SOURCE RANKING DATABASE
Volume 1: Guide and Documentation

Revised Edition

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1. INTRODUCTION

The U.S. Environmental Protection Agency (EPA) has identified indoor air as a major pathway of human exposure to numerous chemicals. Within EPA, the Office of Pollution Prevention and Toxics (OPPT), the Office of Radiation and Indoor Air (ORIA), and the Office of Research and Development (ORD) have collaborated on an Indoor Air Source Characterization Project (IASCP) that will provide information to better define exposures and risks encountered in indoor air (Cinalli et al., 1993). The overall goal of the IASCP is to support EPA actions in the areas of testing, risk management, and pollution prevention. A major component of this effort is the development of a software application called the Source Ranking Database (SRD). The remainder of this section describes the purpose and intended uses of the SRD software, assumptions and limitations, and the contents of this report.

1.1   Purposes and Uses of the SRD

The purpose of the SRD is to provide a means for systematically reviewing a large number of consumer products, building materials, and furnishings that are potential sources of airborne chemicals to which individuals can be exposed while indoors. The software is intended for use as a screening tool, to identify high-priority products or product classes for further evaluation. There are three applications in SRD: (1) ranking products on the basis of acute or chronic hazard ratings, (2) finding products that contain a particular chemical, and (3) identifying the chemicals found in a particular product.

The primary application in the SRD software scores and ranks products and materials using modeled indoor-air concentrations of their chemical constituents in selected types of environments, frequency of use (in the case of products), the fraction of buildings in which products or materials are used, and the relative health hazard associated with inhalation of each chemical. The size of potentially exposed populations in each environment is also taken into account. Products and materials can be ranked based on peak modeled concentrations and acute chemical hazard ratings or time-integrated concentrations together with chronic hazard ratings for chemicals.

Each type of product or material included in the SRD has at least one formulation (i.e., chemical composition). For products or materials with more than one formulation, the score is determined by averaging across the scores calculated for each formulation. Products and materials also are grouped into several classes, and the ranking application can be applied to these classes. Product/material classes are ranked based on average scores across all products or materials in each class.

The SRD also includes applications for determining all products or materials in the database that contain a certain chemical, and for determining all chemicals that are contained in various formulations of a specific product or material. These applications are intended primarily to assist the user in better

1-1

understanding why a certain product or material may have received a relatively high or low score in the ranking application.

1.2   Assumptions and Limitations

The SRD includes a mathematical model, based on the principle of conservation of mass (Nagda et al., 1987), for calculating peak and time-integrated airborne concentrations of the chemicals released from products or materials. The modeling involves some simplifying assumptions while attempting to retain as much "real world" fidelity as possible. Simplifying assumptions are necessary because of the lack of information required to support more complex calculations, coupled with the large number of calculations that are required to ultimately rank product or material classes. For example, a single-chamber model is used, for which analytical solutions have been developed so that peak and time-integrated concentrations can be calculated directly. Potential indoor sinks are ignored in the model. Breathing rates are not included in model calculations. Therefore, the chemical scores are related to airborne concentrations rather than inhalation exposures per se.

The chemical-specific hazard information contained in the SRD includes ratings for both acute and chronic health effects for compatibility with peak and time-integrated concentrations that are calculated by the model. Due to limitations of existing data, a given chemical in the database currently has the same relative hazard rating (high, medium, or low) for acute and chronic health effects. In calculating the score for each chemical in a product formulation, a high hazard rating is assigned a value of 100, as compared to 0.1 for a medium rating and 0.001 for a low rating.

The primary information available for products in the SRD database is their formulation (i.e., weight fractions of various chemicals comprising each product) and duration and frequency of use. For materials and furnishings, some information on time-varying emission rates is available from testing that has been conducted in large chambers to support other EPA projects.

The specific calculations for peak and time-integrated calculations depend on how a product or material is used or applied. There are four types of situations, or "cases," in which a product is used: (1) a product that is discharged directly to air (e.g., spray freshener); (2) a product involving application in water (e.g., laundry detergent) or for which portion ultimately goes "down the drain" (e.g., shaving cream); (3) a product that is applied to a surface (e.g., general purpose cleaner); and (4) a product or material that is placed in an environment (e.g., room deodorizer, building material). To the extent possible, the SRD calculations are made to place the various products and materials on an "equal footing." That is, assumptions generally are oriented toward worst-case estimates of emissions in either case.

As noted previously, a number of products in the SRD database have more than one formulation. In these cases, it is assumed that each formulation has an equal market share. Using this assumption, a simple average across the scores, calculated for each formulation, can be used to develop a score for the product.

1.3   **This Report**

This report (Volume 1: Guide and Documentation) describes the files contained in the SRD, the relationships among these files, and the sources of information and assumptions that were used to develop the data files. It also describes the calculations, assumptions and options available to the user in ranking product/material classes based on acute or chronic chemical hazard ratings. This document also provides guidance for using the SRD application.

Section 2 of this report provides instructions for installing the SRD software together with an overview of SRD data files, relationships and applications. Sections 3 to 6 describe the information sources and contents of each data file. Section 7 provides further details on the three primary SRD applications: (1) ranking products, (2) finding products that contain a chemical, and (3) finding chemicals in a product. Section 8 documents the calculations and associated assumptions involved in ranking products. Section 9 lists the references cited throughout the report.

Supporting materials relating to files, calculations, and assumptions used for the SRD software are presented in Volume 2 (Appendices). These include descriptions of the contents of the data files. Also included in the Appendices are lists of contacts made to solicit product and material usage information, a description of the methodology to derive 50th and 90th percentile product usage factors from the Simmons Market and Media Study, assignment of product IDs to cases, and mathematical documentation for the algorithms used to calculate peak and time-integrated airborne concentrations.

The SRD was reviewed by EPA's Science Advisory Board (SAB) in July 1997. The SAB's final report, received in December 1997, contained recommendations for a variety of changes and improvements to the SRD. The primary comments from the SAB review related to the algorithm used to rank products. In particular, the SAB Committee recommended that the algorithm be reviewed and that attention be paid to several issues such as the overall sensitivity of the algorithm to variability in the component factors and in the hazard scale. In addition, several additional recommendations were made including: a) addition of additional exposure sources to SRD; b) addition of octanol/water partition coefficient and Henry's Law ration so that sorption/desorption and volatilization processes can be better addressed; and c) consideration of the need for regular updates and accessibility of the database to the public. Many of the changes suggested in SAB's report were made during years 1999 and 2000. Specifically, the revised version of the SRD has

an expanded hazard scale, uses Henry's Law constants as the means to estimate product volatilization from aqueous solutions, and incorporates several other capabilities.

This version of the SRD incorporates SAB's comments made during peer review. No further modification of the SRD's structure is expected. Additional data may be added if and when resources become available. Any updates will be posted at:

http://www.epa.gov/oppt/exposure/docs/srd.htm

2.   INSTALLATION AND OVERVIEW

2.1   <u>Installation</u>

The Source Ranking Database is a Windows application developed using Microsoft Visual FoxPro software version 6.0. It has been developed, using the FoxPro distribution kit, as a stand-alone executable program. The minimum hardware requirements are a Pentium computer with Windows 95, Windows 98, Windows ME or Windows NT operating system and 8 MB of memory and 20 MB of free hard disk.

If the software is provided on a CD ROM disk, run setup.exe from the CD ROM. This is accomplished by pressing the START button, followed by selecting the RUN menu item and typing:

    d:\setup.exe

    where d: is the drive of the CD ROM.

If you have downloaded the model from the Internet, make sure that all elements of the program are in the same folder and run setup.exe from that folder. Follow the prompts to complete installation of the program. The default installation places the program files in the c:\PROGRAM FILES\SRD folder, but the user may change the destination folder. A program group called SRD will be created.

The software is opened by locating the program group SRD and double-clicking the SRD icon that is created during the installation procedure described above. The user will then be presented with the introductory screen shown in Figure 2-1. From the introductory screen, the user has the option to access database files or applications in SRD by selecting one of the tabs on this screen. An overview of the files, applications, and ranking methods is provided below.

2.2   <u>Troubleshooting</u>

The SRD's user interface includes two maintenance/troubleshooting functions

Figure 2-1. Introductory Screen for SRD Software

2.2   <u>Applications</u>

There are three applications in SRD. The first application is used to rank products and materials using modeled indoor-air concentrations of their chemical constituents in selected types of environments. The application takes into account the frequency of use (in the case of products), the fraction of buildings in which products or materials are used, the relative health hazard associated with inhalation of each chemical, and the size of the potentially exposed populations in each environment. Products and materials can be ranked based on peak modeled concentrations and acute chemical hazard ratings or time-integrated concentrations, together with chronic hazard ratings for chemicals.

The second application in SRD is used to locate all products or materials in the database that contain a certain chemical. The user selects a chemical by CAS number or chemical name and information is presented about the products (e.g., product name, formulation name, weight fraction, and emission rate).

The third application in SRD is used to determine all chemicals that are contained in various formulations of a specific product or material. The user selects a product by product ID or by product name category and information is presented on the chemical data (e.g., CAS number, chemical name, weight fraction and hazard score).

Help screens are provided in SRD and are easily accessed from each SRD window by clicking on the button with the red question mark and the word "Help". Each help screen provides a summary of the elements within the activated window or screen in SRD. The numbered sections in the Help files correspond to the equivalent sections in this user's manual, which contains more detailed information.

2.3   Files

The SRD software contains eight types of files that are used in calculating relative risk and can be readily accessed by the user under the tab labeled "Browse Database Files."(Figure 2-2)

- CHEMICAL file (CHEMICAL.DBF)
- ENVIRONMENT file (ENVIRNMT.DBF)
- MATERIAL-ENVIRONMENT file (MAT_EVT.DBF)
- PEOPLE-ENVIRONMENT file (PEOP_EVT.DBF).
- PRODUCT-CHEMICAL file (PROD_CHM.DBF)
- PRODUCT-ENVIRONMENT file (PROD_EVT.DBF)
- PRODUCT-FORMULATION file (PROD_FOR.DBF)
- PRODUCT-CATEGORY file (TL_CAT.GRP)

All files have been created in dBASE-compatible format. Thus, they can be accessed or viewed "outside" the SRD software using various dBASE-compatible programs or utilities that are commercially available.   The user is cautioned against using such utilities for updating files, because the internal documentation of file updates obtained through the SRD software would not be utilized in such instances.

The key contents of each file are summarized in Table 2-1. The CHEMICAL file primarily contains physical/chemical properties, as well as acute and chronic hazard ratings, for each chemical.   The PRODUCT-CHEMICAL file contains information on the specific chemicals contained in each product or material, including weight fractions for chemicals in products and emission rates for chemicals in materials. The PRODUCT-ENVIRONMENT and MATERIAL-ENVIRONMENT files contain usage information for products and materials, respectively, for up to nine indoor environments. The PRODUCT-FORMULATION file indicates whether a given item is classified as a product or a material, and also indicates the type(s) of environment in which each product or material is used. The ENVIRONMENT file describes properties of each environment (e.g., residences, office buildings) such as the volume and the rate of air exchange between indoors and outdoors. The PEOPLE-ENVIRONMENT file describes the various subpopulations occupying each environment, including the size of each subpopulation and the average fraction of time spent by that subpopulation in the environment.
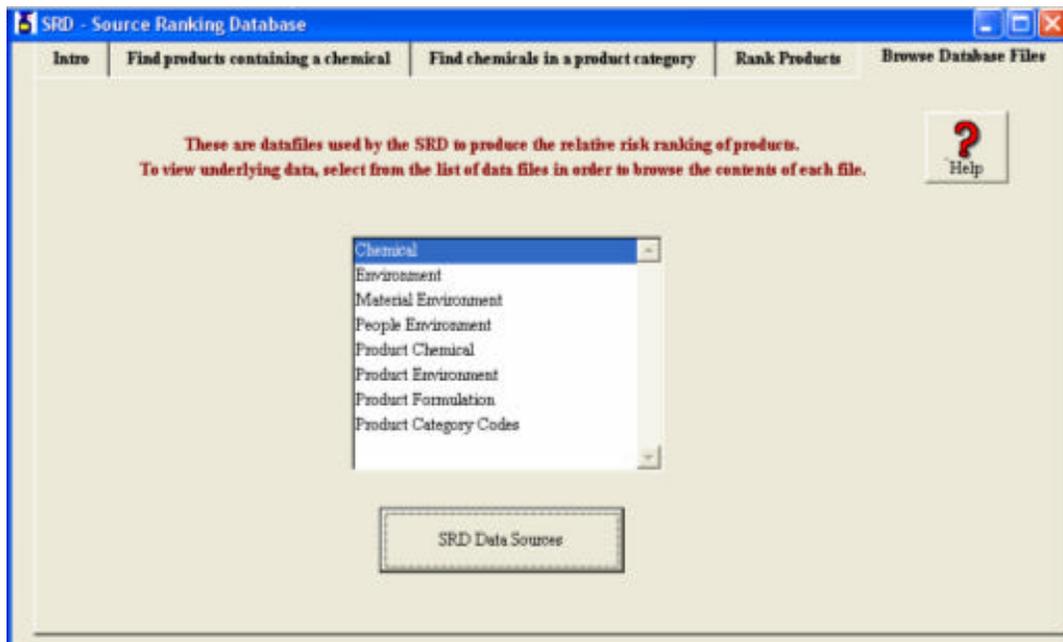
Figure 2-2. SRD Files Accessible to the User

Table 2-1. Key Contents of SRD Files

FILE	KEY CONTENTS (OTHER THAN LINKING VARIABLES)
Chemical	Chemical name, molecular weight, vapor pressure, hazard ratings, fraction volatilized
Environment	Environment description, volume, air exchange rate
Material-Environment	Amount present, duration since installation, fraction of buildings
People-Environment	Type/size of population, fraction of time in environment
Product-Chemical	Weight fraction, emission rate
Product-Environment	Quantity/duration/frequency of use, fraction of buildings
Product-Formulation	Product/material descriptions, applicable environments, case, subcase
Product Category	Codes/descriptions for product/material categories

The SRD software uses relational-database concepts to minimize storage of redundant information. Relationships across the various files are established using the common or linking variables shown in Table 2-2. The "hub" of the database is the PRODUCT-FORMULATION file. This file is linked (i.e., related) to other files using the product ID, formulation ID, or environment ID fields. The PRODUCT CATEGORY file is also linked to the PRODUCT-FORMULATION file using the product ID. A CAS number, assigned to each chemical, provides a linkage between the CHEMICAL and the PRODUCT-CHEMICAL files. The environment ID provides a linkage to the ENVIRONMENT, PEOPLE-ENVIRONMENT, PRODUCT-ENVIRONMENT, and MATERIAL-ENVIRONMENT files.

Further details on the contents of each file and the identifiers for products, chemicals and environments are provided in subsequent sections of the report. Section 3 describes the PRODUCT-FORMULATION file and product-grouping schemes that have been developed to date. Section 4 describes the CHEMICAL and PRODUCT-CHEMICAL files, Section 5 describes the PRODUCT-ENVIRONMENT and MATERIAL-ENVIRONMENT files, and Section 6 describes the ENVIRONMENT and PEOPLE-ENVIRONMENT files. These descriptions include the file contents, coding schemes that were developed or utilized for certain fields, sources of information, and assumptions or judgments that were made in cases of limited information.

Section 7 of the report provides details on SRD applications, which are reviewed briefly here. The files in Table 2-1 can be viewed using the Browse Database Files tab (Section 7.1); data are displayed on a screen (Figure 2-3) and the user may navigate through the tables, search for a partcular item, or export the tables in a variety of file formats. Ranking products (Section 7.2) involves choosing a classification scheme, selecting all or some product/material categories associated with that scheme, choosing sources of data on product formulations, selecting environments, and using acute or chronic hazard ratings as a basis for ranking. An overview of the ranking methodology is provided in Section 2.4. The Find products containing a chemical tab (Section 7.3) allows the user to extract data pertaining to a specific chemical by entering a name or CAS number. The find chemicals in a product category tab (Section 7.4) allows a user to extract data pertaining to a product name or ID.

Table 2-2. Common/Linking Variables for SRD Files

FILE	COMMON/LINKING VARIABLES				
	PRODUCT ID	FORMULATION ID	CAS NUMBER	MATERIAL/ PRODUCT	ENVIRONMENT ID
Chemical			X		
Environment					X
Material-Environment	X				X
People-Environment					X
Product-Chemical	X	X	X		
Product-Environment	X				X
Product-Formulation	X	X		X[1]	X[2]
Product Category	X				

[1] Indicates whether information on quantity/amount is to be found in the PRODUCT-ENVIRONMENT file or the MATERIAL-ENVIRONMENT file

[2] Indicates which of the nine environments the formulation applies to

Figure 2-3. SRD Screen Following Selection of a File

2.4   Ranking Methodology

This section provides an overview of the procedures used in the "Rank Products" application within SRD. Additional information on ranking products may be found in Section 7.2, and the calculations and assumptions associated with the procedure are provided in Section 8.

