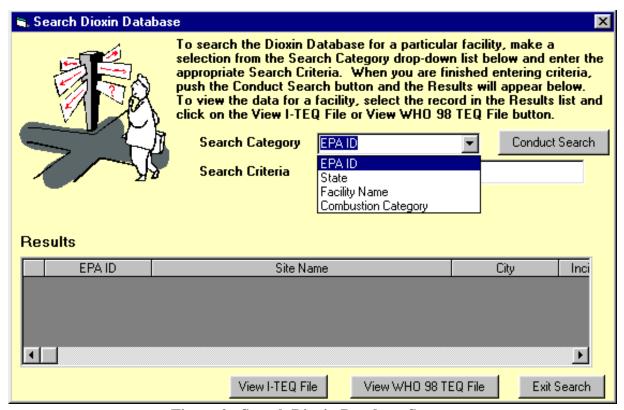


Figure 2. Search Dioxin Database Screen

To search the database, the user should first select the desired **Search Category** from the drop-down list. If the user decides to search for data based EPA ID and Facility Name, a text box will appear that will allow the user to enter the EPA ID or facility name. If the user chooses to search for data based on a State of interest or a Combustion Category, a drop-down list will appear providing the user with applicable choices (Figure 3). Next, the user should enter or select the appropriate **Search Criteria** in the text box or drop-down list which appears and push the **Conduct Search** button. The results of the search will appear in the **Results** table (Figure 4). If none of the records in the *National Database* meet the criteria entered, the **Results** table will appear blank.

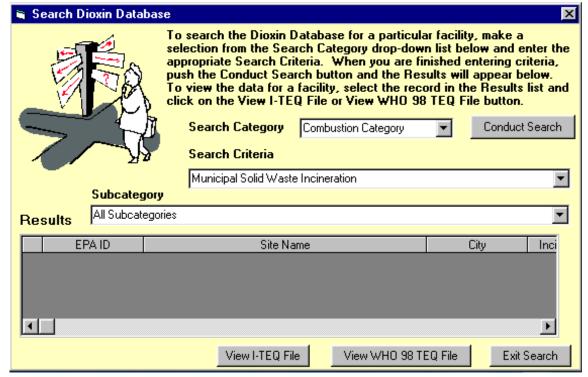


Figure 3. Search Dioxin Database based on Combustion Category

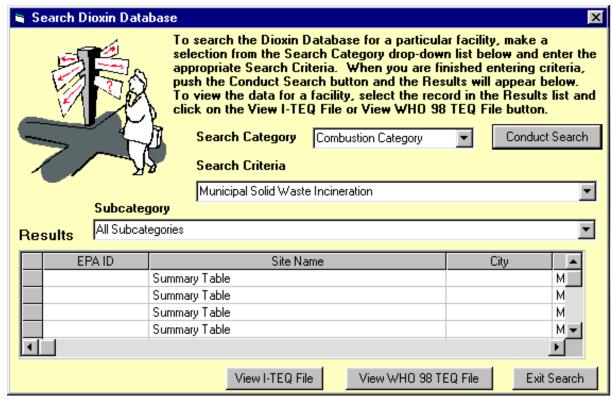


Figure 4. Search Dioxin Database Results

After the results of a search have been displayed, the user can go to the Excel 97[©] data file by highlighting the row with the result of interest and pushing the **View I-TEQ File** or the **View WHO 98 TEQ File** button. To exit the Search Dioxin Database screen, the user should simply press the **Exit Search** button at the bottom of the screen.

2.2 SOURCE CATEGORY INTERFACE

The *National Database* contains Excel 97[©] files that permit the user to view data based on the combustion source. These files can be accessed by selecting the **I-TEQ Data** button or the **WHO 98 TEQ Data** button on the introductory screen for the *National Database* program, or can access them from Excel 97[©]. An example of the Source Category Interface is depicted in Figure 5.

To access the Source Category Interfaces from Excel 97[©]

- Place the CD into the CD-ROM drive and open the Excel 97[©].
- Click the menu **File** and the selection **Open**.
- Select the drive which represents the CD-ROM and open the interface by clicking **Filetree**, the file name of the main table.
- Select the source category of interest in the interface by clicking with a mouse or moving the cell pointer to the source category followed by hitting the key **Enter**.
- Click the facility name listed in the summary table to access facility data.
- Click the button located at the up-right corner of the first worksheet in the facility file to return to the summary table, or click the bar located under the facility inventory in the summary table of summary files to return to the introductory screen.

The emission source categories listed in the Source Category Interface have been linked to source category summary files. By clicking a source category, the user will open the summary table worksheet in the summary file for that category. A more detailed description and discussion of each source category is provided in U.S. EPA(2000). An example of a summary table is shown in Table 1. This summary table lists the average emission factors and average TEQ emission factors of congener-specific and total CDD/CDF data. The facility names in the summary files have been further linked to facility data files in the Database. The user can further access individual facility data by clicking the corresponding facility names. The other