As illustrated in Figure 2-5, the user has certain choices or options that affect how the ranking of products, or product categories, is performed by the SRD software:

- Products or categories can be ranked at the 4-digit, 5-digit or 7-digit (most detailed) level of classification for SIC codes (see Section 3)

- All or a subset of the data sources on product/material formulations can be chosen

- All or a subset of environments in which products/materials are used can be chosen

- Average or upper-end values can be chosen for amount of product used, or material present, and for the duration and frequency of product use

- The ranking can be based on chronic or acute hazards, but not both

- All chemicals in product/material formulations can be used in the ranking, or just those (i.e., the program leaves out calculations for these chemicals) without a value for chronic/acute hazard rating (see Section 4)

The user selections for these items can be saved for retrieval on subsequent SRD ranking applications.
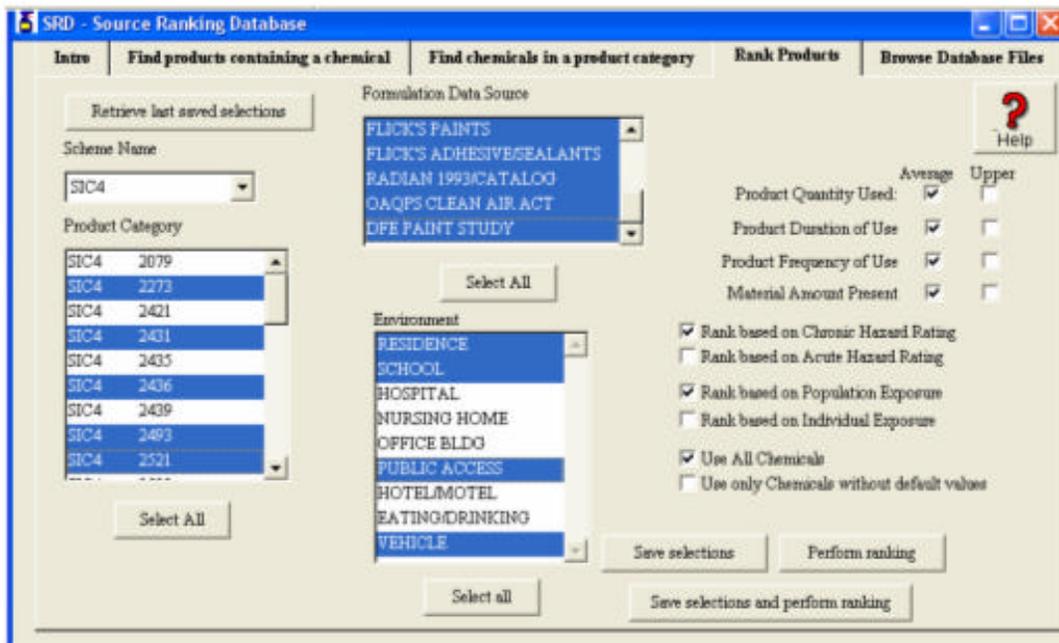
Figure 2-5. User Inputs/Choices for Ranking Products

The ranking procedure begins with a chemical contained in a specific product formulation. A formulation is roughly equivalent to a brand. Based on analytical solutions to a single-chamber model for indoor-air concentrations over time, either a peak concentration (for acute hazards) or a time-integrated concentration (for chronic hazards) is calculated for each environment chosen by the user. The form of the calculation depends on how the product/material is used -- direct discharge to air, application/disposal in water, application to a surface, or placement in an environment. The "score" for the chemical is obtained for each environment by multiplying the calculated concentration by the hazard rating, the percent of buildings in which the product/material is used, and (for products) by the annual frequency of use.

Next, an average score across environments is calculated, using the relative population in each environment as a weighting factor. The average score so derived for each chemical is then summed across all chemicals in the formulation to derive a "formulation score." Many products or materials have more than one formulation. In those cases, then a simple average across formulations is taken to derive a "product score." This approach assumes equal market share for each formulation. Formulations are associated with the 7-digit classification of products and materials. If the user chooses a higher level of aggregation (e.g., a 4-digit or 5-digit classification), then a simple average is taken across scores for each 7-digit product ID associated with the higher-level class. The ranking is based on the average score for each product category. A higher score is assumed to indicate a higher risk and assigned a higher rank.

3. PRODUCT CATEGORY AND PRODUCT-FORMULATION FILES

The Product-Category and Product-Formulation files contain information on sources of data for products and materials contained in SRD. This section provides a description of the classification scheme used for SRD and a description of the contacts of the Product-Category and Product-Formulation files.

3.1   Background - AEERL Classification Scheme

The Classification of Materials as Potential Sources of Indoor Air Pollution (USEPA 1990), prepared by the Air and Energy Engineering Research Laboratory (AEERL) of EPA, systematically identified and classified materials brought into or used to construct and renovate homes and office buildings. The objective of the study was to design a foundation for a systematic analysis of the role of materials in influencing indoor air quality. The approach taken in the report involved identification and categorization of products that are:

- Components of construction of buildings;
- Used as fixtures and furnishings; and
- Consumer goods that are brought into buildings in the course of normal use.

A number of sources containing information on categorization or classification of materials were identified during the course of the study, and are described in the classification report. The report concluded that the Census of Manufactures presented the most comprehensive list of products covering all three categories of interest in the study, and employed categories useful to indoor air quality study. Data presented in the Industry Series Reports of the Census of Manufactures (USDOC 1990) were therefore used as a basis for the classification system. The census data are based on the Standard Industrial Classification (SIC) system, which is commonly used by industry and government agencies.

USEPA (1990) also identified products or materials in the classification thought to be potential sources of indoor air emissions. This was a subjective process, based on consideration of the three following factors:

- The quantity produced. How pervasive is the product in the environment?

- Compositional information. Based on readily available published information, how harmful are the emissions likely to be?

- The nature of its use. What is the likelihood of human exposure to materials emitted?

In the list presented in the classification, the subset of products judged to be potential sources of emissions to indoor air was identified. The report, Indoor Air Pollutant Source Catalog (Radian 1993)

subsequently prepared for AEERL, presents more complete information on this subset of material sources of indoor air pollution, and presents available constituent and emissions data for ten priority product categories of sources. The classification system developed in USEPA (1990) (i.e., SIC code-based system) was used as the starting point for classifying the products in each product category. However, in order to develop the most useful scheme for presenting the usage, constituent, and emissions data for the variety of products in each category, refinements were made to the classification system. Depending on the category, the scheme was revised to account for either how the products are used in the home, the manufacturing process for the product, or the component parts of the product.

3.2   SRD Product Classification Scheme: The PRODUCT CATEGORY File

For purposes of defining a product classification scheme for SRD, an expanded version of the classification scheme developed by AEERL (USEPA 1990) was developed. Those products identified in USEPA (1990) as "thought to contribute to indoor air pollution" were used as the starting point for the scheme. This list was then supplemented with additional products based on a review of the product coding scheme utilized in the report, Numerical List of Manufactured and Mineral Products (USDOC 1989). This review was subjective and considered the same factors used by AEERL in developing the 1990 classification scheme.

The Numerical List of Manufactured and Mineral Products (USDOC 1989) includes the principal products and services of the manufacturing and mining industries in the United States. The data for these products and services were collected in the 1987 Census of Manufactures on 205 long and 77 short report forms (forms MC-2001 through MC-3912) and the 1987 Census of Mineral Industries on 10 long and 1 short form (MC-1001 through MC-1403). Each report form covers one or more industry and includes a product inquiry that lists the primary products for the industries and the chief secondary products frequently reported by establishments classified in the industries on that report form.

Products and services in USDOC (1989) are arrayed generally in ascending seven-digit numerical order followed by alphabetical characters within their respective five-digit codes (product classes), the product classes in order within their four-digit codes (industries), and the industries within their three-digit industry groups and two-digit major groups. Major groups, industry groups, and industries, as presented in this manual, correspond with both title and content of the Standard Industrial Classification Manual: 1987 edition, published by the Office of Management and Budget (OMB 1987). In addition to more than 6,600 products for which information is collected primarily in the Censuses of Manufactures and Mineral Industries, the list contains approximately 4,400 products for which information is collected monthly, quarterly, and annually in the Census Bureau's Current Industrial Reports (CIR) program.

The SRD product classification scheme encompassing the three product groups developed by AEERL (USEPA 1990) (i.e., building materials; consumer products; and furnishings and equipment) is based on the product coding system developed by the Bureau of the Census in USDOC (1989) and further refined in USDOC (1993) for the 1992 Census of Manufacturers and Census of Mineral Industries. The Bureau of the Census system operates so that the coverage is progressively narrower (i.e., more specific) with the successive addition of digits. This is illustrated as follows:

SIC Code	Level	Description
24	Major group	Lumber and wood products
249	Industry group	Miscellaneous wood products
2493	Industry	Reconstituted wood products
24931	Product class	Particleboard
2493105	Product	Mobile home decking

In addition, the SRD scheme employs a two-digit extension of the seven-digit Product code to allow for future refinements to accommodate the needs identified in Radian (1993).

The product classification scheme for SRD has been entered into the PRODUCT CATEGORY file. Table 3-1 presents information on the principal data elements of the file. Appendix A contains all 328 records in the PRODUCT CATEGORY file.

Table 3-1. Contents of the PRODUCT CATEGORY File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
Product, Product Class, or Industry ID	Character	--	4-digit SIC industry code or 5-digit SIC product class code or 7-digit SIC product code to which has been added an additional 2 digits to enable additional product classification.
Description	Character	--	Definition used by U.S. Dept. of Commerce.

3.3　　PRODUCT-FORMULATION File

Formulation and/or chemical emission data have been obtained from a variety of sources for hundreds of products or materials (discussed in detail in Section 4.1). The PRODUCT-FORMULATION file contains records for each product/material having formulation or emission data in SRD. Each record contains a name or description of the product/material, based on information provided in the source documents, and a unique identification code (i.e., the Formulation ID) that identifies the data source and the location of the data within the source document. Table 3-2 presents information on the principal data elements in the PRODUCT-FORMULATION file. Appendix B contains all 12,595 records in the PRODUCT-FORMULATION file.

Table 3-2. Contents of the PRODUCT-FORMULATION File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
Product ID	Character	--	SIC product code[1].
Formulation ID	Character	--	Unique formulation/material[2] code for each product/material.
Formulation Description	Character	--	Name/description of specific formulation or material as reported in the data source.
Formulation Applicability	Logical	--	Repeating field; one field for each of nine defined environments. T = formulation data apply F = formulation data do not apply
Product/Material Indicator	Character	--	P = product M = material
Case	Numeric	--	Refers to how formulation/material is used.
Subcase	Numeric	--	Refers to specific use for products dissolved in water. (Case 2).

[1] The SIC Code is defined in Section 3.2. This SIC Code consists of seven characters with two additional characters to enable additional product classification.

[2] The formulation/material code is discussed in Section 3.3.

4. PRODUCT-CHEMICAL AND CHEMICAL FILES

4.1 PRODUCT-CHEMICAL File Overview

Formulation and emission data have been obtained from a variety of sources as described in detail in Section 4.2. All product formulation and emission data were entered into spreadsheets to enable efficient data entry, quality control, ease of entry into SRD, and use as standalone spreadsheets. These spreadsheets were then combined to form the PRODUCT-CHEMICAL file. Each record of this file contains data for a specific chemical within an individual product (e.g., CAS number and weight fraction of the chemical in the product). Each of the 30,914 records in this file contains information on one chemical in one product. Table 4-1 presents detailed information on the data elements of the PRODUCT-CHEMICAL file.

4.2 Data Sources for the PRODUCT-CHEMICAL File

Information for the product formulations was obtained from a variety of sources.

4.2.1 Advanced Cleaning Product Formulations (Flick 1989a)

This book presents more than 800 cleaning product formulations for household, industrial, and automotive applications. The formulation data were obtained by Flick from numerous companies and other organizations. The book states that the data represent selections made at no cost to, nor influence from, the makers or distributors of the materials. The book also states that only the most recent formulations are presented.

Each formulation in the book lists the following information, as available, in the manufacturer's own words:

- Description of end use and, if applicable, typical dilution(s) for various applications;
- The percent by weight or volume of each component of the formulation;
- Key properties of the product that may differentiate it from other similar products; and
- The name of the manufacturer or organization that supplied the formulation.

The formulations in the book are divided into the following sections and chapters (parenthetical numbers indicate the number of products in each chapter):

Table 4-1. Contents of the PRODUCT-CHEMICAL File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
Product ID	Character	--	SIC product code.
CAS Number	Character	--	Chemical-specific Chemical Abstract Service number.
Formulation ID	Character	--	Unique formulation/material code for each product/material.
Weight Fraction	Numeric	--	Weight fraction of specific chemical in a specific formulation as reported in the data source or as calculated based on information provided in the data source.
Initial Emission Rate	Numeric	Materials: μg/m^2-hr or μg/unit-hr Products:μg/g-hr	Based on data reported in literature or from actual chamber testing results.
Rate Constant for Decline	Numeric	hr^{-1}	Currently based on assumptions related to emissions life (see Section 8). In the future, could be based on data reported in the literature or from actual chamber testing results.
Deposition Rate	Numeric	hr^{-1}	For possible future use; assumed zero value for now.

I.   Household/Industrial Cleaners (# of products in each section/chapter)

1.   Bathroom Cleaners (16)
2.   Dishwashing Detergents (57)
3.   Disinfectants (11)
4.   Floor Cleaners and Wax Strippers (41)
5.   General Purpose Cleaners (73)
6.   Laundry Products (143)
7.   Metal Cleaners (73)
8.   Oven Cleaners (10)
9.   Rinse Additives and Aids (96)
10.   Rug, Carpet and Upholstery Cleaners (40)
11.   Wall and Hard Surface Cleaners (49)
12.   Window and Glass Cleaners (25)
13.   Miscellaneous Cleaners (129)

II.   Automotive Cleaners

14.   Car and Truck Washes (51)
15.   Whitewall Tire Cleaners (8)
16.   Miscellaneous Cleaners (21)

All formulations in this book, except for a small number for which the data presented were unclear (e.g., total weight fractions of components did not total to a value of 1), were extracted and entered into the PRODUCT-CHEMICAL file.

4.2.2   Printing Ink and Overprint Varnish Formulations (Flick 1990)

This book is a collection of more than 300 formulations for printing inks, overprint varnishes, and related products. The formulation data were obtained by Flick from numerous companies and other organizations. The book states that the data represent selections made at no cost to, nor influence from, the makers or distributors of the materials. The book also states that only the most recent formulations are presented.

Each formulation in the book lists the following information, as available, in the manufacturer's own words:

- Description of end use;
- The amount of each raw material included in the formulation as presented by the supplier;
- Any description of the product; and
- The name of the manufacturer or organization that supplied the formulation.

The formulations in the book are divided into the following sections (parenthetical numbers indicate the number of products in each section):

4-3

      I.   Printing Inks (179)

     II.   Overprint Varnishes (73)

    III.   Miscellaneous (18)

All formulations in this book, except for a small number for which the data presented were unclear (e.g., total weight fractions of components did not total to a value of 1), were extracted and entered into the PRODUCT-CHEMICAL file.

4.2.3   Cosmetic and Toiletry Formulations (Flick 1989b)

More than 1,800 cosmetic and toiletry formulations are presented in this book. The formulation data were obtained by the author from numerous companies and other organizations. The author of the book states that the data represent selections made at no cost to, nor influence from, the makers or distributors of the materials. The author also states that only the most recent formulations are presented in the book.

Each formulation in the book lists the following information, as available, in the manufacturer's own words:

- Description of end use;
- The percent by weight of each component of the formulation;
- Suggested formulation procedure; and
- The name of the manufacturer or organization that supplied the formulation.

The formulations in the book are divided into the following 14 sections (parenthetical numbers indicate the number of products in those sections which were extracted for inclusion in SRD):

       I.   Antiperspirants and Deodorants
      II.   Baby Products
    III. Bath and Shower Products
    IV.   Beauty Aids
     V.   Creams
    VI.   Fragrances and Perfumes (12)
   VII. Hair Care Products (378)
 VIII. Insect Repellents
    IX.   Lotions
     X.   Shampoos
    XI.   Shaving Products
   XII. Soaps (88)
  XIII. Sun Care Products
  XIV. Miscellaneous

All formulations in section VI (Fragrances and Perfumes - 12 formulations), section VII (Hair Care Products - 378 formulations), and section XII (Soaps - 88 formulations) of this book, except for a small number for which the data presented were unclear (e.g., total weight fractions of components did not total to a value of 1), were extracted and entered into the PRODUCT-CHEMICAL file.

4.2.4   Water-Based Trade Paint Formulations (Flick 1988)

This book presents 562 water-based trade paint formulations. The formulation data were obtained by Flick from numerous companies and other organizations. The book states that the data represent selections made at no cost to, nor influence from, the makers or distributors of the materials. The book also states that only the most recent formulations are presented in the book.

Each formulation in the book lists the following information, as available, in the manufacturer's own words:

- The percent by weight or volume of each component of the formulation;
- Key properties of the product which may differentiate it from other similar products; and
- The name of the manufacturer or organization that supplied the formulation.

The formulations in the book are divided into the following sections and chapters (for those chapters from which formulation data were extracted, parenthetical numbers indicate the number of product formulations extracted):

   I.   Exterior Paints, Enamels and Coatings

   1.   Exterior paints (28)
   2.   Exterior tint base paints (10)
   3.   Exterior tinted paints
   4.   Exterior trim tint-base enamels
   5.   Exterior white paints
   6.   Exterior white and light tint paints
   7.   Exterior white semi-gloss paints and enamels
   8.   Roof coatings
   9.   Miscellaneous exterior paints

   II.   Interior Paints, Enamels and Coatings

   10.   Interior flat paints (85)
   11.   Interior flat tint bases (16)
   12.   Interior flat white paints (33)
   13.   Interior flat white and tint bases (17)
   14.   Interior semi-gloss paints and enamels (32)
   15.   Interior tint base semi-gloss paints and enamels (7)

16. Interior tinted paints (6)
17. Satin/sheen/eggshell paints and enamels (11)
18. Stipple and texture paints (8)

III. Exterior and/or Interior Paints, Enamels, Primers and Stains

19. Colored enamels (15)
20. Gloss enamels and paints (42)
21. Intumescent fire retardant paints (4)
22. Primers and primer/sealers (27)
23. Semi-gloss paints and enamels (20)
24. Stains (41)
25. White enamels (16)
26. Miscellaneous paints and enamels (15)

All extracted formulations were entered into the PRODUCT-CHEMICAL file.

4.2.5   Adhesive and Sealant Compound Formulations (Flick 1984)

This book presents a collection of 444 adhesive and sealant formulations. The formulation data were obtained by Flick from numerous companies and other organizations. The book states that the data consist of selections of manufacturers' formulations made at no cost to, nor influence from, the makers or distributors of the materials. The book also states that only the most recent formulations are presented in the book. There are no solvent-based formulations presented in the book, although a small amount of solvent is present in some formulations as an additive to improve product performance.

Each formulation in the book lists the following information, as available, in the manufacturer's own words:

- Description of end use and, if applicable, typical dilution(s) for various applications;
- The percent by weight or volume of each component of the formulation;
- Key properties of the product which may differentiate it from other similar products; and,
- The name of the manufacturer or organization that supplied the formulation.

The formulations in the book are divided into various sections corresponding primarily to adhesive end use. Listed below are the various sections of the book and those chapters from which formulation data were extracted for inclusion in the SRD (parenthetical numbers indicate the number of products in each chapter):

I. Water-Based Industrial Type Adhesives

1. Construction Adhesives (3)

3. Flocking Adhesives (11)
5. General Purpose Adhesives (13)
6. Industrial Adhesives (15)

III. Water-Based Coatings

8. Industrial Coatings (6)

VI. Epoxy Adhesives, Castings and Coatings

14. General Purpose (111)

VIII. Miscellaneous Compounds

20. Caulking (9)
24. Sealants (23)

All formulations in these chapters, except for a small number for which the data presented were unclear (e.g., total weight fractions of components did not total to a value of 1), were extracted and entered into the PRODUCT-CHEMICAL file.

4.2.6 "Canadian" Caulks and Sealants (Eyre and Jennings 1986)

In 1986, the Home Energy Program of Energy, Mines and Resources Canada commissioned a study to identify the substances in caulk and sealant products that present the greatest hazard when these products are used in residential interiors. Although the objective of the first part of the study, to obtain formulations of the entire range of caulk and sealant products from four manufacturers, could not be met for various reasons, Eyre and Jennings (1986) did obtain formulation data from various other industry sources and published material.

The formulations in the report are divided into the following sections and chapters (for those chapters from which formulation data were extracted, parenthetical numbers indicate the number of product formulations extracted):

I. Mastic Sealants

4. Oleoresinous products (2)
5. Polysulfide products, one-part gun-grade (1)
6. Polysulfide products, two-part gun-grade (2)
7. Butyl rubber products (4)
8. Acrylic water-based emulsion products (2)
9. Acrylic solvent-based, one-part, gun-grade products (2)
10. Polyvinyl acetate-based products (1)

11. Vinyl acrylic emulsion products (1)
12. Asphaltic one-part products, gunnable and pourable (2)
13. Neoprene products, two-part gun-grade (1)
14. Hypalon, one-part gun-grade (1)
15. Polyurethane one-part products (1)
16. Polyurethane two-part products (1)
17. Silicone products
18. Polybutene caulks
19. Styrene butadiene rubber (SBR) products (1)
20. Nitrile products

II. Glazing Compounds/Putties

21. Professional glazing compound (1)
22. Putties (2)

III. Aerated Sealants

23. Two-part expanded polyurethane foam (1)

IV. Rope-Type Sealants

24. Rubber or polymer-based rope caulks (1)
25. Fibre-based rope

V. Specialty Products

26. Intumescent sealants

No quantitative formulation data were reported in Chapters 17, 18, 20, 25, and 26. All extracted formulations were entered into the PRODUCT-CHEMICAL file.

4.2.7 IACS System (USEPA 1992)

The IACS System is a database of product formulation and emission rate data compiled by EPA's Office of Pollution Prevention and Toxics. IACS was a precursor to the SRD and a description of the data sources that came from IACS is provided below. All information from the May 1992 version of the database was extracted and entered into the PRODUCT-CHEMICAL file.

Bayer 1990   Bayer, Charlene. 1990. Large environmental chamber techniques were used to determine if VOC and formaldehyde emissions from modular office partitions and particle boards before, during and after "building bakeout".

CCMS 1989   Analytical tests carried out among several European laboratories on emissions from a single carpet-coated particle board. Emission rates and compounds not quantified are given.

USEPA 1988   GC/MS analysis of headspace air above heated building materials and consumer products for volatile organic chemicals. Materials which emitted target chemicals found in monitoring study were selected for an emission rate study using an environmental chamber.

HEP 1986   Eyre, D. and D. Jennings. 1986. The identification of toxic materials in caulks and sealants, and the selection of short listed substances for outgas tests. Report submitted to Home Energy Program; Energy, Mines and Resources Canada. SRC Publication No. R-823-6-E-86. Identification of substances in caulk and sealant products based primarily on the listing of ingredients provided in Frost & Sullivan Study of the USA caulk & sealant market. One manufacturer supplied information as well. Additional information was gathered from other various literature.

JAPCA 1988   GC/MS analysis of headspace air above product in a 1-liter Teflon-lined container.

MRI 1989   This study reviews the mass spectra data for 1,159 household products collected by MRI during 1987. During the early study, samples of household products were tested directly by purge and trap gas chromatography/mass spectrometry (GC/MS) and the full mass spectra were archived into an analytical database. This database was reviewed during this study for 25 analytes and may be used in the future to estimated other analytes assuming the appropriate response factors can be generated.

RTI 1990   Emissions of organic vapors from 31 consumer products were characterized by headspace purging followed by GC/MS analysis; 127 chemicals were identified.

USEPA 1990   Evaluating organic emissions from building materials and products (Selected results from technical support projects). U.S. EPA Indoor Air Branch AEERL, RTP, NC. IAB Report 90-2, January 1990. Contains reports from five studies conducted to evaluate the organic emissions from consumer product and building material sources. Small chamber tests using Tenax collection media and GC/MS analysis.

Versar 1990   Memo dated August 3, 1990 to Pat Kennedy from Carl D'Ruiz, Subject: Results of Shelf Survey of Consumer Products that may contain hazardous or toxic ingredients. Versar purchased various consumer products from K-mart and Hechinger and reports listed ingredients, product name and manufacturers.

4.2.8 Formulations of Aerosol Products (Radian 1989)

This report discusses the experience of the U.S. aerosol products industry in converting from chlorofluorocarbon propellants to alternative aerosol formulations. Detailed examples of non-CFC formulations are provided in the report for 28 categories of aerosol products. All extracted formulations were entered into the PRODUCT-CHEMICAL file. The IACS system discussed in Section 4.2.7 contained some of the formulations reported in Radian (1989) and referenced Radian (1989). Those formulations were removed from the IACS input to the PRODUCT-CHEMICAL file to avoid duplicate records.

4.2.9 Washington State Indoor Air Quality Study (AQS 1992; AQS 1993a; AQS 1993b)

In 1989, the State of Washington responded to an incident of "sick building syndrome" in a state office building by instituting an "Indoor Air Quality" program applicable to new office building construction. As part of the program, the state specified pollutant-emission-limit parameters for furniture and building materials used in the construction and furnishings of these buildings. The standards addressed several categories of pollutants including (1) formaldehyde, (2) total VOCs, and (3) particulates. Vendors who bid for state contracts to provide construction materials, furniture, and furnishings for these buildings were required to certify, through product testing, that their offerings complied with the specified emission standards.

As a cooperative project involving the U.S. Environmental Protection Agency and the State of Washington, a study was undertaken aimed at evaluating the effectiveness of Washington's program in meeting its goal of ensuring high indoor air quality in office buildings. The purpose of the study was to evaluate the impact of using low pollutant-emitting source materials and institute special building-preparation techniques on indoor air quality.

As part of this project, all industry-submitted and other product emissions data available from the State of Washington were obtained. Also, data were generated by Air Quality Sciences, Inc. (AQS) on products obtained by AQS from prospective product bidders and on products obtained from the NRB during its construction. These data were provided to EPA under separate projects under EPA Contract No. 68-D3-0013. The data include those products actually used in the building with additional data on three workstation units. Also, emissions data were obtained for 15 other products not used in the NRB but used in another Washington State office building. The data

include information on 95 products ranging from modular furniture to paint and fireproofing. Of the 95 products, 67 have emission testing data and the remaining 28 have only MSDS sheets or letters of compliance sheets indicating that their products met IAQ requirements without supporting test data. Limited product formulation information was also available for 10 of the products (3 sealants/caulks, 2 plasters, 1 adhesive, and 4 paints/coatings). The duration of the emission rate testing ranged from days to weeks depending on the product being tested.

For purposes of the SRD, the maximum emission rate reported for a given material (μg/h per m^2 surface area) or furnishing (μg/h per unit) tested under this project was assumed to be its initial emission rate when placed into an indoor environment. The limited set of products tested under the project were not included in the SRD because the amount of product applied in the test was not known and, hence, the initial emission rate could not be normalized to the quantity used.

4.2.10 EPA/AEERL Catalog of Materials as Potential Sources of Indoor Air Emissions (Radian 1993)

This report (two volumes), prepared by Radian Corporation for EPA's Air and Energy Engineering Research Laboratory, is intended to be used as a tool by researchers to help organize the study of 12 categories of materials as potential sources of indoor air pollution. In addition to providing sales and usage volume data, and qualitative data on product composition, this report has compiled VOC emission data from several sources. In addition to providing formaldehyde emission data for the wood product category, the report had emission rate data suitable for inclusion into SRD for 19 products (5 insulation products, 2 wall coverings, 3 resilient floor coverings, 7 carpets, 1 wood product, and 1 fabricated rubber product).

4.2.11 Office of Air Quality Planning and Standards Consumer and Commercial Products Survey (WESTAT 1987a, 1987b, 1987c)

Under authority of Section 183(e) of the Clean Air Act, EPA's Office of Air Quality Planning and Standards (OAQPS) conducted a survey of consumer products manufactured in 1990 that contain volatile organic compounds (VOCs). Information provided by the companies included product name, product form, volatile chemical, and chemical amount (percentage) in the product.

4.2.12 Design for the Environment (DfE) Paint Project (GEOMET, 2000)

The U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) initiated a Design for the Environment (DfE) Project to develop a wall paint exposure assessment model for interior latex and alkyd paints. The purpose of the model is to allow industry product developers and health and safety officials to more easily and accurately identify chemicals in paint formulations that pose potential exposure problems. Although fairly extensive testing had was performed previously by EPA's Air Pollution and Prevention Control Division (APPCD) to characterize emissions through chamber tests, additional data were deemed necessary to cover a broader sample of paints and associated chemicals.

Methods for and results of the data collection effort been documented in a recent report (ARCADIS 1998). As part of a related effort to develop a Wall Paint Exposure Model (WPEM), GEOMET (2000) fit the chamber concentration data for chemicals that were measured to empirical emission models, assuming a first-order decay rate for the chemical emissions. To put the emission rates in a format suitable for use in the SRD, the rates were normalized to the amount of paint applied.

4.3   CHEMICAL File Overview

The CHEMICAL File contains chemical-specific physical/chemical property data and hazard data for those chemicals listed in the PRODUCT-CHEMICAL File (i.e., chemicals detected in emissions or reported to be formulation components). Table 4-2 presents detailed information on the data elements of the file. Appendix C contains all 1,377 records in the CHEMICAL file.

Chemical Abstract Service (CAS) numbers were obtained from standard reference sources as well as computerized searches of CAS On-Line using the chemical or mixture names reported in the PRODUCT-CHEMICAL file data sources. CAS numbers could not be obtained for some of the reported chemical or mixture names, many of which are trade names. Chemicals/mixtures for which CAS numbers could not be obtained are not included in the current version of the SRD CHEMICAL File.

For chemicals with CAS numbers, molecular weight and vapor pressure values were obtained from both standard reference sources (i.e., ChemFinder, 2000) and computerized searches of the Envirofate Data Base maintained by the Syracuse Research Corporation (SRC).

Human health hazard ratings developed by the Health and Environmental Review Division (HERD) of OPPT are the basis of the hazard scores in the CHEMICAL file. A rating of 100 indicates a high hazard,

0.1 a medium hazard, and 0.001 a low hazard. For chemicals without a HERD-assigned hazard score, a default value of 0.00099 was used. This value is close to that for a low hazard (0.001), but distinguishes chemicals for which a hazard rating has not yet been assigned. The scoring system is described in Section 4.4.

The fraction volatilized was calculated for each chemical found in products whose use involves dissolution in water (i.e., case 2 products). The fraction volatilized is the fraction of the mass of the chemical in the product that is expected to volatilize into air during product use. This quantity was estimated using physical-chemical properties such as the Henry's Law coefficient, as well as information on the characteristics of typical use. As such, the fraction volatilized is use specific, therefore, it was calculated for the following six Case 2 use scenarios:

     (2)   laundry detergents,
     (3)   toilet bowl cleaners,
     (4)   dish wash liquid,
     (5)   hair shampoo and body lotion,
     (6)   liquid hand soap, and
     (7)   detergents and powders for dish washers.

The fractions are zero for non-applicable products. See Section 8.2.2 and Appendix H for more detail about how these values were calculated.

Table 4-2. Contents of the CHEMICAL File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
CAS Number	Character	--	Chemical-specific Chemical Abstract Service number.
Chemical Name	Character	--	Name of the chemical as reported in the data source or a synonym of the reported name to maintain name consistency within SRD.
Molecular Weight	Numeric	Grams/mole	Value reported in SRC's Envirofate database or standard references.
Molecular Weight Reference	Character	--	Source of information on molecular weight.
Vapor Pressure	Numeric	Torr	At approximately 23 to 25°C. Value reported in SRC's Envirofate database or standard references.
Vapor Pressure Reference	Character	--	Source of information on vapor pressure.
Reactivity Rate/ Sink Effect	Numeric	hr^{-1}	For possible future use; assumed zero value for now.
Acute Hazard Rating	Numeric	--	Supplied by EPA.* Chemical-specific value of 0.001, 0.1, or 100.
Chronic Hazard Rating	Numeric	--	Supplied by EPA.* Chemical specific value of 0.001, 0.1, or 100.
Combined Overall Hazard Rating	Numeric	--	Supplied by EPA.* Chemical specific value of 0.001, 0.10, or 100.0.
Fraction Volatilized	Numeric	--	One value for each of 6 types of usages for products dissolved in water.

*   If EPA has supplied no value, then a default value of 0.00099 was used; a value of 0 was assigned to water (CAS number 7732185).

4.4   SRD Human Health Effects Scoring Methodology

The Source Ranking Database (SRD) uses the human health portion of the Chemical Use Cluster Scoring Methodology (UCSS) (US EPA 1993) to systematically evaluate and then place chemicals into one of three potential human health hazard categories (i.e., "high", "medium", and "low"). The hazard of a chemical is based on its inherent toxicological properties. In the UCSS, the criteria for the category thresholds for levels of high (i.e., 100), medium (i.e., 0.1), and low (i.e., 0.001) concern were set by professional toxicologists after a review of the data distributions of reference doses (RfD), reference concentrations (RfC), and cancer potencies (q_1*). The specific cutoff points are based on these distributions and an approximate distribution of 1:2:1 for the chemicals in the high, medium, and low categories, respectively.

The potential human health hazard category to which a chemical is assigned is determined from several sources of chemical toxicity information. These sources are arranged into a hierarchy of data quality (quality being based on the degree of peer review to which a study or specific value has been subjected). If human health data elements of high quality are available, the highest of the scores is taken as the chemical's overall health hazard score. If data of high quality are lacking, medium quality data elements are used and the highest of these available scores is taken as the chemical's overall health hazard score. Comparably, if data of medium quality are lacking, low quality data are used. Because the health hazard score is based on the data available at the time of evaluation, it is possible that the score will change as new data of higher quality becomes available.

Each chemical is scored separately for both non-carcinogenic and carcinogenic health effects. The higher of these two scores is taken as the chemical's final human health hazard score. Values of the human health data elements used in the assignment of categories are shown in Tables 4-3 and 4-4. These human health data elements and the method used to assign categories are described below (US EPA 1993).

4.4.1.   Human Health Data Elements of High Quality - Noncarcinogens

Reference Dose and Reference Concentration -- The chronic reference dose (RfD) is an estimate of the highest daily exposure that can be incurred by individuals in the general population (including highly susceptible subgroups) without significant risk of deleterious effects during a lifetime. The chronic reference concentration (RfC) is a comparable estimate of the concentration of a chemical in air. Both values are published by EPA in the Health Effects Assessment Summary

Table 4-3. Human Health Hazard Ranking - Noncarcinogens (from U.S. EPA, 1993)

Data Element	Data Quality	Ranking		
		High (3)	Medium (2)	Low (1)
Reference Dose (RfD)	High	<0.001 mg/kg/day	0.001 - 0.1 mg/kg/day	>0.1 mg/kg/day
Reference Concentration (RfC)	High	<0.002 mg/m^3	0.002 - 0.2 mg/m^3	>0.2 mg/m^3
Reportable Quantity (RQ)	High	1, 10 lb	100, 1,000 lb	5,000 lb
Threshold Planning Quantity (TPQ)	High	1, 10 lb	100, 500 lb	1,000, 10,000 lb
Human Health Water Quality Criteria (HWQC)	High	<1 mg/l	1 - 10 mg/l	>10 mg/l
Chronic NOAEL	Medium	<0.1 mg/kg/day	0.1 - 10 mg/kg/day	>10 mg/kg/day
Chronic LOAEL	Medium	<1 mg/kg/day	1 - 100 mg/kg/day	>100 mg/kg/day
Subchronic NOAEL	Medium	<1 mg/kg/day	1 - 100 mg/kg/day	>100 mg/kg/day
Subchronic LOAEL	Medium	<10 mg/kg/day	10 - 1,000 mg/kg/day	>1,000 mg/kg/day
Human Health Structure Activity Team Rank	Low	High	Medium-high, medium	Low-medium, low
Chemical Category Human Toxicity Estimate	Low	3	2	1
TSCA §8(e) Submission	Low/Consistency	3	2	1

Table 4-4. Human Health Hazard Ranking - Carcinogens (from U.S. EPA, 1993)

Data Element	Data Quality	Ranking		
		High (3)	Medium (2)	Low (1)
If WOE = A or B then				
q_1 (Cancer Potency)	High	>1 mg/kg/day	0.01 - 1 mg/kg/day	<0.01 mg/kg/day
RQ Potency Factors	High	>10 mg/kg/day	0.2 - 10 mg/kg/day	<0.2 mg/kg/day
Structure Activity Team Rank	Low	High	Medium, medium-	Low, low-medium
Chemical Category Human Toxicity	Low	3	high	1
Estimate	Low/Consistency	3	2	1
TSCA §8(e) Submission			2	
If WOE = C then				
q_1 (Cancer Potency)	High	>10mg/kg/day	0.1 - 10mg/kg/day	<0.1 mg/kg/day
RQ Potency Factors	High	>8 mg/kg/day	1 - 80 mg/kg/day	<1 mg/kg/day
Structure Activity Team Rank	Low	High	Medium, medium-	Low, low-medium
Chemical Category Human Toxicity	Low	3	high	1
Estimate	Low/Consistency	3	2	1
TSCA §8(e) Submission			2	
If WOE = Unclassified				
Structure Activity Team Rank	Low	High	Medium, medium-	Low, low-medium
Chemical Category Human Toxicity	Low	3	high	1
Estimate	Low/Consistency	3	2	1
TSCA §8(e) Submission			2	

Tables (HEAST) or in the Integrated Risk Information System (IRIS). The limits of the UCSS category ranks were established using the set of chemicals with RfDs and RfCs reported in IRIS and creating classifications of low, medium, and high based on an approximate distribution of 1:2:1 for these chemicals.