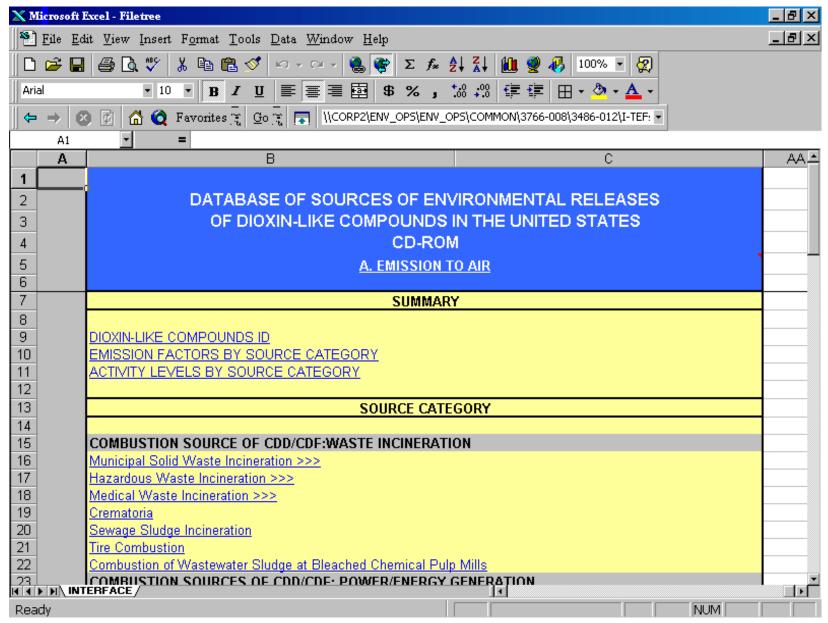
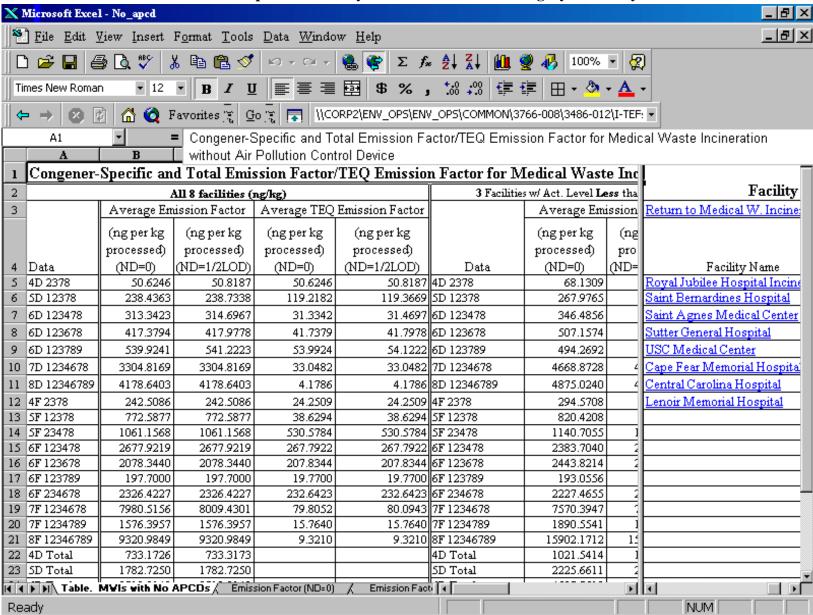


Figure 5. Source Category Interface

Table 1. A Sample of Summary Table in the Source Category Summary File



worksheets included in summary files can also be accessed by clicking worksheet tabs located at the bottom of the screen.

The Source Category Interfaces were created in Excel 97[©] and, as such, will only operate using Excel 97[©], or a later version. Any attempt to use these interfaces with earlier versions of Excel[©] will result in disabling the interfaces.

2.3 FACILITY DATA FILES

Upon opening a facility data worksheet, Excel 97[©] will inform the user that the worksheet contains links and will ask the user if they wish to re-establish the links. The user should only reestablish the links in a worksheet if they intend to update the worksheet with new available test data or changed TEF values in the chemical data worksheet (**Chemid**) and then recalculate EFs and TEQs. The user should keep in mind that re-establishing links may take a few minutes, depending on the speed of their computer.

The links in the worksheets retrieve congener-specific data contained in a chemical data worksheet. This chemical worksheet contains information on the chemical's name, abbreviations, and toxic equivalency factors so that the chemical data only needs to be entered once.

Excel[©] creates the link between this chemical worksheet and facility data files through the *Vlookup* function. The *Vlookup* function searches the chemical data in the chemical worksheet, matches the corresponding row, and inserts a particular congener's Toxic Equivalency Factor, a 2378 Toxicity flag, the Congener flag, and the Homologue flag to the facility data file.

A workbook for each facility contains three worksheets (see Section 3.3 for more details). The user can move around in a worksheet by using the arrow keys on the keyboard or by using the mouse and the vertical and horizontal slide bar located at the right and bottom of the screen, respectively. The user can move from worksheet to worksheet by moving the mouse to the appropriate tab in the lower portion of the screen and pressing the mouse button.

The EF and TEQ worksheets were created through the use of Excel®'s Pivot Table function. A pivot table is an interactive worksheet table that enables the user to summarize and analyze data from existing tables¹. Pivot tables were created from the facility data worksheets to determine the average, maximum, and minimum EF and TEQ values and count of test runs for each congener identified. For more information on Excel®'s Pivot Table command, please consult Excel®'s Help screens.

¹ Chester, Thomas. Mastering Excel 5 for Windows. Sybex, Inc. Alameda, CA. 1995

2.4 USER NOTES

Users can conduct data analysis directly on the files contained on the CD-ROM. However, any analysis or changes to the data cannot be saved back to the CD-ROM, but must be saved to a separate disk or drive.

The summary files on the CD-ROM were created by using the Data Consolidate command provided by Excel 97[©]. Data from the EF and TEQ worksheets were pulled from each of the data files and consolidated into the summary files. For more information on Excel 97[©]'s Data Consolidate command, please consult Excel 97[©]'s Help screens.

3. DATABASE STRUCTURE

3.1 OVERALL STRUCTURE

The overall structure of the database is a series of linked spreadsheets contained within Excel® "workbooks". This structure was selected over several others because of its versatility for entering data from the original test reports, standardizing the data, and calculating emission factors. An overarching criterion for the design of this database was that the data storage and calculations using the data be transparent to users of the database. ORD believes that this transparency is better achieved through the use of spreadsheets which allows the user to follow the calculations, than through the use of a custom database application.

Version 3.0 of the *National Database* consists of two databases which differ only in the toxicity equivalency factor (TEF) scheme used. One database uses the International TEF approach (U.S. EPA, 1989d); the other uses the 1998 World Health Organization approach (Van den Berg et al., 1998) (see Table 2).

Each of the two databases consists of approximately 270 spreadsheet files, distributed among over 30 directories and subdirectories. Figure 6 illustrates the directory structure. Each directory/subdirectory was given a unique name to indicate the type of emission source that was being analyzed. For instance, the directory name "CK-NHW" was used for Cement Kilns Burning Non-Hazardous Waste. Table 3 lists the directories/subdirectories which make up the *National Database* and the category/subcategory to which directory refers.