Reportable Quantity -- The Reportable Quantity (RQ) of a chemical is that amount of a hazardous substance necessary to trigger reporting under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) in the event of a chemical release. A RQ value is assigned by EPA to a chemical substance based on the substance's intrinsic chemical, physical and toxicological properties. The UCSS category ranks were established based on a comparison of chemicals in IRIS with RfDs and RfCs. Limits were selected to distribute the chemicals in the same levels as if they had been using RfDs.

Threshold Planning Quantity -- The Threshold Planning Quantity (TPQ) is the amount of an extremely hazardous substance present at a facility above which the facility's owner/operator must give emergency planning notification to the State Emergency Response Commission (SERC) and Local Emergency Planning Committee (LEPC) under the Superfund Amendments and Reauthorization Act, Section 302. The quantity is primarily based on the chemical's acute toxicity, but also accounts for the chemical's tendency to become airborne. UCSS category limits were based on the values in the Toxic Chemical Release Inventory Risk Screening Guide.

Human Health Water Quality Criteria -- EPA's human health ambient water quality criteria (HWQC) are estimates of the ambient concentrations of chemicals in surface water that will not cause adverse effects to human health. For chemicals with multiple values, the lowest (most conservative) was chosen. The UCSS category limits are those used for water quality criteria in the Toxic Chemical Release Inventory Risk Screening Guide for water quality criteria.

4.4.2. Human Health Data Elements of High Quality - Carcinogens

Weight-of-Evidence -- Each chemical is first evaluated to determine the weight-of-evidence group to which it has been assigned by EPA. The EPA weight-of-evidence groups that are used in the UCSS are:

- Group A -   known human carcinogen -- evidence in humans is sufficient;

- Group B -   probable human carcinogen -- evidence in humans is inadequate or there is no evidence in humans, but animal evidence is sufficient;

- Group C -   possible human carcinogen -- inadequate or no evidence in humans and animal evidence is limited; and
- Group D -   not classifiable as to human carcinogenicity.

Once the weight-of-evidence groups have been established, the chemical is categorized using the data elements below (slope factor and RQ potency).

Slope Factor (q_1*) -- For cancer risk assessments, EPA has developed standard methods of predicting incremental lifetime risk of cancer resulting from the exposure to a chemical. Typically, EPA uses a linearized multistage model of carcinogenesis to quantitatively model the dose-response function of the carcinogen. The upper bound linear term of this model is the q_1*. The higher the value of the q_1*, the greater the potency of the chemical. These values are documented in HEAST and IRIS. The UCSS category limits were established by comparing chemicals with slope factors reported in IRIS with a database of 80 to 90 chemicals and analogous compounds that was developed for EPA's TSCA New Chemicals Program. The combined set was ordered by potency and assigned to high, medium, and low groups using an approximate ratio of 1:2:1.

RQ Potency -- The RQ potency factor is based on a multi-stage dose response model using quantitative evidence from animals studies to develop an estimated dose for a 10 percent lifetime cancer risk (ED_{10}) for animals. The human potency factor is derived by applying a multiplier based on the relative body weights of the test species and humans. RQ potency factors are given in EPA's background document for CERCLA Section 102 rulemaking. The UCSS category limits were set by comparing a set of IRIS chemicals having information for both q_1* and RQ potency factors, then selecting RQ potency values to achieve the same distribution of high, medium, and low values as that for the q_1* category limits.

4.4.3.   Human Health Data Elements of Medium Quality - Noncarcinogens

Effects Levels -- Four data elements of medium quality relating to effects levels are used. They are:

- Chronic No Observed Adverse Effects Level (Chronic NOAEL) - the highest experimental dose at which there is no significant increase in a toxicologically important effect in an organism after exposure to a chemical for a major portion of its lifetime;

- Chronic Lowest Observed Adverse Effects Level (Chronic LOAEL) - the lowest experimental dose at which there is a significant increase in a toxicologically important effect in an organism after exposure to a chemical for a major portion of its lifetime;
- Subchronic No Observed Adverse Effects Level (Subchronic NOAEL) - the highest experimental dose at which there is no significant increase in a toxicologically important effect in an organism after exposure to a chemical for about 10 percent of its lifetime; and

- Subchronic Lowest Observed Adverse Effects Level (Subchronic LOAEL) - the lowest experimental dose at which there is a significant increase in a toxicologically important effect in an organism after exposure to a chemical for about 10 percent of its lifetime.

The effects levels data were collected from HEAST or IRIS. The UCSS category limits were chosen using the limits chosen for the reference dose (RfD) and 'back-calculating' to an effects level using an average uncertainty factor. The average uncertainty factors are 100 for a chronic NOAEL, 1,000 for both the chronic LOAEL and subchronic NOAEL, and 10,000 for the subchronic LOAEL.

4.4.4.   Human Health Data Elements of Low Quality

Human Health Structure Activity Team Rank -- EPA/OPPT's Structure Activity Team (SAT) has evaluated a number of chemicals for both non-carcinogenic and carcinogenic effects based on available test data, the structure of the compound, and toxicological data available for chemical analogs. The outcome of this deliberation is a human health hazard rating of the chemical on a five step scale of low, medium-low, medium, medium-high, and high. These ratings were converted into a three step category scale of high (SAT high rank), medium (SAT high-medium and medium ranks), and low (SAT low-medium and low ranks).

Rank Based on Chemical Category -- Chemicals are first divided into two groups based on the relative complexity of the molecular structures using professional judgement. 'Complicated' chemicals (e.g., those with more than two or three functional groups, exotic substitutions, or are obviously biologically active) are set aside for evaluation by an expert panel of chemists and toxicologists.

'Uncomplicated' chemicals are evaluated using the following steps:

- All functional groups of the chemical are identified based on its molecular structure;

- Each functional group is assigned a score based on the health rating of the chemical category/subcategory, as documented in the Use Cluster Health Hazard Ratings Database (US EPA 1994); and

- The chemical is assigned the rating of the highest rated functional group.

TSCA Section 8(e) Submission -- Under TSCA Section 8(e), companies must report to EPA information that "reasonably supports" a conclusion of substantial risk for any chemical substance or mixture that the company manufactures, processes, or distributes in commerce. EPA reviews this information as part of an initial hazard screening review and assigns a high, medium, or low level of concern. These values are used as categories of low quality data in the UCSS.

5. PRODUCT-ENVIRONMENT AND MATERIAL-ENVIRONMENT FILES

5.1 Sources of Data

During the period of performance of this project, efforts were directed at obtaining and reviewing sources of information on:

- Product/material use frequency;
- Product/material use duration; and
- Product/material use quantities or material loadings.

Six readily available data sources were obtained for review. All six sources reviewed deal solely with consumer usage almost entirely in the residential setting. The six sources are as follows:

Reference No.	Reference	Title
001	WESTAT, Inc. (1987a)	Household solvent products survey
002	WESTAT, Inc. (1987c)	Household cleaning products survey
003	WESTAT, Inc. (1987b)	Household survey of interior painters
004	RTI (1992)	National home and garden pesticide use survey
005	CFTA (1983)	Survey of cosmetic products usage
006	SMRB (1992)	Simmons 1992 study of markets and media

The following on-line data bases were also searched for product usage information: *NTIS*, *Thomas New Industrial Products*, *Magazine ASAP*, *Pollution Abstracts*, and *Enviroline.* Abstracts were retrieved and evaluated for 147 citations. Several potentially useful documents were ordered but none contained the specific product usage data required for SRD.

In addition, numerous trade associations, industry groups, trade unions and other organizations and individuals were contacted for relevant published or citable information concerning product and material usage.

5.2 Available Compiled Data

Appendix D presents a listing of all contacts made with trade associations, unions, etc., and the results of all contacts. Most information within this data file was determined using professional judgement, since attempts to obtain this information from various trade associations was futile.

Table 5-1 describes the data elements in the PRODUCT-ENVIRONMENT file. Appendix E presents a compilation of the product usage data obtained to date from the six sources listed above in Section 5.1. The data were compiled into PRODUCT-ENVIRONMENT files, one for each of the nine environmental settings (see Section 6). The files contain, for each 9-digit SRD Product ID, the available or estimated frequency data (i.e., mean, 50th percentile and 90th percentile values), the available or estimated product use event duration data (i.e., mean, 50th percentile and 90th percentile values), and the available or estimated data (i.e., mean, 50th percentile and 90th percentile values) on amount of product used annually or per event.

Only Westat (1987a) provided frequency <u>and</u> duration <u>and</u> amount used information for products. However, many of the references provided frequency and amount used information. Also, often more than one source provided information on the same product or for multiple activities using that product. The current configuration of SRD assumes that only one set of data will be provided for each 9-digit SRD code. Therefore, professional judgement was used to select the most appropriate values to use in the PRODUCT-ENVIRONMENT file. In addition, professional judgment was used to estimate frequency, duration, and amount used values for all relevant Product IDs for which published product usage data were not available. A panel of three members was used to reach consensus or majority opinion on estimated values.

One of the data sources, the Simmons Market and Media Study (SMRB 1992), contains data on frequency of use reported as the percent of respondents within four or more ranges of use. Therefore, to derive estimates of the 50th and 90th percentiles, linear interpolation of the reported data was performed. Appendix F presents details on the methodology employed to perform this interpolation.

Table 5-2 describes the data elements in the MATERIAL-ENVIRONMENT file. As discussed in Sections 4.2.9 and 4.2.10, chemical-specific emission rate data, as opposed to non-specific data such as VOC emission rates, were available for only a relatively small number of materials. Table 5-3 lists the materials and furnishings in the MATERIAL-ENVIRONMENT file together with their associated loading units. Most of these tested materials (i.e., carpet, ceiling tiles, subflooring, vinyl flooring) can be found in any of the nine environmental settings, with the exception of vehicles.

Table 5-1. Contents of the PRODUCT-ENVIRONMENT File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
Environment ID	Character	--	Environment-specific 2-digit code.
Product ID	Character	--	SIC product code.
Quantity Used (avg.)	Numeric	Grams/event	Product-specific value; used median value if average value was not available.
Quantity Used (upper)	Numeric	Grams/event	Product-specific value.
Quantity Used Reference	Character	--	Source of information on quantity used. PJ indicates "professional judgment."
Duration of Use (avg.)	Numeric	Hours/event	Product-specific value; used median value if average value was not available.
Duration of Use (upper)	Numeric	Hours/event	Product-specific value.
Duration of Use Reference	Character	--	Source of information on duration of use. PJ indicates "professional judgment."
Frequency of Use (avg.)	Numeric	Events/yr	Product-specific value; used median value if average value was not available.
Frequency of Use (upper)	Numeric	Events/yr	Product-specific value.
Frequency of Use Reference	Character	--	Source of information on frequency of use. PJ indicates "professional judgment."
Fraction of Buildings (avg.)	Numeric	--	Fraction of buildings in the specific environment in which the product is used.

Table 5-2. Contents of the MATERIAL-ENVIRONMENT File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
Environment ID	Character	--	Environment-specific 2-digit code.
Product ID	Character	--	SIC product code.
Amount Present (avg.)	Numeric	*	Agrees with emission-rate units in Product-Chemical File. Amount present (average) describes how values were selected from chamber studies. Eg. The 1st 8 hr TWA used for average.
Amount Present (upper)	Numeric	*	Agrees with emission-rate units in Product-Chemical File. . Amount present (average) describes how values were selected from chamber studies. Eg. The peak initial concentration was used for upper values.
Amount Present Units	Character	*	Agrees with emission-rate units in Product-Chemical File.
Duration Since Installation (avg.)	Numeric	Hours	Estimate of the typical age of a material in a specific environment. Estimated by dividing the service life of the material by a factor of 2.
Duration Since Installation (peak)	Numeric	Hours	Estimate of the age of a new material when individuals are first exposed to it in a specific environment setting.
Fraction of Buildings (avg.)	Numeric	--	Fraction of buildings in the specific environment that contain the existing (i.e., aged) material.
Fraction of Buildings (peak)	Numeric	--	Fraction of buildings in the specific environment into which the new (i.e., unaged) material is introduced every year.

Table 5-3. Loading Units for Materials and Furnishings
in the MATERIAL-ENVIRONMENT File

PRODUCT ID	TYPE OF MATERIAL/FURNISHING	LOADING UNITS
227320100	Carpet or carpet tile	m^2/m^3
242120000	Softwood lumber	m^2/m^3
243144500	Particleboard core door w/veneer	m^2/m^3
243520000	Hardwood plywood paneling	m^2/m^3
243660000	Urea formaldehyde softwood plywood	m^2/m^3
243909800	Self-leveling floor or sub-floor	m^2/m^3
249310300	Floor underlayment	m^2/m^3
249310500	Manufactured home decking	m^2/m^3
249312000	Particleboard	m^2/m^3
249331400	Medium density fiberboard	m^2/m^3
249341200	Hardboard (basic-standard)	m^2/m^3
249341400	Hardboard (basic-tempered)	m^2/m^3
252100000	Furniture composite (built-in furniture)	unit/m^3
252101100	Comfort secretarial/task chair	unit/m^3
252107300	Complete workstation	unit/m^3
252211400	Chair (neutral posture chair)	unit/m^3
252211500	Chair (comfort lowback & manager's)	unit/m^3
259131100	Levelor window shade (polyester & vinyl)	m^2/m^3
267910000	Vinyl wallcovering	m^2/m^3
306942600	Rubber floor tile	m^2/m^3
308631000	Polystyrene rigid foam insulation	m^2/m^3
329611100	Monokote fireproofing	m^2/m^3
329613000	Glass wool insulation	m^2/m^3
329616100	Ceiling tile	m^2/m^3
399601100	Vinyl flooring	m^2/m^3
399602100	Vinyl flooring (tile)	m^2/m^3
399602600	Vinyl composition tile	m^2/m^3

Table 5-4 lists the average loading rates for each of the 28 materials or furnishings previously listed in Table 5-3 (these loading rates carry the loading units listed in Table 5-3). Most of the these loading rates were developed by considering a 10 foot by 10 foot room (i.e., 100 square feet of floor area). Differences across environments in loading rates for many of the materials reflect differences in assumed ceiling heights, as described in Section 6. For example, residences have an assumed ceiling height of eight feet (2.44 meters). The floor area of a 10 foot by 10 foot room is 9.29 m^2, and the volume with an 8-foot ceiling height is 22.64 m^3. Thus, the loading rate (if fully carpeted) is 9.29 m^2/22.64 m^3, or 0.41 m^2/m^3. By comparison, a school with an assumed ceiling height of 10 feet (3.05 meters) has a volume of 28.3 m^3, and a loading rate of 0.33 m^2/m^3 if fully carpeted. The average loading rates in Table 5-4 are half the maximum loading rate, or 0.205 m^2/m^3 for residences and 0.165 m^2/m^3 for schools. The MATERIAL-ENVIRONMENT file also contains upper values for the loading rate (see Table 5-2), which are twice the values given in Table 5-4.

For most of the materials used for floors, walls or ceilings, the differences across environments are largely due to differences in ceiling heights. Certain other items such as complete workstations or secretarial/task chairs were assumed to have higher loadings in office buildings than in any of the other environments. Eating and drinking establishments were assigned the highest loading rate for built-in furniture. For certain wood products such as softwood lumber, particleboard core doors and hardwood plywood paneling, arbitrarily low loading rates were uniformly assigned to all environments except vehicles.

Table 5-5 lists the fraction of buildings/vehicles for each type of environment in which the materials or furnishings are assumed to be used. Particleboard, for example, was assumed to be routinely present in all environments except vehicles. Items such as workstations and secretarial/task chairs were assumed to be routinely present in schools, hospitals, nursing homes and office buildings. Glass wool and rigid foam insulation were collectively assumed to be present in 100 percent of all environments except vehicles, with glass wool insulation having a much higher fraction (0.9). Carpeting was assumed to be most prevalent in residences, office buildings and hotels/motels. Certain materials were assumed to be uniquely associated with single environments, such as manufactured home decking with residences and self-leveling floors with office buildings.

Table 5-4. Average Material/Furnishing Loading Rates for Each Environment

PRODUCT ID	ENVIRONMENT								
	RESIDENCE	SCHOOL	HOSPITAL	NURSING HOME	OFFICE	PUBLIC ACCESS	HOTEL/ MOTEL	EAT/ DRINK	VEHICLE
227320100	0.205	0.165	0.165	0.165	0.165	0.135	0.165	0.135	1.000
242120000	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.000
243144500	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.000
243520000	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.000
243660000	0.205	0.165	0.165	0.165	0.165	0.135	0.165	0.135	0.000
243900800	0.000	0.000	0.000	0.000	0.165	0.000	0.000	0.000	0.000
249310300	0.205	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
249310500	0.205	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
249312000	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.000
249331400	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.000
249341200	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.000
249341400	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.000
252100000	0.000	0.000	0.018	0.018	0.018	0.000	0.000	1.000	0.000
252101100	0.005	0.010	0.010	0.010	0.035	0.010	0.010	0.000	0.000
252107300	0.000	0.005	0.005	0.005	0.018	0.000	1.000	0.000	0.000
252211400	0.000	0.010	0.010	0.010	0.035	0.000	0.000	0.000	0.000
252211500	0.000	0.010	0.010	0.010	0.035	0.000	0.000	0.000	0.000
259131100	0.044	0.018	0.018	0.018	0.018	0.015	0.018	0.015	0.000
267910000	0.650	0.650	0.650	0.650	0.650	0.150	0.650	0.150	0.000
306942600	0.005	0.020	0.020	0.020	0.020	0.020	0.020	0.020	0.000
308631000	0.210	0.055	0.060	0.070	0.070	0.035	0.070	0.100	0.000
329611100	0.015	0.015	0.015	0.015	0.015	0.015	0.015	0.015	0.000
329613000	0.210	0.055	0.060	0.070	0.070	0.035	0.070	0.100	0.000
329616100	0.100	0.165	0.165	0.165	0.165	0.135	0.165	0.135	0.000
399601100	0.205	0.165	0.165	0.165	0.165	0.135	0.165	0.135	0.000
399602100	0.205	0.165	0.165	0.165	0.165	0.135	0.165	0.135	0.000
399602600	0.205	0.165	0.165	0.165	0.165	0.135	0.165	0.135	0.000

Table 5-5. Fraction of Buildings/Vehicles in Which Materials/Furnishings are Used

PRODUCT ID	ENVIRONMENT								
	RESIDENCE	SCHOOL	HOSPITAL	NURSING HOME	OFFICE	PUBLIC ACCESS	HOTEL/ MOTEL	EAT/ DRINK	VEHICLE
227320100	0.90	0.50	0.20	0.20	0.90	0.10	0.90	0.10	0.50
242120000	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
243144500	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.00
243520000	0.20	0.10	0.10	0.10	0.10	0.05	0.10	0.30	0.00
243660000	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
243900800	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
249310300	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
249310500	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
249312000	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00
249331400	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.00
249341200	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.00
249341400	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.00
252100000	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.50	0.00
252101100	0.05	1.00	1.00	1.00	1.00	1.00	1.00	0.00	0.00
252107300	0.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	0.00
252211400	0.00	1.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00
252211500	0.00	1.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00
259131100	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.00
267910000	0.25	0.10	0.10	0.10	0.10	0.10	0.75	0.10	0.00
306942600	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.25	0.00
308631000	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
329611100	0.05	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.00
329613000	0.90	0.90	0.90	0.90	0.90	0.90	0.90	0.90	0.00
329616100	0.25	0.90	0.90	0.90	0.90	0.90	0.50	0.50	0.00
399601100	0.75	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00
399602100	0.75	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00
399602600	0.75	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00

As previously indicated in Table 5-2, the fraction of buildings in which materials or furnishings are used is split into two fields--average, representing aged materials, and peak, representing new or unaged

materials. The latter category would apply to newly built or remodeled buildings. Within the SRD, 90 percent of each fraction in Table 5-5 is assumed to be for aged materials and the remaining 10 percent for new materials. Thus, for carpeting in residences, for example, the fraction of 0.90 for residences is composed of 0.81 for aged materials and 0.09 for new materials.

6.   ENVIRONMENT AND PEOPLE-ENVIRONMENT FILES

6.1   File Contents

The contents of the ENVIRONMENT file are summarized in Table 6-1. Nine types of environments, each listed in the table, are used for the SRD. All but one of these environments--vehicles--can be viewed as a type of building. Aside from the environment ID and description, the information contained in the file includes the indoor volume, the air exchange rate, and the replication factor. The replication factor refers to the number of buildings (or vehicles) in the United States that are associated with each type of environment.

The PEOPLE-ENVIRONMENT file (Table 6-2) describes the major subpopulations occupying each of nine environments. For residences and vehicles there is only one subpopulation, referred to as "occupants." The only subpopulation for office buildings is "workers." All other environments have two major subpopulations, including "employers" and "customers" for environments such as restaurants, "staff" and "students" for schools, and "staff" and "patients" for hospitals. In addition to the environment ID, population ID and population description, the information in the file includes the size of each subpopulation and the fraction of time spent by that subpopulation in the environment. Multiplication of the size of a subpopulation by the fraction of time in the environment and the replication factor (number of buildings) yields the number of full-time-equivalent (FTE) people occupying that type of environment throughout the United States. The final field in the PEOPLE-ENVIRONMENT file -- breathing rate -- is not currently used in any SRD calculations (see Section 8) but may be used in the future for estimation of potential inhaled dose.

6.2   Information Sources and Assumptions

Various sources of information and assumptions have been used in developing values for certain fields in the ENVIRONMENT and PEOPLE-ENVIRONMENT files. Those pertaining to the PEOPLE-ENVIRONMENT file are described first, as the size of the subpopulations occupying each environment are used in estimating one of the fields (air exchange rate) for the ENVIRONMENT file.

Table 6-1. Contents of the ENVIRONMENT File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
Environment ID	Character	--	Nine environments of interest with the following IDs: 01 - residences 02 - schools 03 - hospitals 04 - nursing homes 05 - offices 06 - public access buildings 07 - hotels 08 - restaurants 09 - vehicles
Environment Name	Character	--	See ID above.
Indoor Volume	Numeric	m^3	Environment-specific default value.
Air Exchange Rate	Numeric	hr^{-1}	Environment-specific default value.
Replication Factor	Numeric	--	Environment-specific default value for number of buildings or vehicles.

Table 6-2. Contents of the PEOPLE-ENVIRONMENT File

FIELD NAME	FIELD TYPE	UNITS	FIELD DESCRIPTION
Environment ID	Character	--	Environment-specific 2-digit code.
Population ID	Numeric	--	ID for a subpopulation in a specific environment.
Population Description	Character	--	Description of the subpopulation
Size of Population	Numeric	--	Number of people in the subpopulation
Fraction of Time	Numeric	--	Fraction of time spent by the subpopulation in the environment.
Breathing Rate	Numeric	m^3/day	Breathing rate of the subpopulation while in the specific environment.

6.2.1 PEOPLE-ENVIRONMENT File

Two of the primary sources of information for this file are a national study (Robinson and Thomas 1991) and a California study (Robinson and Wiley 1989) of people's activity patterns, from which estimates were developed of how an individual's 24-hour time period is allocated to various activities and microenvironments. Although the national study is more representative, the California study was used as the primary data source because the environment-specific information from that study was developed at a finer level of detail, providing greater compatibility with the nine types of environments defined for the SRD. Information on the number of buildings (or vehicles) associated with each environment, as well as the size of certain subpopulations such as patients and staff in hospitals and nursing homes, was also utilized; this information was obtained from the 112th edition of the *Statistical Abstract of the United States* (USDOC 1992).

Table 6-3 lists the average number of people in the population subgroups occupying each environment, the average fraction of time spent by each subgroup in the environment, and the number of buildings (or vehicles) for each environment. Multiplication of these three quantities yields the number of FTE people associated with each environment, which can be thought of as the number of people that one would expect to find across the United States in each type of environment at any point in time, if each environment were accessible 24 hours a day. The derivation of these numbers is described below.

Table 2 of USDOC (1992) lists an estimated 253 million U.S. residents as of 1991, and Table 1223 lists 92 million occupied housing units, for an average of 2.75 people per residence. The California activity study estimates 892 minutes a day at home, 27 minutes of which are spent in the yard, plus 61 minutes per day at other's residences, for a total of 926 minutes per day in a residence; this equates to 64.3 percent of the total time budget (1440 minutes). The national study estimates 954 minutes a day at home but provides no estimate of time spent in the yard.

Table 210 of USDOC (1992) estimates about 60 million students as of 1990 and 110,000 schools (elementary, secondary and college) as of 1988, for an average of 545 students per school. Table 212 estimates about 3.6 million teachers/faculty as of 1990, for an average of 33 per school. Assuming students are in school for 30 hours per week for 75 percent of the year, each spends 30 hours/week x 52 weeks x .75, or 1170 hours per year, or 13.4 percent of the 8750 hours in a year. For teachers, assuming 40 hours per week for 75 percent of the year, the corresponding value is 17.8 percent.

Table 6-3. Estimates of Number of People and Time Spent per Environment

ENVIRONMENT	SUBPOPULATION	AVERAGE PEOPLE PER ENVIRONMENT[1]	AVERAGE % TIME IN ENVIRONMENT[2]	REPLICATION FACTOR[1]
Residence	Occupants	2.75	64.3	92,000,000
School	Students Staff	545 33	13.4 17.8	110,000 110,000
Hospital	Patients Staff	127 535	100 25.0	7,000 7,000
Nursing Home	Patients Staff	85 50	100 25.0	16,000 16,000
Office Building	Workers	66	25.0	680,000
Public Access Building (retail store)	Customers Employees	227 12	5.3 25.0	1,100,000 1,100,000
Hotel/Motel	Customers Employees	70 35	50.0 25.0	40,000 40,000
Eating/Drinking Establishment	Customers Employees	633 14	2.8 25.0	400,000
Vehicle	Occupants	1.6	6.7	125,000,000

[1]   Source: USDOC 1992 (Statistical Abstract of the United States).
[2]   Sources: Robinson and Wiley 1989; Robinson and Thomas 1991.

Table 166 of the Statistical Abstract estimates about 7,000 hospitals as of 1989 with 3.5 million full-time personnel and 4 million total personnel. Treating the difference (0.5 million) as half-time personnel yields 3.75 million FTE personnel, or 535 staff members per hospital spending 25 percent of their time per week. At an average of 182 beds per hospital and an occupancy rate near 70 percent, there is an average of 127 patients at any point in time. Table 180 of the USDOC (1992) estimates about 16,000 nursing homes as of 1986. With an average of 92 beds and an occupancy rate near 92 percent, there is an average of 85 patients at any point in time. Assuming nearly 600 full-time employees per 1,000 patients (Table 179 of the abstract), the average nursing home (85 patients) has 50 employees spending 25 percent of their time at work.

For the remaining environments, the California activity data were used as a starting point to develop time estimates. On average, California adults spend 86 minutes per day in offices (working or visiting), which translates to 523 hours per year. Multiplication by the U.S. population of 253 million, about 75 percent of which are adults (USDOC (1992), Table 19) yields a total of 99,000 million hours per year. Division by 8,760 hours per year yields 11.3 million FTEs in office buildings. Division by 680,000 office buildings (Table 1239 of the abstract) yields 16.5 FTEs per building, the equivalent of 66 workers spending 25 percent of time each.

On average, California adults spend 76 minutes per day (462 hours per year) in grocery stores, shopping malls, and other retail outlets and public places. Applying this estimate to the entire U.S. population of 253 million yields 117,000 million hours per year. Division by 1.1 million retail establishments (USDOC (1992), Table 1282, after netting out 0.4 eating/drinking places that are treated separately below), yields 106,000 customer hours per year per store, or 12 FTE customers. At 76 minutes per day, each customer spends 5.3 percent of the day in stores, such that the 12 FTE customers equate to 227 at 5.3 percent of time each. Assuming one FTE worker for every three FTE customers, there are 3 FTE workers, or 12 employees working 25 percent of the time each. The estimate of 12 employees per store, multiplied by 1.1 million stores, yields 13.2 million employees, very close to the number (12.7 million) in Table 1282 of the abstract (after netting out employees of eating/drinking places).

California adults spend 8 minutes per day, on average, in hotels or motels. Multiplication by the U.S. population of 253 million yields 12,310 million hours per year. Division by 40,000 hotels/motels (USDOC (1992), Table 1309) results in 307,825 hours per year per establishment, or 843 hours per day, equivalent to 35 FTE customers. Assuming that each customer spends 50 percent of his or her time in the hotel or motel, there are 70 customers per day on average. Assuming one FTE worker for every 4 FTE customers, there are 8.75 FTE employees per hotel/motel, or 35 workers spending 0.25 of time each. This estimate, when multiplied by 40,000 establishments, yields 1.4 million employees nationwide, consistent with the estimate of 1.4 million in Table 1309 of the abstract.

California adults spend 40 minutes per day on average in restaurants or lounges, which correspond to the category of eating/drinking establishments in the SRD. Multiplication by the U.S. population of 253

million yields 61,560 million hours per year. Division by 400,000 establishments (USDOC (1992), Table 1282) results in 153,908 hours per year per establishment, or 422 hours per day, equivalent to 17.6 FTE customers. Since each person spends 40 minutes per day, this is equivalent to 633 people spending 2.8 percent (40/1440 minutes) of the time each. Assuming one FTE worker for every 5 FTE customers, there are 3.5 FTE workers per establishment, or 14 workers spending 25 percent of the time each. This number, when multiplied by 400,000 establishments, yields 5.6 million employees nationwide, close to the estimate of 6.3 million in Table 1282 of the abstract.

California adults spend 96 minutes per day (584 hours per year) on average in cars or vans. Multiplication by the U.S. population of 253 million yields 147,750 million hours per year. Division by 125 million cars in use (USDOC (1992), Table 1000) yields 1182 hours per year per car, or 13.5 percent of a person's time. The 96 minutes per day in cars by the California population accounts for half this percentage (6.7 percent of time), implying that the average vehicle occupancy is 2 persons. This average occupancy is higher than the estimate of 1.6 provided by the U.S. Department of Commerce (USDOC 1992).

The national activity study did not provide an estimate of time spent in cars and vans, but did estimate 81 minutes per day in cars, vans and while walking; the corresponding California estimate is 105 minutes. This national/California ratio of 0.77, when multiplied by the California-based estimate of 2 persons per vehicle, yields a number very close to the 1.6 persons/vehicle from the Department of Commerce.

6.2.2   ENVIRONMENT File

Table 6-4 lists estimates of the volume and air exchange rate for each environment. The replication factor, or number of buildings (or vehicles) associated with each environment, is also part of this file; estimates of the replication factor were previously shown in Table 6-3, as these estimates were used in developing some of the values for the PEOPLE-ENVIRONMENT file. The primary source of information for building volume is the 112th edition of the *Statistical Abstract of the United States* (USDOC 1992), which provides estimates of floor area for most environments; multiplication by an assumed ceiling height yields the estimated indoor volume. The primary source of information for air exchange rates is *Ventilation for Acceptable Indoor Air Quality*, ASHRAE Standard 62-1989 (ASHRAE 1989), which lists outdoor air requirements for ventilation for various commercial and institutional facilities.

Table 6-4. Estimates of Volume and Air Exchange Rate per Environment

ENVIRONMENT	VOLUME, m^3	AIR EXCHANGE RATE, ACH
Residence	390	0.5
School	8,125	1.7
Hospital	13,075	1.0
Nursing Home	5,225	1.0
Office Building	4,925	0.85
Public Access Building	3,300	1.15
Hotel/Motel	7,025	0.85
Eating/Drinking Establishment	1,625	0.85
Vehicle	2	5.0

Table 1213 of USDOC (1992) estimates the average floor area of one-family U.S. residences at 2,075 square feet; multiplication by an assumed ceiling height of 8 feet and by 0.0283 (to convert to cubic meters) yields an estimate of 470 cubic meters for the indoor volume. One-family residences account for 65 percent of all housing units (Table 1223 of USDOC (1992)); the remainder are multi-unit structures (apartments) or mobile houses. Assuming that multi-unit structures have half the volume of one-family structures (i.e., 235 cubic meters), the weighted average for volume of residences is 390 cubic meters. Based on an analysis of more than 3,000 measurements in U.S. residences, Koontz and Rector (1993) estimated a median air exchange rate of 0.5 air changes per hour (ACH); this estimate is preferred over the average rate because the mean is heavily affected by the upper tail of the distribution, which is believed to represent cases where occupants open windows or doors for a significant fraction of the time.

Estimates for the volumes of most other types of buildings are based on an assumed ceiling height of 10 feet; for eating/drinking establishments and public access buildings (retail stores), a ceiling height of 12 feet was assumed. Table 1239 of the USDOC (1992) lists average floor areas of 28,700 square feet for schools, 25,700 square feet for health-care facilities, 17,400 square feet for office buildings, 9,700 square feet for mercantile/services (assumed to apply to retail stores), 24,800 square feet for lodging facilities (hotels/motels) and 4,800 square feet for food services (eating/drinking establishments). The collective estimate for health-care facilities applies to hospitals and nursing homes; their respective estimates were derived by assuming that hospitals (7,000 buildings) had 2.5 times the volume of nursing homes (16,000 buildings) because of higher patient and staff counts, coupled with requirements for ancillary facilities such as operating and emergency rooms. These assumptions result in an estimated average floor area of 46,180 square feet for hospitals and 18,472 square feet for nursing homes. For vehicles, the passenger compartment was assumed to be 4 feet wide, 6 feet long, and 3 feet high, resulting in an estimated volume of 2 cubic meters.

The outdoor-air requirements developed by ASHRAE (1989) are based on either the number of occupants (most cases) or the floor area. For office buildings, for example, the requirement is 15 cfm (25.5 m^3/h) per occupant. Earlier (1981) ASHRAE criteria are considerably lower (5 cfm per occupant). To reflect the varying ages of the building stock, two-thirds of the 1989 criterion, or 10 cfm, was used to estimate the air exchange rate. Since buildings are designed to accommodate maximum occupancy and office buildings typically have some vacant offices as well as visitors, the average of 66 workers per building (see Table 6-3) was increased by 50 percent, to 99 occupants. Multiplication by 10 cfm (17 m^3/h) yields 1,683 m^3/h as the outdoor air requirement; division by the building volume (4,925 m^3) yields an air exchange rate of about 0.35 ACH due to requirements for mechanical ventilation. This rate, when added to the infiltration rate (0.5 ACH, assumed to be similar to residences), results in an estimated air exchange rate of 0.85 ACH. This value is very close to the median value of 0.89 ACH reported by Persily (1989), based on measurements of air exchange rates in 14 office buildings.