Table 2. TEF Schemes for CDD/CDFs

International TEF Scheme

CDD Congeners	TEF	CDF Congeners	TEF
2,3,7,8-TCDD 1,2,3,7,8-PeCDD 1,2,3,4,7,8-HxCDD 1,2,3,6,7,8-HxCDD 1,2,3,7,8,9-HxCDD 1,2,3,4,6,7,8-HpCDD OCDD	1.0 1.0 0.1 0.1 0.1 0.01 0.001	2,3,7,8-TCDF 1,2,3,7,8-PeCDF 2,3,4,7,8-PeCDF 1,2,3,4,7,8-HxCDF 1,2,3,6,7,8-HxCDF 1,2,3,7,8,9-HxCDF 2,3,4,6,7,8-HxCDF 1,2,3,4,6,7,8-HpCDF 1,2,3,4,7,8,9-HpCDF OCDF	0.1 0.05 0.5 0.1 0.1 0.1 0.01 0.01 0.001

1998 World Health Organization Scheme

CDD Congener	TEF	CDF Congener	TEF
2,3,7,8-TCDD 1,2,3,7,8-PeCDD 1,2,3,4,7,8-HxCDD 1,2,3,6,7,8-HxCDD 1,2,3,7,8,9-HxCDD 1,2,3,4,6,7,8-HpCDD OCDD	1.0 0.5 0.1 0.1 0.1 0.01 0.001	2,3,7,8-TCDF 1,2,3,7,8-PeCDF 2,3,4,7,8-PeCDF 1,2,3,4,7,8-HxCDF 1,2,3,6,7,8-HxCDF 1,2,3,7,8,9-HxCDF 2,3,4,6,7,8-HxCDF	0.1 0.05 0.5 0.1 0.1 0.1 0.1
		1,2,3,4,6,7,8-HpCDF 1,2,3,4,7,8,9-HpCDF OCDF	0.01 0.01

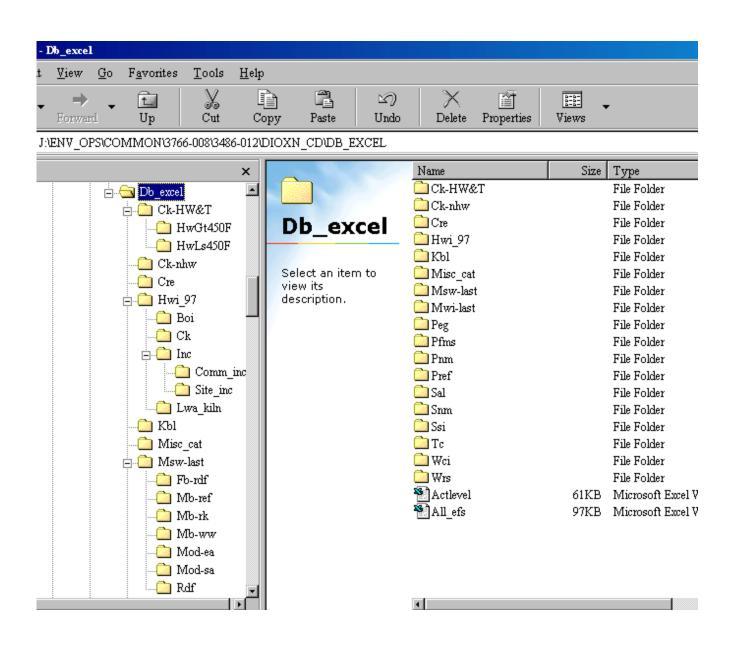


Figure 6. Database Directory Structure

Table 3. Database Directory Breakdown

Directory	Subdirectory	Subdirectory	Category
Ck-HW&T	HwGt450F		Cement Kilns Burning Hazardous Waste with inlet temp of APCD> 450F
	HwLs450F		Cement Kilns Burning Hazardous Waste with inlet temp of APCD< 450F
Ck-nhw			Cement Kilns Burning Nonhazardous Waste
Cre			Crematoria
Hwi-97			Hazardous Waste Incinerators
	Boi		Boilers - Haz Waste
	Ck		Cement Kilns - Haz Waste
	Inc		Incinerators - Haz Waste
		Comm_inc	Commercial Incinerators
		Site_inc	On-site Incinerators
	Lwa_kiln		Lightweight Aggregate Kilns
Kbl			Kraft Black Liquor Recovery Boilers
Misc-cat			Miscellaneous Sources
MSW-last			Municipal Solid Waste Incinerators
	Fb-rdf		Fluidized Bed - refuse-derived fuel
	Mb-ref		Mass burn - refractory-wall
	Mb-rk		Mass burn - rotary kiln
	Mb-ww		Mass burn - water-wall
	Mod-ea		Modular excess-air
	Mod-sa		Modular starved-air
	Rdf		Refuse derived fuel
Mwi-last			Medical Waste Incinerators
Peg			Power Energy Generation
Pfms			Primary Ferrous Metal Smelting
Pnm			Primary Non-ferrous Metal Smelting
Pref			Petroleum Refining Catalyst Regeneration
Sal			Secondary Aluminum Smelting
Snm			Secondary Non-ferrous Metal Smelting
Ssi			Sewage Sludge Incineration
Тс			Tire Combustion
Wci			Industrial Wood Incineration
Wrs			Combustion of Wastewater Sludge at Bleached Chemical Pulp Mills

Each directory/subdirectory contains two types of files: summary files (typically one) and data files. The summary file was constructed to provide a consolidated view of the facilities within a particular emission source category. The data files in each directory/subdirectory contain raw data and calculations for determining emission factors (EFs) for CDD/CDFs both in chemical-specific units and dioxin toxicity equivalent (TEQ) units.

3.2 SUMMARY FILE STRUCTURE

As discussed earlier, summary files located in each directory/subdirectory display consolidated data from each of the facilities within a particular emission source category. The nomenclature used for the summary files is typically:

***-sum.xls

where, *** indicates an abbreviation for the category or subdirectory in which the file is located. In the case of the municipal solid waste incinerator and medical waste incinerator categories, summary files were based on the type of air pollution control device, and are so named. For example, a summary file of facilities with a dry scrubber and fabric filter would be called: ds-ff.xls.

Figure 7 presents an example of the second sheet in a summary file for the source category "cement kilns not burning hazardous waste." There are typically five sheets in a summary file. They are: Emission Factor (nondetects (ND)=0); Emission Factor (ND=half limit of detection (LOD)); TEQ Emission Factor (ND=half LOD); and Table. The Emission Factor and TEQ Emission Factor sheets present the average emission factor and corresponding TEQ emission factor for each congener (from all of the facility test runs) from the emission factor and TEQ worksheets within each data file. These sheets were formed using the "Data Consolidate" command in Excel 97°. The Table worksheet presents the average emission factor and corresponding TEQ emission factor for each congener across all facilities in the summary file. The Table sheet was created by linking the values from the last row of data in the four sheets mentioned above. In addition, the Table worksheet includes the facility inventory from which the users can link to individual facility data files. This facility inventory was created for the database in the Excel 97° version only.