Schools have the highest estimated air exchange rates among the various building environments, due to the relatively high occupant density. Multiplication of 578 occupants (545 students and 33 teachers) by 17 m^3/h yields 9,826 m^3/h, and division by the volume of 8,125 m^3 yields 1.2 ACH due to mechanical ventilation; addition of 0.5 ACH due to infiltration results in 1.7 ACH as the estimated air exchange rate. For hospitals and nursing homes, ASHRAE (1989) lists 25 cfm per occupant as the outdoor air requirement. Two-thirds of this value was multiplied by the number of occupants to provide an estimate of 0.5 ACH due to mechanical ventilation, resulting in an estimated air exchange rate of 1.0 ACH after adding 0.5 ACH due to infiltration. For eating/drinking establishments, the ASHRAE requirement of 25 cfm (multiplied by two-thirds) resulted in an overall air exchange rate of 0.85 ACH (0.35 ACH due to mechanical ventilation).

For public access buildings, the ASHRAE requirement is 0.2 cfm per square foot of floor area. Multiplication by an average floor area of 9,700 square feet and by two-thirds yields 1,293 cfm, or 2,198 m^3/h; division by the volume of 3,000 m^3 results in 0.65 ACH due to mechanical ventilation, or 1.15 ACH in total. For hotels and motels, the requirement is 30 cfm per room; multiplication by 70 rooms and by two-thirds yields 1,400 cfm, or 2,380 m^3/h; division by the volume of 7,025 m^3 results in 0.35 ACH due to mechanical ventilation, or 0.85 ACH in total. There is little quantitative basis from which to develop an estimate for vehicles; given the rate of speed at which vehicles travel, coupled with occupants' abilities to provide fresh air by opening windows or vents, an arbitrarily large value of 5.0 ACH was assumed.

7. APPLICATIONS

There are three applications in SRD. The first and primary application is used to rank products and materials using modeled indoor-air concentrations of their chemical constituents in selected types of environments. The second application is used to determine all products or materials in the database that contain a certain chemical. The third application is used to determine all chemicals that are contained in various formulations of a specific product or material. The second and third applications are used to browse information about chemicals in products, and materials.

7.1   File Review and Update

Reviewing and updating files are treated here as SRD applications. When SRD is first started, the introductory screen appears. Five tabs line the top of this screen: Intro, Find products containing a chemical, find chemicals in a product category, Rank Products, and Browse Database Files (Figure 7-1). The Browse Data Files tab can be selected using one click of the mouse. This will display a list of seven data files (Figure 7-2). Any of the files listed can be selected with one click of the mouse. For purposes of this discussion, it is assumed that the "Product Chemical" file has been selected by the user.

The screen in Figure 7-3 will appear after the "Product Chemical" file has been selected. The screen displays the contents of the first record in the file. Commands at the bottom of the screen can be accessed with the mouse, the Tab key (to move forward across screen items), or the Shift-Tab key combination (to move backwards). The Top, Previous, Next, and Bottom commands enable the user to access various records in the file. Using the Find command the user can locate the first record in the file that matches a specific value for one of the fields (Product ID, CAS Number, etc.). For example, if the user specifies the CAS Number as the search field and 64175 as the value for the field (Figure 7-4) and uses the mouse to click the Search button, the first record in the file with this CAS Number will be displayed. To view the list of Product IDs containing this CAS Number the user will need to click on the Print button and then chose the output type (Figure 7-5) by clicking on the drop box arrow next to output type. To view the list on the screen, the user should select Preview (filename) as the output type by clicking once to highlight the selection. In this case the user will be selecting Preview (Prod_chm) as the output type. Once the output type is selected, click on the OK button and the Report Preview screen will appear. The user can then scroll through the list using the up or down arrows on the keyboard or else by clicking the up or down arrows at the right of the screen. To exit this screen, click on the X in the upper right corner of the screen. To print out the list of Product Id's containing this CAS Number, the user will need to click on the Print button and then select Print list from table (filename) as the output type by clicking on the drop box arrow next

Figure 7-1. SRD Introductory Screen
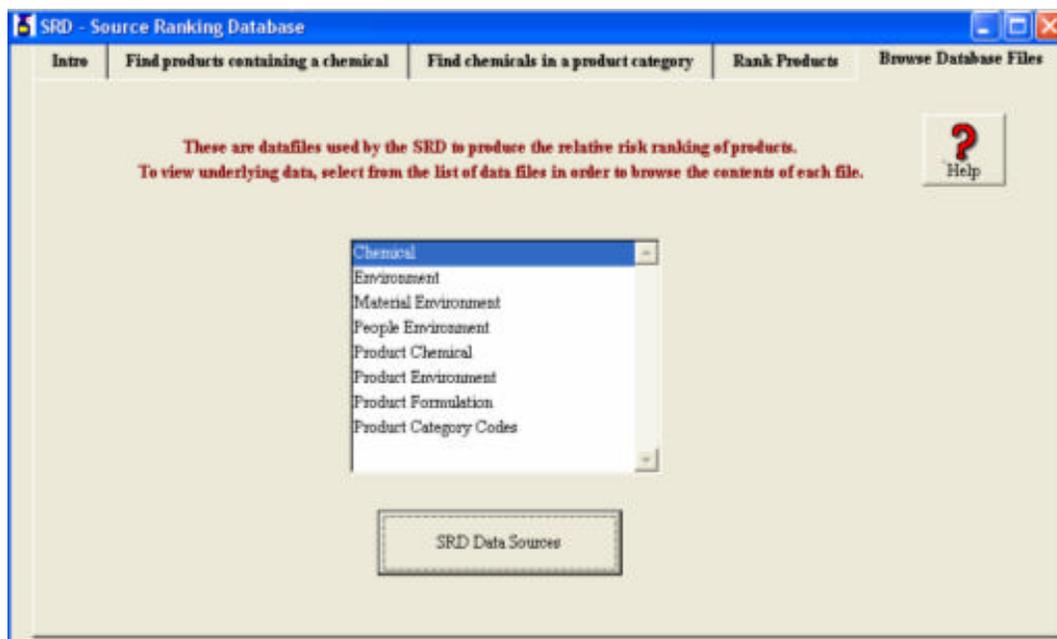
Figure 7-2. SRD Data Browsing Screen

Figure 7-3. First Record in "Product Chemical" File
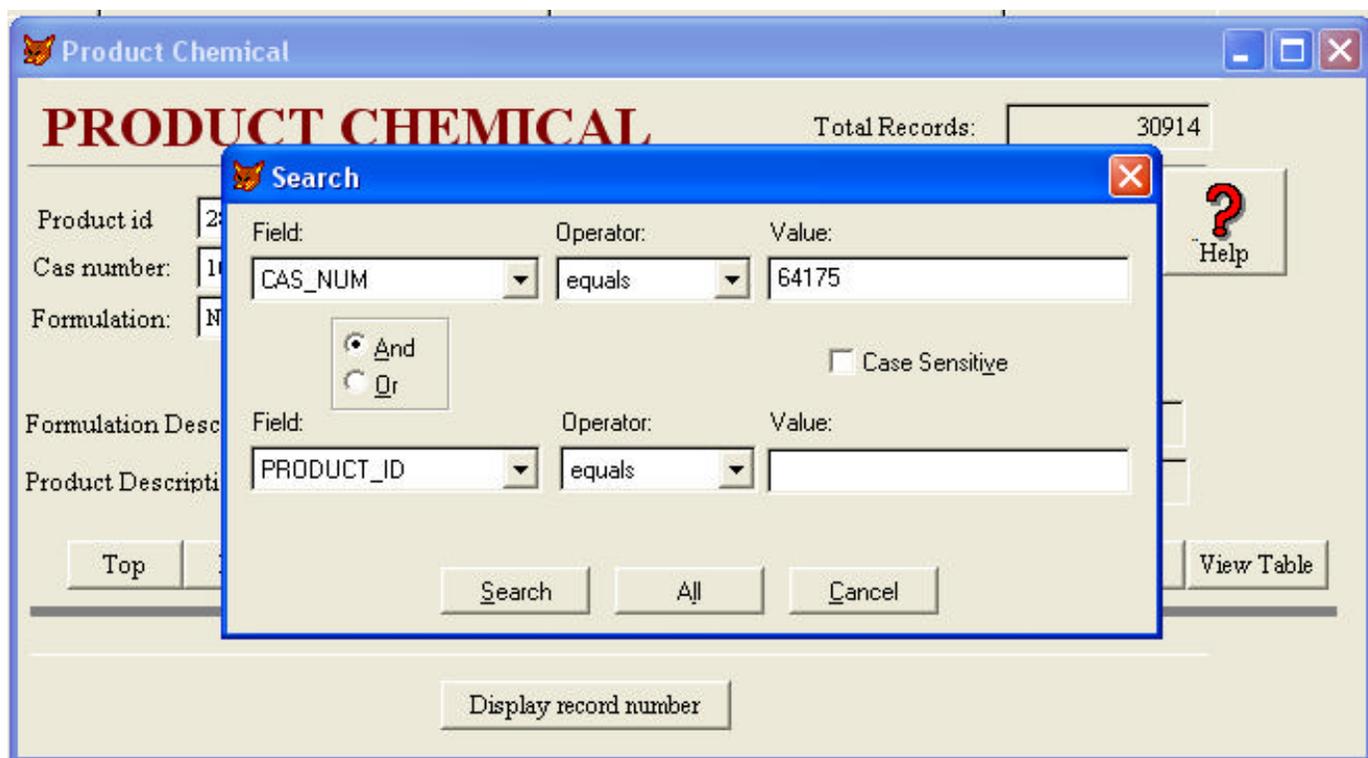
Figure 7-4. Screen Associated with the Find Command
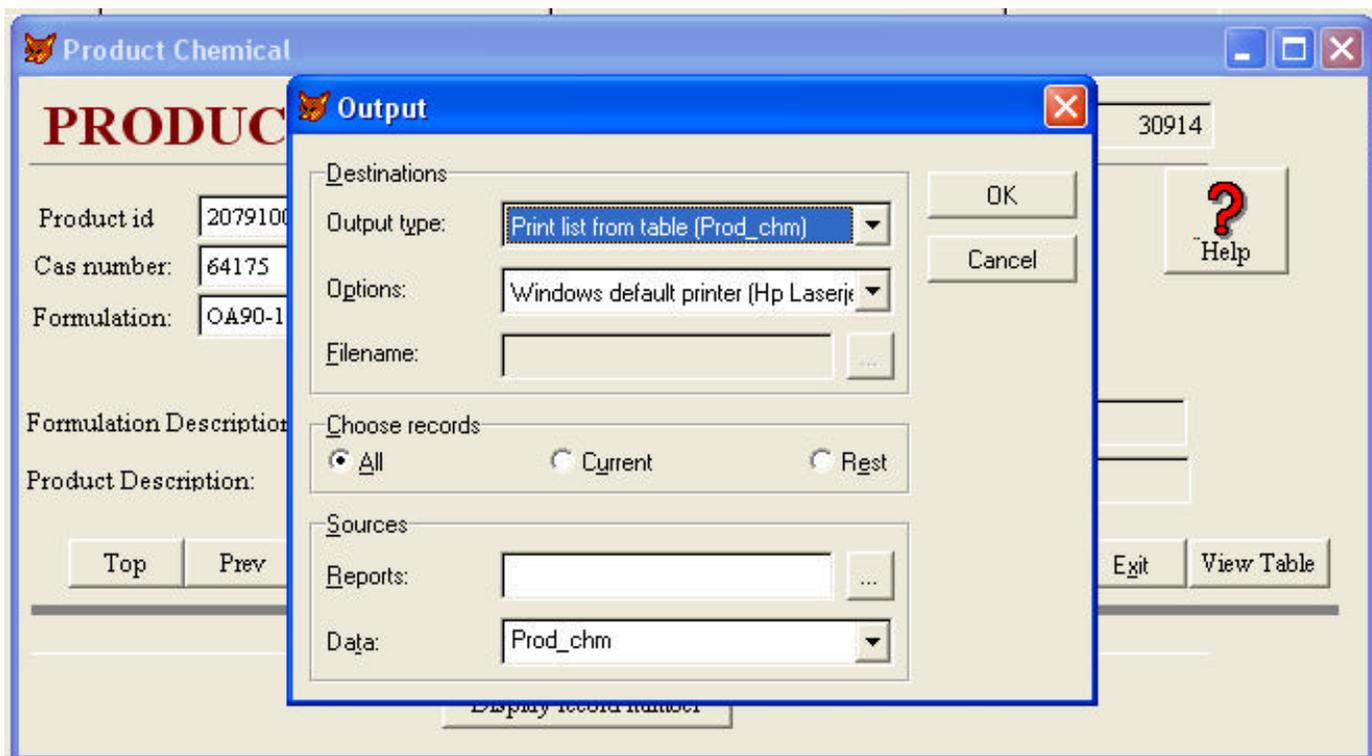
Figure 7-5. Selecting Output Type to Print or Display Records From Database File

to the output type and clicking once to highlight the selection. In this case the user will be selecting Print list from table (Prod_chm) as the output type. Once this output type is selected, click on the OK button and the table will be sent to the printer.

In the browse mode, the user can rapidly view all of the field contents of the database file by moving up or down using the mouse (by clicking the up or down arrows at the right of the screen) or using the up/down arrow keys or PgUp/PgDn keys on the keyboard. An expanded view of the file can be obtained by clicking the maximize symbol at the upper right of the screen; with the keyboard, this can be accomplished using the Ctrl-F10 key combination. Even with the expanded view, all fields cannot be viewed simultaneously. The user can move across fields with the mouse, by clicking the left or right arrows at the bottom of the screen, or with the keyboard, using the Tab key or the Shift-Tab key combination. Exiting the browse function is accomplished using the mouse to click on the "X" in the upper right corner of the window to close the screen or else hit the Esc key on the keyboard. Selecting the Exit button at the bottom of the next screen displayed returns the user to the Data Browsing screen previously shown in Figure 7-2.

7.2   **Ranking Products**

When the Rank Products tab is selected, the window shown in Figure 7-6 appears. Criteria for ranking must be specified before the ranking can be performed. There are six types of criteria to be addressed:

- Product classification scheme and associated categories

- Formulation data sources to be included

- Environment(s) to be included

- Average versus upper values for selected items in the PRODUCT- ENVIRONMENT and MATERIAL-ENVIRONMENT files

- Ranking based on chronic hazards or acute hazards

- Ranking based on all chemicals or the subset without default values for hazard ratings.
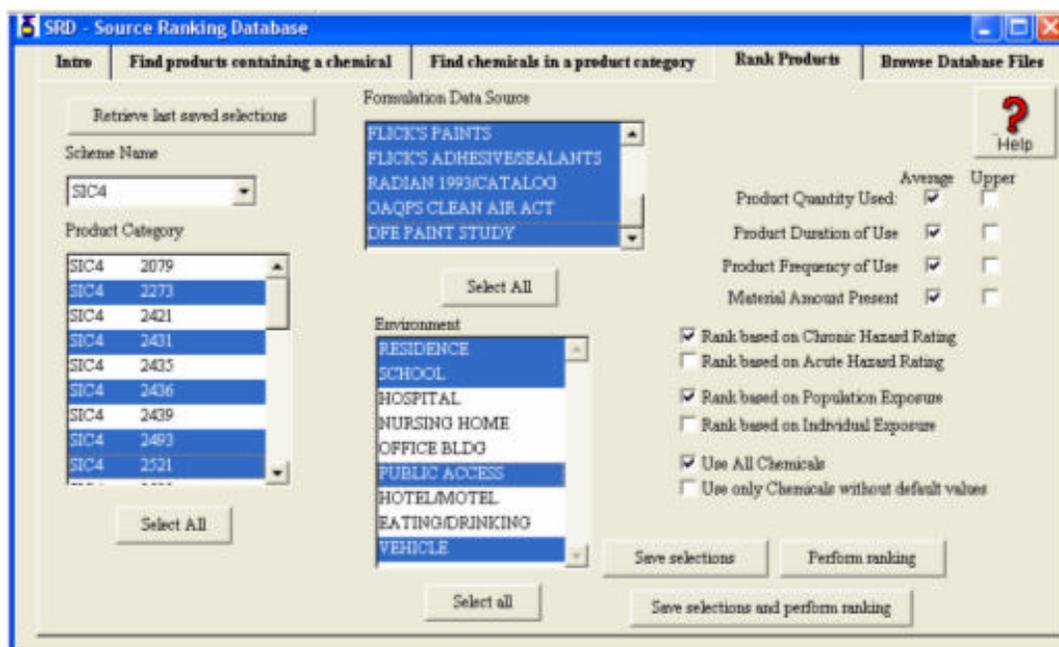
Figure 7-6. Ranking Products Screen

A scheme for product categories is first selected using a drop-down list. Three options are available: SIC4, SIC5 or SIC7. Click the desired scheme and the corresponding list in the Product Category box will be displayed. The user can select an individual product category or a subset of product categories. To select multiple categories, use the mouse to click and hold on the first selection and then move the mouse to sequentially highlight additional categories. To select non-sequential categories, use the mouse to highlight the first selection and then, with the Ctrl key depressed, click each additional category desired. The "Select All" button under the Product Category box will select all categories in the list. The same selection procedure is used when selecting the Formulation Data Sources and desired Environments. At the right-hand side of the screen, the user may choose either average (Avg.) or high-end (Upper) values for each of the first four items -- Product Quantity Used, Product Duration of Use, Product Frequency of Use, and Material Amount Present. Care should be taken to ensure that the choices are consistent; for example, if a high-end value is chosen for quantity used, then a high-end value should also be chosen for duration of use. Next, the user can opt to rank based on chronic hazard ratings or acute hazard ratings. The user can also opt to base the ranking on all chemicals or only those that do not have a default value for hazard ratings; at present, about 70 percent of the chemicals have a default (low) value for hazard ratings. Finally, the user can elect to save the current selections and perform the ranking or not save the selections. To save the current selections, the user can either click on the "Save selections" or the "Save selections and perform ranking" button. Clicking on the "Perform ranking" button will perform the ranking without saving the settings for future retrieval. If

selections are saved, then the current selections can be retrieved the next time the user sets ranking criteria by clicking on the "Retrieve last saved selections" button at the top left corner of the Rank Products window. This button may not be used until at least one ranking has been performed and saved since the installation of the program.