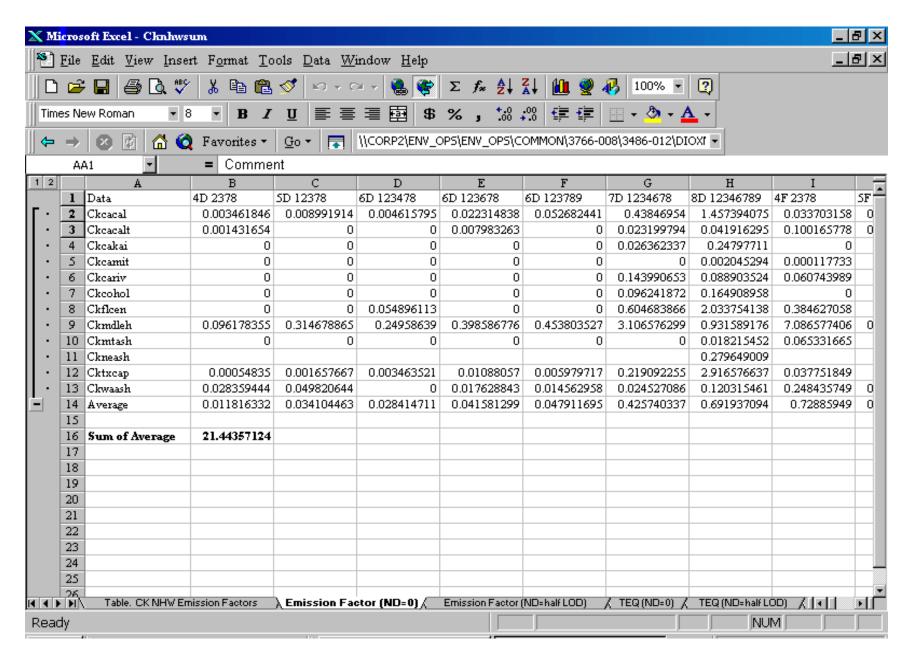


Figure 7. Example of a Summary File

The user should note that the number of significant figures displayed in this worksheet and other worksheets in the database do not necessarily reflect the level of certainty in the data. EPA recommends using no more than three significant figures for any emission factor estimates derived from these data.

In some cases, the summary files contain profile worksheets (for ND=0 and ND=half LOD). These sheets present the ratio of a specific congener's emission factor relative to the total CDD/CDF emission factor for a specific facility in the summary file.

3.3 DATA FILE STRUCTURE

Data files located in each directory/subdirectory are the repositories of the raw data compiled from various facility test reports and other sources. Data files also contain some calculations and manipulations of data to determine EFs. Data files were named using the following nomenclature:

- 1. The first 2-3 characters of the name represent the category or subcategory (e.g., CK for cement kiln);
- 2. The next 2 characters represent the state abbreviation where the facility is located; and
- 3. The remaining letters are comprised of the first 3-4 characters from the facility name.

For example, the file CKARASH.XLS was derived from

CK - cement kiln,

AR - Arkansas, and

ASH - Ash Grove Cement Company.

Data files normally contain three separate worksheets: the facility data worksheet; the EF worksheet; and, the TEQ EF worksheet.

3.3.1 Worksheet 1 - Facility Data

The first worksheet, the facility data worksheet, in each data file contains the raw data obtained from a facility's test report or similar source. The raw data were used to calculate congener and homologue group emission factors and the corresponding TEQ emission factors, generally in units of ng/kg of material combusted, for each congener in each test run. This spreadsheet is "linked" to other data containing standard chemical names, abbreviations, and toxic equivalency factors. In some cases, the emission factors could not be calculated because the

facility data were incomplete (e.g., missing activity level, or volumetric flow rate). Table 4 provides a listing of the data fields contained in the facility data worksheet. For the category of cement kiln burning hazardous waste, one additional column for the inlet temperature of the air pollutant control device was created for facilities with available data. Figure 8 presents an example of the facility data worksheet.

3.3.2 Worksheet 2 - Emission Factor (EF)

The second worksheet, the EF worksheet, is based on data from the facility data worksheet and presents the average, maximum, and minimum EF as well as the count of test runs for a particular congener at the given facility. Excel®'s Pivot Table function was used to create this worksheet. Table 5 provides a listing of the data fields calculated in this worksheet. Figure 9 presents an example of an EF worksheet. Many of the EF worksheets include a row that calculates congener profiles, which are the ratio of a specific congener's emission factor relative to the total emission factor (for all homologue groups) for that facility.

In several cases, insufficient data were available in the facility data worksheet to properly perform the EF analysis. In these cases, the EF worksheets were not developed. For those cases where the EF worksheets were developed, the pivot tables need to be "refreshed" (a command provided by Pivot Table) should the source data be revised.

3.3.3 Worksheet 3 - TEQ Emission Factors

The third worksheet, the TEQ emission factor worksheet, is based on data from the facility data worksheet and presents the average, maximum, and minimum TEQ emission factors as well as the count of test runs for a particular congener at the given facility. Excel[®]'s Pivot Table function was used to create this worksheet. Table 6 provides a listing of the data fields calculated in this worksheet. Figure 10 presents an example of a TEQ worksheet.

As was the case with the congener EF Worksheet, there were several cases where not enough data were available in the facility data worksheet to properly run the TEQ emission factor analysis. In these cases, the worksheets were not developed. For those cases where the TEQ worksheets were developed, as with the EF Worksheet, the pivot tables need to be "refreshed" should the source data be revised.

3.3.4 Miscellaneous Worksheets

Some of the data files contain several miscellaneous worksheets not yet discussed. These include profile worksheets which may be contained in the summary files or in the facility data files.

Table 4. Data Fields for Facility Data Worksheet

Field	Units	Comments/Explanation
EPA ID Number	unitless	
Facility	unitless	
City	unitless	
State	unitless	
Latitude	degrees, minutes, seconds	
Longitude	degrees, minutes, seconds	
Release Media	unitless	air, water, or land
Number of Incinerators	Combustion Units	applicable for releases to air
Total Annual Combustion Capacity	tons per day	applicable for releases to air
Activity Level	kilograms (kg) or liters (L) per unit time	
Source Category	unitless	
Source Subcategory	unitless	
Technology Design Category	unitless	
Technology Design Subcategory	unitless	
Air Pollution Control Device 1	unitless	applicable for releases to air
Air Pollution Control Device 2	unitless	applicable for releases to air
Pipe or Stack Number	unitless	applicable for releases to air
Stack Height	feet (ft)	applicable for releases to air
Stack Diameter	inches (in)	applicable for releases to air
Stack Flow (Volumetric Flow Rate)	dry standard cubic feet per minute (dscfm)	applicable for releases to air
Stack Flow (Volumetric Flow Rate)	dscfm standardized to 7% O ₂	applicable for releases to air

Table 4. Data Fields for Facility Data Worksheet (continued)