After the user selects either the "Perform ranking" or the "Save selections and perform ranking" button the window displayed in Figure 7-7 appears. Here the options for output formats are listed. The user can request results with all details or results without chemical details or results without chemical and formulation details. The user also has the option to return to the previous (ranking criteria) screen. Choosing all details will result in a large output file, but will enable the user to determine how specific chemicals, environments and product formulations have contributed to the overall score for each product category (see Section 8 for discussion of the calculations involved in scoring product categories). As scores are being developed to enable ranking of product categories, progress will be displayed at the top right corner of the screen. When all scores and ranks have been calculated, the message "Formatting output data" will be displayed, after which the Printing/Viewing Screen will appear. Figure 7-8 displays an example of an output with all details requested. This screen enables the user to view, print, or save detailed and summary reports. The two tabs at the top of the Printing/Viewing Screen allow the user to view the Detailed Results or Summary Results by clicking on the desired tab. To save the detailed report, click on the "Save Detailed Results to a File" button. The user will be prompted to select the folder in which the file is to be saved, and to supply a file name. Depending on the size of the outputs for detailed and summary results, additional tabs may appear at the top of the output screen. Each tab represents one page of results. The user need not save each page; all detailed results pages will be saved. To save the summary results, select the Summary Results tab to display the summary results and then click on the "Save Summary to a File" button and follow the same procedure as described for the detailed results. An example of the first page of a detailed listing, with the previously selected option to obtain results with all details, is shown in Figure 7-9. An environment-specific value of 0.0 for a given product's chemical indicates that the environment has not been selected by the user, that the product is not used in that environment, or that some variable involved in the calculation (e.g., weight fraction) has a value of zero. An environment-specific value of 0.0000 indicates that a small, non-zero value has resulted from the calculations. An example of the first page of a summary listing is provided in Figure 7-10. For each product category, the product ID, product description, product score and product rank are provided.

For product categories with the same scores, the rank is determined by averaging across the relative positions occupied by the tied categories. For example, if three different products each had the third lowest score and, thus, occupied the third, fourth, and fifth positions. As a result, the rank assigned to each of these categories would be (3+4+5)/3, or 4.0.

Once the detailed or summary listing has been saved, it can be viewed or printed "outside" the SRD software. If the user selects the final choice ("Return to Previous Menu") in the menu for output options, then he or she will no longer have the ability to view, print or save listings within the SRD, except by choosing to perform the ranking again.
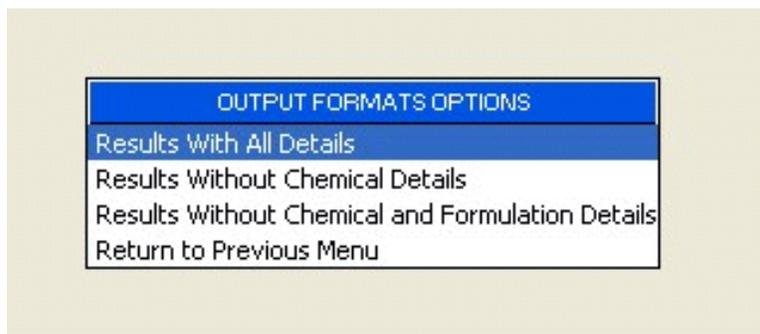
Figure 7-7. Options for Level of Output Detail
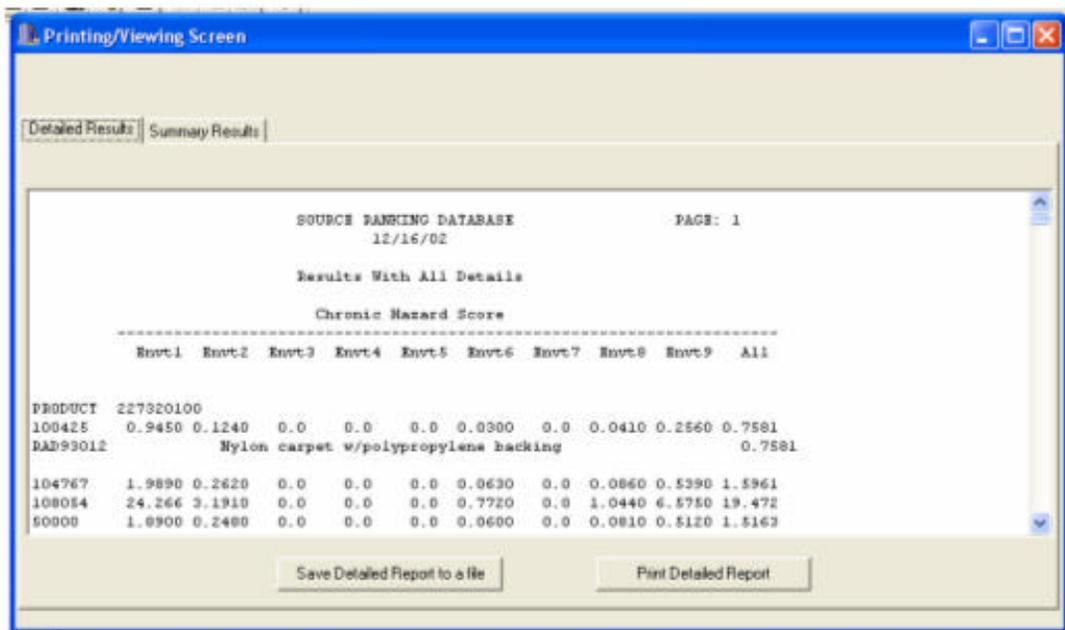
Figure 7-8. Printing/Viewing and Saving Outputs

Results With All Details

Chronic Hazard Score

```
--------------------------------------------------------------------
     Envt1   Envt2   Envt3   Envt4  Envt5   Envt6  Envt7  Envt8  Envt9    All


               `   PRODUCT  227320100
100425   0.9450 0.1240   0.0     0.0    0.0  0.0300   0.0    0.0  0.2560  0.7884
RAD93012          Nylon carpet w/polypropylene backing               0.7884


104767   1.9890 0.2620   0.0     0.0    0.0  0.0630   0.0    0.0  0.5390  1.6598
108054   24.266 3.1910   0.0     0.0    0.0  0.7720   0.0    0.0  6.5750  20.249
50000    1.8900 0.2480   0.0     0.0    0.0  0.0600   0.0    0.0  0.5120  1.5768
75070    0.7960 0.1050   0.0     0.0    0.0  0.0250   0.0    0.0  0.2160  0.6639
RAD93013          Nylon carpet w/polypropylene&PVC backin            24.150


128370   0.0990 0.0130   0.0     0.0    0.0  0.0030   0.0    0.0  0.0270  0.0825
34590948 0.0100 0.0010   0.0     0.0    0.0   0.0     0.0    0.0  0.0030  0.0086
71363    0.8450 0.1110   0.0     0.0    0.0  0.0270   0.0    0.0  0.2290  0.7054
95501    0.2980 0.0390   0.0     0.0    0.0  0.0090   0.0    0.0  0.0810  0.2489
RAD93014          Nylon carpet w/polypropyl&polyureth bac            1.0456


100425   0.4970 0.0650   0.0     0.0    0.0  0.0160   0.0    0.0  0.1350  0.4149
RAD93015          Nylon carpet w/SBR latex backing                   0.4149


100425   6.8120 0.8960   0.0     0.0    0.0  0.2170   0.0    0.0  1.8460  5.6848
RAD93016          Nylon carpet w/polypropyl&SBR latex bac            5.6848


100414     0.0    0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0     0.0
100425     0.0    0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0     0.0
103651     0.0    0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0     0.0
106467     0.0    0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0     0.0
108678   0.0010   0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0    0.0008
1120214  0.0050 0.0010   0.0     0.0    0.0   0.0     0.0    0.0  0.0010  0.0041
112403   0.0020   0.0     0.0     0.0    0.0   0.0     0.0    0.0  0.0010  0.0020
124185   0.0030   0.0     0.0     0.0    0.0   0.0     0.0    0.0  0.0010  0.0024
526738     0.0    0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0     0.0
611143     0.0    0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0    0.0004
71432    49.725 6.5390   0.0     0.0    0.0  1.5820   0.0    0.0  13.473  41.495
95476    0.0500 0.0070   0.0     0.0    0.0  0.0020   0.0    0.0  0.0130  0.0414
95636      0.0    0.0     0.0     0.0    0.0   0.0     0.0    0.0   0.0    0.0004
```

Figure 7-9. First Page of Detailed Report

Ranking Results

Product Category	Description	Chronic Score	Chronic Rank
2493	Reconstituted Wood Products	18.992	1.0
2521	Wood Office Furniture	12.295	2.0
2273	Carpets and Rugs	8.735	3.0
2431	Millwork	0.987	4.0
2436	Softwood Veneer and Plywood	0.093	5.0

Figure 7-10. First Page of Summary Report

7.3 Finding Products Containing a Chemical

The second application available to the user provides useful information concerning which products a given chemical is found in as well as information about the products (i.e., Product Name, Formulation Name, Weight Fraction, and Emission Rate). To access this application, select the "Find products containing a chemical" tab. The two boxes in the middle of the screen will be empty until the user chooses to select a chemical by CAS number or by chemical name. After making this selection, a drop-down list appears (Figure 7-11). At this point the user can scroll through the list in alphabetical order to identify the desired chemical. To expedite the identification of the desired chemical, the user can type in the initial digits of the CAS number or the first letters of the chemical name. The list will immediately scroll to the point where the CAS numbers or chemical names begin with the digits or letters typed in. The user can then scroll from there to identify the desired chemical in less time. Once the desired chemical is located and selected using the mouse, the user may click on the "View matches and info" button or the "View matches only" button. The "View matches and info" button will bring up a search results window which will show the search results for CAS # 100425 (Figure 7-12).

The search results screen displays the chemical name, the hazard score for the chemical, the total number of product records in which the chemical is found, the number of product records where the weight fraction of the chemical within the product is greater than 0, the weight fraction values (average, median, minimum, and maximum) and information about the first product in which the chemical is found. The buttons near the bottom of the screen (Next, Bottom, etc.) provide access to the remaining records containing the desired chemical. The "View Table" button at the bottom right of the screen allows the user to view both detailed and summary results for the CAS # of interest (in this case CAS# 100425 - Styrene). The detailed results table provides a listing of all the identified products as well as information about each product, while the summary results table provides a brief overview of all the results (Figure 7-13). To exit the browse screen, click on the "X" in the upper right corner of the screen. The "Exit" button at the bottom right corner of the search results screen will take the user back to the "Find products containing a chemical" screen.

Figure 7-11. Finding Products Containing a Chemical

SEARCH RESULTS FOR CAS#100425

Help

Chemical name:	STYRENE		
Hazard Score:	0.10000		
Total Records:	24	Median weight fraction:	0.16000
Total records with wt. fraction > 0:	16	Minimum weight fraction:	0.09000
Average weight fraction:	0.25600	Maximum weight fraction:	0.99800

Product ID:	227320100
Product name:	Tufted carpets and rugs (no
Formulation ID:	RAD93012 Source Radian 1989, 19
Form name:	Nylon carpet w/polypropylene backin
Weight fraction:	0.00000 Emission Rate: 19.00000

Top   Prev   Next   Bottom   Find   Print   Exit   View Table

Display record number

Figure 7-12. Example Search Results for CAS # 100425 Search

Figure 7-13. Browse Listing of Detailed and Summary Results
of All Products Containing CAS # 100425

Record	PROD ID	PROD NAME	FORM ID	FORM NAME	WT FRAC	EM RATE
1	227320100	Tufted carpets and rugs [	RAD93012	Nylon carpet w/polypropylene backin	0.00000	19.000
2	227320100	Tufted carpets and rugs [	RAD93015	Nylon carpet w/SBR latex backing	0.00000	10.000
3	227320100	Tufted carpets and rugs [	RAD93016	Nylon carpet w/polypropy&SBR latex	0.00000	137.000
4	227320100	Tufted carpets and rugs [	RAD93017	Polypropylene carpet	0.00000	0.000
5	285150000	Unknown	0A90-15519	CBI521718	0.99800	0.000
6	289140000	Synthetic resin and rubbe	0A90-16467	CBI671713	0.09000	0.000

Summary Results For CAS #100425

Chemical Name	STYRENE
Total Records	24
Total Records w/ Wt Frac.:	16
Average Weight Fraction	0.256000
Median Weight Fraction	0.160000
Minimum Weight Fraction	0.090000
Maximum Weight Fraction	0.998000
Hazard Score	0.100000

7-17

The user will notice at this point that the center box is no longer empty, but contains a recap of the product ID's and formulation descriptions in which the desired chemical is found. In order to view this list without first going through the results screen, the user can click on the "View matches only" button instead of the "View matches and info" button after identifying the chemical of interest. From this list in the center box (see Figure 7-14) the user can select the desired products (by highlighting them) and then clicking on the "View info of highlighted matches" button. Once the "View info of highlighted matches" button has been activated, the search results for a chemical screen will appear with information for just the highlighted products.
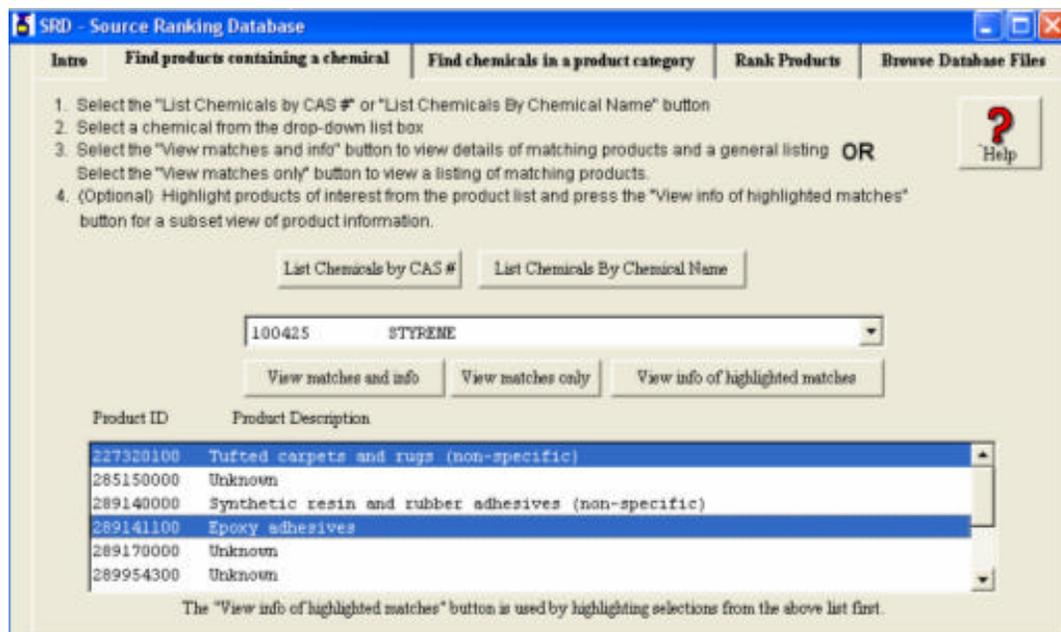
Figure 7-14. Highlighting Only the Desired Products from the List Box

7.4   Finding Chemicals in a Product Category

This third application available to the user provides useful information concerning which chemicals are found in a given product category.   To access this application, select the tab called "Find chemicals in a product category" (Figure 7-1) and click on one of the boxes to access a listing "By Product ID" or "By Product Category Name." (Figure 7-15) The user can scroll through either list in alphabetical order to identify the desired product category. To expedite the identification of the desired product category the user can type in the initial digits of the product ID or the first letter of the product category. This will cause the list to scroll immediately to the corresponding point in the list. The user can then scroll from there to identify the desired product ID or category. Once the desired product ID number or product category name is located and selected using the mouse, the user has the option to click on the "View matches and info" button or the "View matches only" button. The "View matches and info" button will take the user directly to the search results for a product screen.

Figure 7-16 shows search results for the product name Household Hard Surface Cleaners (dry), Product 2841206. The search results page provides the product name, general statistics on weight fraction per CAS number, and chemical data for the first chemical found in the desired product. The chemical data includes the formulation ID and formulation description in which the chemical is found, the CAS number, the chemical name, the weight fraction and the hazard score. The buttons near the bottom of the screen (Next, Bottom, etc.) provide access to the remaining records for each chemical found in each formulation. The "Browse" button at the bottom right of the screen allows the user to view both detailed and summary results for the selected Product ID. The detailed results table provides a listing of all the identified chemicals and formulations. The summary results table provides information on each chemical found in the desired Product ID (Figure 7-17). To exit the browse screen, click on the "X" in the upper right corner of the screen. The "Exit" button at the bottom right corner of the search results screen will return the user to the "Find chemicals in a product category" screen. The larger box in the center of the screen contains a recap of all the formulations (ID number and description) for the selected product category. In order to view this list without first going through the results screen, the user can click on the "View matches only" button instead of the "View matches and info" button after identifying the product category of interest. From this list of formulations in the center box (see Figure 7-18) the user can select the desired formulations (by highlighting them) and then clicking on the "View using highlights" button. Once the "View using highlights" button has been activated, the search results for a product screen will appear with information for just the highlighted formulations.