Field	Units	Comments/Explanation
Stack Exit Velocity	feet per second	applicable for releases to air
Stack Temperature (Exit Temperature)	degrees Fahrenheit (°F)	applicable for releases to air
Stack O ₂	percent (%)	applicable for releases to air
Stack CO ₂	percent (%)	applicable for releases to air
Stack Moisture	percent volume (%V)	applicable for releases to air
Chlorine Content of Waste Feed	percent (%)	
Pipe Flow	cubic feet per second	applicable for releases to water
Run ID	unitless	
Test Date	unitless	
Report Date	unitless	
COC (Chain of Custody) Date	unitless	
Substance	unitless	CDD/CDF congeners
Detect - Non-Detect Flag	unitless	
Emission Amount - Concentration as Reported	see next field	When "Concentration as Calculated" is shown, it indicates that a concentration has been calculated from raw data reported.
Concentration Units (as Reported)	units vary depending on data source	
Standardized Emission Amount	see next field	
Standardized Units	ng/dscm @ 7% O ₂	applicable for releases to air
Emission Rate, as Reported	units vary depending on data source	
Conversion Factor	units necessary to convert "Emission Rate, as Reported" to pounds per hour	

Table 4. Data Fields for Facility Data Worksheet (continued)

Field	Units	Comments/Explanation	
Emission Rate	pounds per hour (lbs/hr)		
Concentration (ND=0)	ng/dscm @ 7% O ₂	applicable for releases to air	
Concentration (ND=1/2 LOD)	ng/dscm @ 7% O ₂	applicable for releases to air	
Toxic Equivalency Factor (TEF)	unitless: developed from Lookup file		
TEQ Emission Factor (ND=0)	varies depending on activity level units		
TEQ Emission Factor (ND=1/2LOD)	varies depending on activity level units		
2378 Toxicity Flag	unitless: developed from Lookup file	"Y" indicating a toxicity equivalency factor (TEF) is available	
Congener Flag	unitless: developed from Lookup file		
Homologue Flag	unitless: developed from Lookup file		
Emission Factor (ND=0)	varies depending on activity level units		
Emission Factor (ND=1/2LOD)	ng/kg processed		
Receiving Stream	unitless	applicable for releases to water	
Reach Number	unitless	applicable for releases to water	
Data Source Reference	unitless		
Comments	unitless		

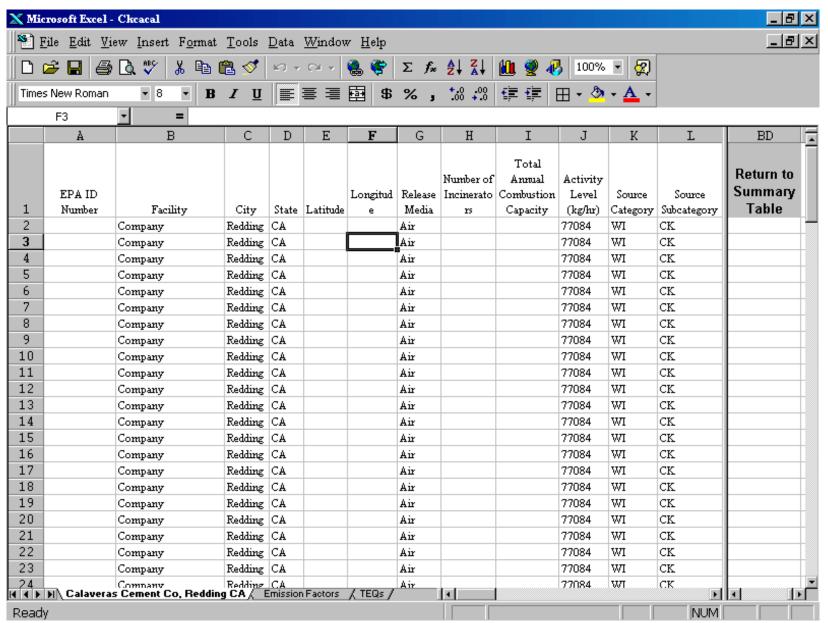


Figure 8. Example of the Facility Data Sheet in a Facility Data File

Table 5. Emission Factor (EF) Worksheet Contents

Data Analysis	Typical Units
at Non-Detect $(ND) = 0$	
Average Emission Factor (EF)	ng/kg processed
Maximum EF	ng/kg processed
Minimum EF	ng/kg processed
Count of EFs	
at $ND = 1/2 LOD$	
Average EF	ng/kg processed
Maximum EF	ng/kg processed
Minimum EF	ng/kg processed
Count of EFs	

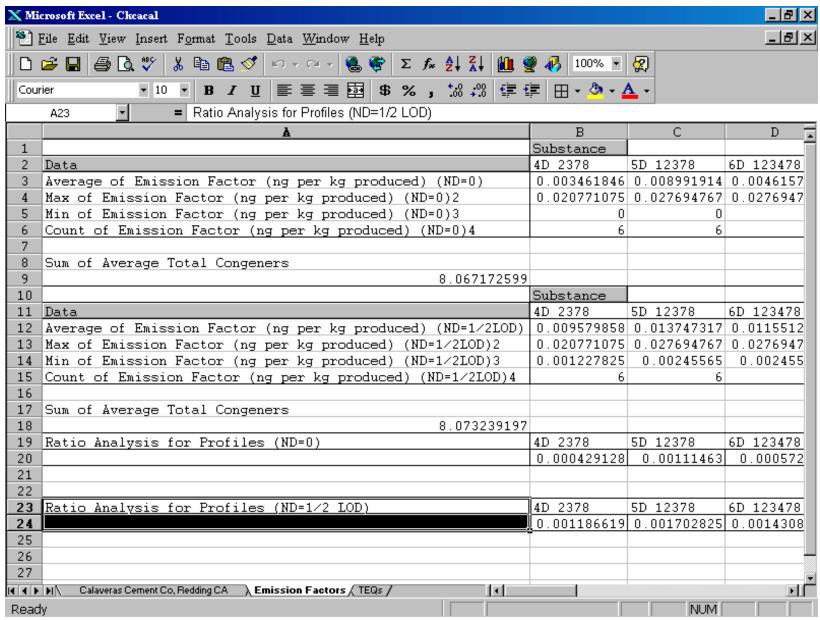


Figure 9. Example of an Emission Factor Sheet in a Facility Data File

Table 6. TEQ Emission Factor (EF) Worksheet Contents

Data Analysis	Typical Units
at Non-Detect (ND) = 0 Average TEQ Maximum TEQ Minimum TEQ Count of TEQs	ng/kg processed ng/kg processed ng/kg processed
at ND = 1/2 LOD Average TEQ Maximum TEQ Minimum TEQ Count of TEQs	ng/kg processed ng/kg processed ng/kg processed

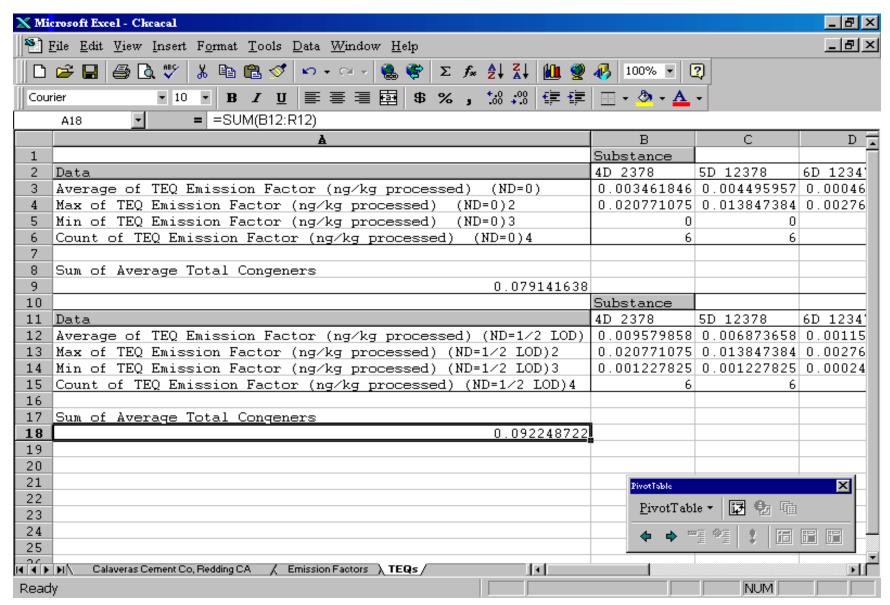


Figure 10. Example of a TEQ Sheet in a Facility Data File

4. CALCULATIONS AND QUALITY CONTROL MEASURES

4.1 STANDARDIZATION

Data underwent a process of standardization after they were extracted from the original test reports and before they were entered into the *National Database*. Three areas in particular were standardized -- chemical names, treatment of detects and non-detects, and concentration units of measure.

Chemical names were standardized by matching compounds to a "master" list of dioxinlike compounds. These standard values are linked to the "master" spreadsheets, allowing other parameters (e.g., TEFs, homologue groups) to be retrieved into the facility-specific spreadsheet.

Measured CDD/CDF concentrations are presented in the test reports in a number of ways (e.g., ng/sample, ng/dscm, ng/dscm @ 12% CO₂, etc.). For comparison purposes, stack gas concentrations were generally standardized to units of ng/dscm at 7 percent oxygen. As needed, the volumetric flow rates were standardized to dry standard cubic feet per minute (dscfm) at 7 percent oxygen using the following equation:

flow (dscfm) =
$$\frac{(20.9\% \ O_2 - test \ run \ O_2)}{(20.9\% \ O_2 - 7\% \ O_2)}$$

Figure 11 presents sample calculations that demonstrate the estimation of a proxy concentration for a nondetected congener and standardization of that concentration to ng/dscm @ $7\% O_2$.

Two sets of data were generated to address congeners that were reported as nondetected in the test reports. In the first set, nondetected congeners were assigned a value of zero; while in the second set of data, nondetected congeners were assigned a proxy concentration of half the detection limit for that congener.

<u>Congener</u>	Non-detect Flag	Concentration (ng/sample)	Sample Volume (dscm/sample)	Percent O ₂		
2378 TCDD	ND	0.05	4.5	10		
Proxy concentration for n	ondetected 2378 TC	DD:				
Concentration (ng/dscm):	:	imple $\div 2 = 0.025 \text{ ng}$ $\div 4.5 \text{ dscm/sample} =$	•			
The general equation for	standardization to 79	% O ₂ is:				
ng/dscr	n @ 7%O ₂ = Sample	Conc. (ng/dscm) * ${(20)}$	(20.9% O ₂ - 7% O ₂) .9% O ₂ - Sample % O ₂)			
Standardized concentration	on (ng/dscm @ 7% (O ₂):				
$ng/dscm @ 7\%O_2 = 0.006 (ng/dscm) * \frac{(20.9\% O_2 - 7\% O_2)}{(20.9\% O_2 - 10\% O_2)}$						
= 0.006 (ng/dscm) * $\frac{(13.9\% \text{ O}_2)}{(10.9\% \text{ O}_2)}$						
	= 0.006 (ng/dscm) * 1.28					
= 0.008 ng/dscm @ $7\%O_2$						

Figure 11. Sample CDD/CDF Concentration Standardization Calculation

4.2 CALCULATION OF EMISSION FACTORS

Congener- and homolog-specific emission factors are calculated for each facility in units of nanograms emitted per kilogram of material combusted/processed. These emission factors are based on sample concentration, volumetric air flow rate, and activity level (i.e., material throughput). Test runs from single or multiple test reports are averaged for each facility. Two sets of emission factors are presented to reflect nondetected congener concentrations valued at zero, and those estimated at half the detection limit. Figure 12 shows the process for estimating an emission factor for a nondetected congener concentration valued at half the detection limit (when the concentration is valued at zero, the emission factor for that congener is zero). The

calculation of TEQ emission factors involves an additional equation that multiplies the congenerspecific emission factor by the TEF for that congener.

<u>Congener</u>	$\frac{\text{Concentration}}{\text{(ng/dscm @ 7% O2)}}$ $\frac{\text{ND} = 0}{\text{ND}}$	$\frac{\text{Concentration}}{\text{(ng/dscm @ 7% O2)}}$ $\frac{\text{ND} = \frac{1}{2} \text{LOD}}{\text{ND}}$	Volumetric Flow Rate (dscf/min)	Activity Level (kg/hr)
2378 TCDD	0	0.025	237	48.5

The general equation for estimation of emission factor is:

$$ng/kg \ = \ \frac{Conc. (ng/dscm) \ * \ Flow \ Rate \ (dscf/min) \ * \ cf(min/hr)}{cf(\frac{ft^3}{m^3}) \ * \ Activity \ Level \ (kg/hr)}$$

Substituting values from the above table and using ½ LOD concentration:

$$ng/kg = \frac{0.025 \ (ng/dscm) \ * \ 237 \ (dscf/min) \ * \ 60 \ (min/hr)}{35.31 \ (\frac{ft^3}{m^3}) \ * \ 48.5 \ (kg/hr)}$$

$$= \frac{355.5}{1712.5} \ = \ 0.208 \ ng/kg$$

Figure 12. Sample Emission Factor Calculations

In some cases, oxygen content data in the stack exhausts were not provided. Without knowing the oxygen content, standardized emission concentrations and volumetric air flow rates can not be calculated. However, in several cases, non-standardized reported flow rates and non-standardized reported emission concentrations along with reported activity levels were used to calculate emission factors (EF) and TEQ emission factors (TEQ-EF) assuming that the reported concentrations and flow rates were at the same oxygen content.

4.3 QUALITY CONTROL MEASURES

EPA conducted a data quality audit of the September 1997 draft version of the *National Database* under a contract with Research Triangle Institute (RTI). To conduct the audit, RTI

was provided with a copy of the draft *National Database* on CD-ROM and the draft User's Manual. The draft data base consisted of over 100 Megabytes (Mb) of data in more than 270 individual worksheets. RTI randomly selected 58 of the hard-copy and computer-readable data sources used to construct the data base. These data sources included EPA reports, reports from State environmental agencies, and independent laboratory reports, among others. RTI personnel audited 64 (28%) of the site-specific worksheets using these source documents. The audit searched for data input errors, errors present in the source documents and how these errors were addressed in the data base, spreadsheet formula errors, and cosmetic and other minor problems. The audit report (RTI, 1998) recommended a series of corrective actions all of which were subsequently addressed in developing Version 1.1 of the *National Database*.

5. ANNUAL CDD/CDF EMISSION CALCULATIONS

Because only a few U.S. facilities in most source categories have been tested for CDD/CDF emissions, an extrapolation is needed to estimate national emissions for most source categories. Many of the national emission estimates developed from this database that are presented in EPA's *Sources of Dioxin-Like Compounds in the United States* (U.S. EPA, 2001), were, therefore, developed using a "top down" approach. The first step in this approach is to derive from the available emission test data an emission factor (or series of emission factors) deemed to be representative of the source category (or segments of a source category that differ in configuration, fuel type, air pollution control equipment, etc.). As described in Section 4.2, the emission factor relates mass of CDD/CDFs released into the environment per some measure of activity (e.g., kilograms of material processed per year, vehicle miles traveled per year, etc.). The emission factor was then multiplied by a national value for the activity level basis of the emission factor (e.g., total kg of material processed in the United States annually).

Although no categories had estimates developed in Volume 2 from a true "bottom up" approach (i.e., estimates developed using site-specific emissions and activity data for all individual sources in a category and then summed to obtain a national total), existing facility-specific emissions testing and activity level data for some source categories in the database (e.g., municipal solid waste incinerators) supported a semi- "bottom up" approach. In this approach, facility-specific annual emissions were calculated for those facilities with adequate data. For the untested facilities in the class, a subcategory (or class) emission factor was then developed by averaging the emission factors for the tested facilities in the class. This average emission factor was then multiplied by the measure of activity for the non-tested facilities in the class. Emissions were summed for the tested facilities and non-tested facilities. In summary, this procedure can be represented by the following equations:

$$E_{total} = \sum_{tested,i} E_{tested,i} + \sum_{tested,i} E_{untested,i}$$
 $E_{total} = \sum_{tested,i} E_{tested,i} + \sum_{tested,i} (EF_i * A_i)_{untested}$

Where: E_{total} = annual emissions from all facilities (g TEQ/yr)

 $E_{tested,i}$ = annual emissions from all tested facilities in class i (g TEQ/yr) $E_{untested,i}$ = annual emissions from all untested facilities class i (g TEQ/yr) Ef_{i} = mean emission factor for tested facilities in class i (g TEQ/kg)

A_i = activity measure for untested facilities class i (kg/yr)

Some source categories are made up of facilities that vary widely in terms of design and operating conditions. For these sources, as explained above, an attempt was made to create subcategories that grouped facilities with common features and then to develop separate emission factors for each subcategory. Implicit in this procedure is the assumption that facilities with similar design and operating conditions should have similar CDD/CDF release potential. For most source categories, however, the specific combination of features that contributes most to CDD/CDF or dioxin-like PCB release is not well understood. Therefore, how to best subcategorize a source category was often problematic. For each subcategorized source category in this report, a discussion is presented about the variability in design and operating conditions, what is known about how these features contribute to CDD/CDF or dioxin-like PCB release, and the rationale for subcategorizing the category.

As discussed above, each source emission calculation required estimates of an "emission factor" and the "activity level." For each emission source, the quantity and quality of the available information for both terms vary considerably. Consequently, it is important that emission estimates be accompanied by some indicator of the uncertainties associated with their development. For this reason, a qualitative confidence rating scheme was developed as an integral part of the emission estimate in consideration of the following factors:

• *Emission Factor* - The uncertainty in the emission factor estimate depends primarily on how well the tested facilities represent the untested facilities. In general, confidence in the emission factor increases with increases in the number of tested facilities relative to the total number of facilities. Variability in terms of physical design and operating conditions within a class or subclass must also be considered. The more variability among facilities, the less confidence that a test of any single facility is representative of that class or subclass. The quality of the supporting documentation also affects uncertainty. Whenever possible, original engineering test reports were used. Peer reviewed reports from the open literature were also used for developing some emission factors. In some cases, however, draft reports that had

undergone more limited review were used. In a few cases, unpublished references were used (such as personal communication with experts) and are clearly noted in the text.

• Activity Level - The uncertainty in the activity level estimate was judged primarily on the basis of the extent of the underlying data. Estimates derived from comprehensive surveys (including most facilities in a source category) were assigned high confidence. As the number of facilities in the survey relative to the total decreased, confidence also decreased. The quality of the supporting documentation also affects uncertainty. Peer reviewed reports from the open literature (including government and trade association survey data) were considered most reliable. In some cases, however, draft reports that had undergone more limited review were used. In a few cases, unpublished references were used (such as personal communication with experts) and are clearly noted in the text.

The confidence rating scheme, presented in Table 7, presents the qualitative criteria used to assign a high, medium, or low confidence rating to the emission factor and activity level terms for those source categories for which emission estimates can be reliably quantified. The overall "confidence rating" assigned to an emission estimate was determined by the confidence ratings assigned to the corresponding "activity level" term and "emission factor" term. If the lowest rating assigned to either the activity level or emission factor terms is "high," then the category rating assigned to either the activity level or emission factor terms is "medium," then the category rating assigned to the emission estimate is medium (also referred to as "B"). If the lowest rating assigned to either the activity level or emission factor terms is "low," then the category rating assigned to either the activity level or emission factor terms is "low," then the category rating assigned to the emission estimate is low (also referred to as "C"). It is emphasized that this confidence rating scheme should be interpreted as subjective judgements of the relative uncertainty among sources, not statistical measures.

Table 7. Confidence Rating Scheme for U.S. Emission Estimates

Confidence Rating	Activity Level Estimate	Emission Factor Estimate				
Categories/Media for Which Releases Can Be Reasonably Quantified						
High	Derived from comprehensive survey	Derived from comprehensive survey				
Medium	Based on estimates of average plant activity level and number of plants or limited survey	Derived from testing at a limited but reasonable number of facilities believed to be representative of source category				
Low	Based on data judged possibly nonrepresentative	Derived from testing at only a few, possibly nonrepresentative facilities or from similar source categories				
Categories/Media for Which Releases Cannot Be Reasonably Quantified						
Preliminary Estimate	Based on extremely limited data, judged to be clearly nonrepresentative	Based on extremely limited data, judged to be clearly nonrepresentative				
Not Quantified	No data available	Argument based on theory but no data, or Data available indicating formation, but not in a form that allows developing an emission factor				

For many source categories, either emission factor information or activity level information were inadequate to support development of reliable quantitative release estimates for one or more media. For some of these source categories, sufficient information was available to make preliminary estimates of emissions of CDD/CDFs; however, the confidence in the activity level estimates or emission factor estimates was so low that the estimates cannot be included in the sum of quantified emissions from sources with confidence ratings of A, B and C. These preliminary estimates were given an overall confidence class rating of D (Table 8, "Preliminary Estimate" column). As preliminary estimates of source magnitude, they can be used, however, to help prioritize future research and data collection. The actual magnitude of emissions from these sources could be significantly lower or higher than these preliminary estimates. Although EPA has chosen not to include them in the more thoroughly characterized emissions of the national inventory, some of these poorly characterized sources have the potential of being major contributors of releases to the environment. As the uncertainty around these sources is reduced, they will be included in future inventory calculations. For other sources, some information exists which suggests that they may release dioxin-like compounds; however, the available data were judged to be insufficient for developing any quantitative emission estimate. These source categories were assigned a confidence category rating of "E" and also were not included in the national inventory (Table 8, "Not Quantifiable" column).

The emission factors developed for the emissions inventory in Volume 1 are intended to be used for estimating the total emissions for a source category rather than for individual facilities. EPA has made uncertainty determinations for each of these emission factors based, in part, on the assumption that by applying them to a group of facilities, the potential for overestimating or underestimating individual facilities will to some extent be self compensating. This means that in using these emission factors one can place significantly greater confidence in an emission estimate for a class than can be placed on an emission estimate for any individual facility. Given the limited amount of data available for deriving emission factors, and the limitations of our understanding about facility-specific conditions that determine formation and control of dioxin-like compounds, the current state of knowledge cannot support the development of emission factors that can be used to accurately estimate emissions on an individual facility-specific basis.

Table 8. List of Known and Suspected CDD/CDF Sources

	Contemporary Formation Sources			Reservoir Sources			
Emission Source Category	Quantifiable	Preliminary Estimate	Not Quantifiable	Quantifiable	Preliminary Estimate	Not Quantifiable	
I. COMBUSTION SOURCES							
Waste Incineration							
Municipal waste incineration	✓						
Hazardous waste incineration	✓						
Boilers/industrial furnaces	✓						
Medical waste/pathological incineration	✓						
Crematoria	✓						
Sewage sludge incineration	✓						
Tire combustion	✓						
Pulp and paper mill sludge incinerators	✓						
BioGas combustion		✓					
Power/Energy Generation Vehicle fuel combustion - leaded ^b	✓ ·						
- unleaded	✓						
- diesel	✓						
Wood combustion - residential	✓						
- industrial	✓						
Coal combustion - residential		/					
- industrial/utility	✓						
Oil combustion - residential		/					
- industrial/utility	√						
Other High Temperature Sources Cement kilns (haz waste burning)	1						
Cement kilns (non haz waste burning)	✓						
Asphalt mixing plants		✓					
Petro. refining catalyst regeneration	✓						
Cigarette combustion	✓						
Carbon reactivation furnaces	✓						
Kraft recovery boilers	✓						
Manufacture of ball clay products			✓				

Table 8. List of Known and Suspected CDD/CDF Sources (continued)

	Contemporary Formation Sources			Reservoir Sources		
Emission Source Category		Preliminary	Not		Preliminary	Not
	Quantifiable	Estimate	Quantifiable	Quantifiable	Estimate	Quantifiable
Minimally Controlled or Uncontrolled Combustion						
Combustion of landfill gas in flares		✓				
Landfill fires		✓				
Accidental fires (structural)		✓				
Accidental fires (vehicles)		✓				
Forest, brush, and straw fires		✓				
Backyard barrel burning	✓					
Uncontrolled combustion of PCBs			✓			
II. METAL SMELTING/REFINING						
Ferrous metal smelting/refining						
- Sintering plants	✓					
- Coke production		✓				
- Electric arc furnaces		✓				
- Ferrous foundries		✓				
Nonferrous metal smelting/refining						
- Primary aluminum			/			
- Primary copper	1					
- Primary magnesium		✓				
- Primary nickel			/			
- Secondary aluminum	✓					
- Secondary copper	1					
- Secondary lead	✓					
Scrap electric wire recovery	✓					
Drum and barrel reclamation	1					
III. CHEMICAL MANUFACTURING						
(Releases to the Environment)						
Bleached chemical wood pulp and paper mills	1					
Mono- to tetrachlorophenols			1			
Pentachlorophenol			1			
Chlorobenzenes			✓			
Chlorobiphenyls (leaks/spills)			✓			
Ethylene dichloride/vinyl chloride	1					

Table 8. List of Known and Suspected CDD/CDF Sources (continued)

	Contemporary Formation Sources			Reservoir Sources		
Emission Source Category		Preliminary	Not		Preliminary	Not
	Quantifiable	Estimate	Quantifiable	Quantifiable	Estimate	Quantifiable
Dioxazine dyes and pigments			✓			
2,4-Dichlorophenoxy acetic acid			✓			
Municipal wastewater treatment		1				
Tall oil-based liquid soaps			✓			
IV. BIOLOGICAL AND PHOTOCHEMICAL PROCESSES			✓			
V. RESERVOIR SOURCES Natural						
- Land					1	
- Air						✓
- Water						✓
- Sediments						✓
Anthropogenic Structures						
- PCP Treated Wood						/

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