Figure 7-15. Finding Chemicals in a Product Category

Figure 7-16. Example Search Results for Household Hard Surface Cleaners (Dry)

View Table

Detailed Results for Product ID #2841206 - HOUSEHOLD HARD SURFACE CLEANERS (DRY)

Formulation	Description	CAS Number	Weight Fraction	Source
OA90-11403	CBI127770	112345	0.0810	OAQPS Consumer and Commercial Product Se
OA90-11469	CBI571250	112345	0.0810	OAQPS Consumer and Commercial Product Se
OA90-11436	CBI251395	112345	0.0810	OAQPS Consumer and Commercial Product Se
OA90-11403	CBI127770	141435	0.2240	OAQPS Consumer and Commercial Product Se
OA90-11462	CBI900276	141435	0.3910	OAQPS Consumer and Commercial Product Se
OA90-11469	CBI571250	141435	0.3190	OAQPS Consumer and Commercial Product Se

Summary Results for Product #2841206 - HOUSEHOLD HARD SURFACE CLEANERS (DRY)

CAS Number	Chem Name	Haz Score	Min	Maximum	Average	Median
112345	DIETHYLENE GLYCOL	100.000	0.0810	0.0810	0.0810	0.0810
141435	ETHANOLAMINE	100.000	0.2190	0.3910	0.2883	0.2240
2244215	sodium dichloroiso	100.000	0.0500	0.0500	0.0500	0.0500
34590948	DIPROPYLENE GLYCOL	0.0010	0.0800	0.0800	0.0800	0.0800
497198	sodium carbonate	0.0010	0.4000	0.4000	0.4000	0.4000
67630	ISOPROPANOL	0.1000	0.0100	0.0100	0.0100	0.0100
6834920	SODIUM METASILICAT	0.0010	0.0500	0.0500	0.0500	0.0500

Figure 7-17. Browse Listing of Detailed and Summary Results
of All Chemicals Found in Product ID # 2841206
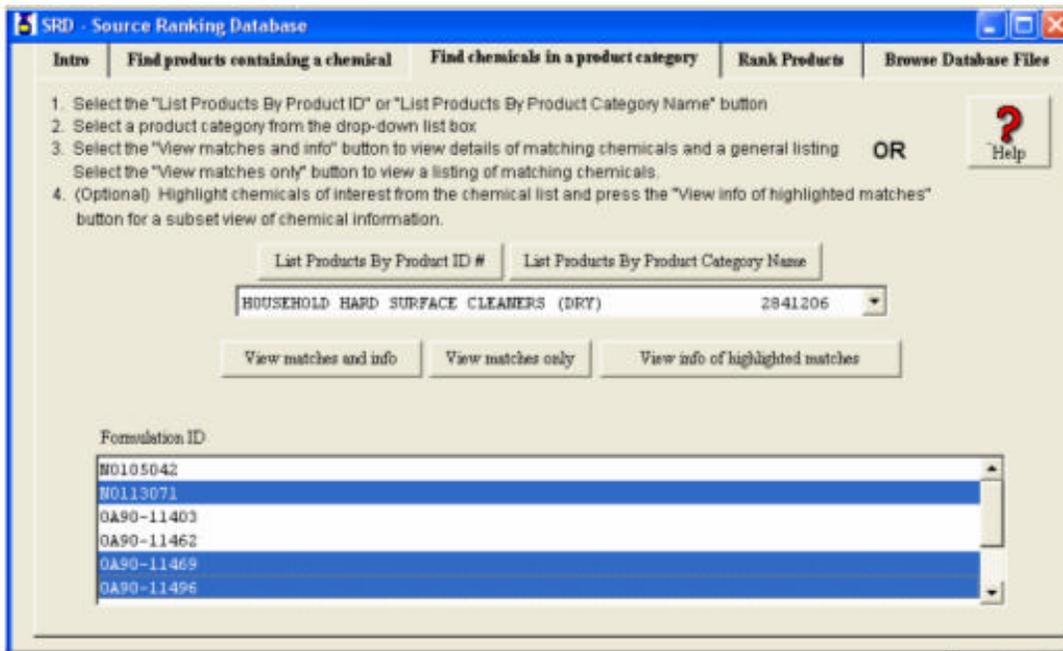
Figure 7-18. Highlighting Only the Desired Formulations from the List Box

8.   CALCULATIONS AND ASSUMPTIONS

8.1   Overview

The SRD application for ranking products involves the calculation of a score for each chemical included in the specific formulation of a product (or material). As shown in Figure 8-1, this score is calculated separately for each environment in which the product is used. Two types of scores can be calculated -- a chronic score or an acute score. The chronic score is obtained by first multiplying a time-integrated indoor-air concentration for the chemical, over a period of one year, by the chronic hazard rating for the chemical; the resultant product then is multiplied by the fraction of buildings in which the product/material is used and (for products) by the annual frequency of use. The acute score is obtained by multiplying a peak indoor-air concentration for the chemical by its acute hazard rating, and then by the fraction of buildings and the annual frequency of use.

The calculations and associated assumptions for time-integrated and peak concentrations are described in Section 8.2. In brief, these calculations use quantities such as the frequency and duration of product use, the amount of product used, the chemical emission rate or weight fraction, and the volume and air exchange rate for each type of environment in which a product is used. The specific calculations are dependent on how a product is applied or used -- direct discharge to air, application/disposal in water, application to a surface, or placement in an environment.

The environment-specific scores for each chemical in a product formulation are used to develop a weighted-average score for the chemical across all environments. As described in Section 8.2, the environment-specific weights used to calculate this average sum to unity, and each environment's weight reflects its relative share of full-time-equivalent (FTE) exposures throughout a year. The FTE exposures are based on the number of people and fraction of time spent in each environment.

As shown in the right-hand column of Figure 8-1, the weighted-average scores for each of the chemicals in a product formulation are summed to obtain a product-formulation score. The score for a specific product is then computed by averaging the scores across different formulations of the product; thus, an equal market share is assumed for each formulation. Finally, the score for a product category is obtained by averaging the product-specific scores across all products associated with the category.

Product 1, Formulation 1

Score for Envt 1	Score for Envt 2	· · ·	Score for Envt 9	Average Score

Weighted Avg Across Envts (based on FTEs)

Chemical 1

Chemical 2

.
.
.

Score for one chemical in one product formulation in one environment
= concentration x hazard rating
x fraction of buildings in which product or material is used

Sum across chemicals to get formulation score

Chemical m

Product 1, Formulation 2

.
.
.

Average across formulations to get product score

Product 2

.
.
.

Average across products to get category score

Product n

Figure 8-1. Flow of SRD Calculations for Product Category Scores

To accomplish the ranking procedure summarized above, the SRD software begins with the user-selected scheme for grouping products. The program selects the first category in the scheme and the first product ID associated with that category. Next, from the PRODUCT-FORMULATION file (see Table 3-2), the program selects the first formulation associated with the product ID and notes the environments to which the formulation applies. The program then accesses the PRODUCT-CHEMICAL file (see Table 4-1) to identify all chemicals (CAS numbers) associated with the product ID and formulation. Based on information pulled from various files (PRODUCT-CHEMICAL, CHEMICAL, PRODUCT-ENVIRONMENT, ENVIRONMENT, AND PEOPLE-ENVIRONMENT), the program calculates the score for the first chemical in each applicable environment. The program then proceeds to the next chemical associated with the product ID and formulation. After completing all the chemical-specific calculations for the first formulation, the program continues with subsequent formulations. When finished with all formulations of a product, the program proceeds to the next product, and so on. Summary values (total/average scores) are computed as calculations are completed for all chemicals in a formulation, all formulations of a product, and all products in a category.

8.2   Peak and Time-Integrated Concentrations

Calculations for both peak and time-integrated airborne concentrations are based on the principle of conservation of mass in indoor environments. Under this principle, indoor concentrations are increased by the chemical mass emitted into the indoor volume from products or materials used indoors and are decreased by the transport of the chemical to the outdoors or to indoor sinks. Indoor concentrations can also be increased by the transport of chemicals from outdoors to indoors. However, because SRD is concerned only with contributions arising from use of products or materials indoors, the outdoor chemical concentration is assumed to be zero for the purpose of SRD calculations. The peak concentration is calculated in units of mg/m^3, and the time-integrated concentration in units of mg/m^3-h.

SRD calculations for peak and time-integrated concentrations depend on assumptions regarding how the product/material is used and how the chemical mass is released over time. There are four types of cases:

1.   Direct release of the chemicals in a product to indoor air from a container, as with an air freshener

2.   Direct release of the chemicals in a product to indoor air from agitated or warm water, as with a laundry or dishwasher detergent

3.   Application of a product to a surface from which the chemicals evaporate, as with an all-purpose cleaner or architectural coating

4.   Release of the chemicals (through diffusion and evaporation) from a material placed indoors, as with furnishings or carpeting.

The distinction between the first and second cases is that all chemical mass is assumed to be released to the indoor air in the first case, whereas some fraction of the mass is assumed to be released in the second case because the product typically is transported to the waste-water stream immediately following its use. Products such as shaving cream, which ultimately are returned to the waste-water stream, also are classified as the second case.

The assignment of each product ID in SRD to one of the four cases listed above is summarized in Appendix G; within SRD, these assignments are contained in the PRODUCT-FORMULATION file (see Table 3-2). The calculations for each case are summarized below; detailed documentation of the mathematical developments underlying these calculations is contained in Appendix H. Although four cases are also described in Appendix H, the cases in the appendix do not correspond identically to those listed above. More specifically, cases 1 and 2 above are variations of case 1 in the appendix, case 3 above corresponds to case 2 in the appendix, and case 4 above corresponds to case 4 in the appendix. Case 3 in the appendix does not currently apply to any of the products contained in the SRD, but may be used in the future.

8.2.1   Case 1: Product Released to Indoor Air From a Container

Calculations for this case involve the quantity of product used (m, in grams), the weight fraction of the chemical in the product (w), the duration of product use (q, in hours), the loss rate (k) for the indoor environment, and the indoor volume (v). The loss rate, in units of inverse hours, is the sum of the indoor-outdoor air exchange rate for the environment, the chemical-specific reactivity rate, and the product- and chemical-specific deposition rate. At present, all reactivity and deposition rates are assigned a value of zero in the SRD, such that the loss rate is equal to the air exchange rate. The indoor volume is expressed in units of m^3.

This case can be viewed as a pulse application with a constant emission rate over the duration of product use (see Appendix H, pp. 7-8). The chemical-specific emission rate, in units of g/h, is the product of the quantity of product used and the chemical weight fraction, divided by the duration of product use. The peak concentration (in mg/m^3) for one episode of product use is calculated as

$$C_{peak} = \frac{m \cdot w}{q \cdot k \cdot v} \cdot (1 - e^{-k \cdot q}) \cdot 1{,}000$$

where 1,000 is a factor to convert the mass from grams to milligrams. The time-integrated concentration (in mg/m^3-h) for one episode of product use is calculated as

$$C_{int} = \frac{m \cdot w}{k \cdot v} \cdot 1{,}000$$

Although more complicated expressions are involved in integrating the indoor concentration over the product-application and post-application phases (see Appendix H, p. 7), the simplified expression used above is obtained by integrating the post-application concentration to infinity. This assumption is reasonable because the application period for a product released from a container is very short (on the order of minutes or hours) relative to the integration period (one year). Because the above expression for the peak concentration is undefined if a value of 0 is found for the duration of product use, this value is arbitrarily reset to 1 hour in such cases.

The expression $m \cdot w$ in the above equations represents the amount of product used, in grams. In some cases the SRD provides an initial emission rate, $s(o)$, that is assumed to be constant over the period of product use and is normalized to the amount of product applied (i.e., $\mu g/h$ per gram of product applied). Multiplication of $s(o)$ by the amount of product used (m, in grams) and by the duration of product use (q, in hours) yields the total mass released, in μg. Division by 1,000,000 converts the mass released to grams, consistent with the units for $m \cdot w$. Thus, in cases where the emission rate is available in the SRD rather than the weight fraction, the expression $[s(o) \cdot m \cdot q]/1{,}000{,}000$ is used instead of $m \cdot w$.

For a limited number of products the SRD provides both an initial emission rate, $s(o)$, and a factor (r) for the assumed rate of decline in the emission rate over time, corresponding to the following expression for the time-varying emission rate, $s(t)$:

$$s(t) = s(o) \cdot m \cdot e^{-r \cdot t}$$

Because this case is treated as a pulse application with a constant emission rate over the duration of product use, the above expression is integrated from time zero to infinity, yielding the total mass released, in μg. The value of this integral is $s(o) \cdot m/r$, which is divided by 1,000,000 to convert the mass units to grams. Thus, in cases where both the emission rate and the rate of decline are available in the SRD, the expression $[s(o) \cdot m/r]/1{,}000{,}000$ is used instead of $m \cdot w$.

The above calculations provide the peak and integrated concentrations for one episode of product use. Because products can be used multiple times during a year, the C_{peak} and C_{int} values are multiplied by the frequency of product use (events per year, see Table 5-1) to provide an annual perspective.

8.2.2 Case 2: Product Released to Indoor Air from Water

This case also is viewed as a pulse application with a constant emission rate over the duration of product use. The same calculations as described above for case 1 are used, with one difference -- only a fraction of the chemical is assumed to volatilize during the application period; the remainder is assumed to go to waste water after application.

In theory, the volatilization of a chemical from aqueous solution can be described by a two-layer film model (Lyman et al., 1983). This model assumes that the bulk water solution is well mixed, with a thin layer immediately adjacent to the interface in which there is a concentration gradient. There is a corresponding layer of air as well in the air phase. The volatilization flux of a chemical from aqueous solution is controlled by the concentration gradients within this two-layer film. The volatilization flux can be described as:

$$\frac{Z \, dC_{water}}{dt} = - \, K_L \, (C_{water} - \frac{C_{air} \, RT_{air}}{H})$$

where:

Z	=	Depth of aqueous solution (cm)
t	=	Time (hours)
C_{water}	=	Concentration of a chemical in aqueous solution (g/m^3)
C_{air}	=	Concentration of a chemical in the air (g/m^3)
K_L	=	Overall liquid mass transfer constant (cm/hour)
R	=	Gas constant (8.206×10^{-5} m^3 atm mol^{-1} K^{-1})
T_{air}	=	Absolute temperature of the air (K)
H	=	Henry's law constant (m^3 atm mol^{-1})

Since the model is used to screen and rank the volatility of chemicals in consumer products, conservative assumptions can be made to simplify the scenario. It is assumed that the chemical will be immediately removed from the liquid/air interface once it volatilizes and the air concentration of a chemical at the liquid/water interface can be assumed to be negligible. As a result, $C_{water} \gg C_{air} RT/H$ and the above equation turns:

$$\frac{Z \, dC_{water}}{dt} = - \, K_L \, C_{water}$$

Integrating this equation yields:

$$C_t = C_o \, e^{-\frac{K_L \, t}{z}}$$

where:

C_0	=	Concentration of a chemical in aqueous solution at $t = 0$.
C_t	=	Concentration of a chemical in aqueous solution at time t.

Based on the above equation, the percent volatilization of a chemical in aqueous solution during its use can be estimated by:

$$Percent_{volatilization} = (1 - e^{-\frac{K_L \, t}{Z}}) * 100$$

Based on this equation and related equations for K_L (discussed in more detain in Appendix H), the percent of loss via volatilization of chemicals during use of household consumer products such as detergents can be estimated solely from molecular weights, Henry's Law constants (or vapor pressure and solubility), and use scenarios of chemicals.

The Henry's Law constants were either found in a chemical database or else they were estimated based on the solubility and vapor pressure of a chemical, using the following equation (Verschueren, 1996):

$$H = \frac{P_{vp}}{S}$$

where:

P_{vp}	=	Vapor pressure of chemical at 25 ^{0}C (atm)
S	=	Solubility of chemical at 25 ^{0}C (mole/m^3)

Note that percent of volatilization is independent of initial concentrations of chemicals in water. This implies that the percent of loss via volatilization is not affected by the amount of chemical products added into water each time during their use. This advantage eliminates the possible uncertainties associated with variation in amounts of chemicals used from one time to another.

Factors associated with the use scenario include the depth, temperature, and velocity of water along with the velocity and temperature of air above the water-air interface. Currently there are six product/use

scenarios for which these factors have been quantified: laundry detergents; toilet bowl cleaners; dishwashing liquids; hair shampoos and body lotions; liquid hand soaps; and detergents/powders for dishwashers. Use-specific volatilization fractions were calculated for those chemicals contained in Case 2 products and were entered into the chemical.dbf file for use in SRD's ranking calculations.

8.2.3   Case 3: Product Applied to a Surface Indoors

This case can be viewed as a linear ramp application with an exponential emission rate (see Appendix H, pp. 9-12). That is, the product is applied to a surface (e.g., floor or counter) at a constant rate, so that the cumulative mass of any chemical in the applied product increases linearly over time. For each differential (infinitely small) area to which the product is applied, the chemical begins to emit immediately, at a rate that declines exponentially over time as the "reservoir" of chemical mass on the surface area is gradually depleted. The parameter describing the rate at which the emission from a differential area declines over time (r, in units of inverse hours) is derived from the time (d, in units of hours) required for 90 percent of a pure chemical "film" to evaporate as follows (see Appendix H, p. 6):

$$r \; = \; \frac{1}{d} \; \cdot \; \ln \; (10)$$

The chemical-specific value for d is based on an empirical relationship, developed by Chinn (1981), between the 90-percent drying (evaporation) time and the chemical's molecular weight (mw) and vapor pressure (vp, in torr):

$$d \; = \; \frac{145}{(mw \cdot vp)^{0.9546}}$$

If either the molecular weight or the vapor pressure is unavailable for a chemical, then a default value of 0.01 is used for d. If the rate of decline in the emission rate is available in the SRD, then it is used directly rather than calculated from the above equations.

Although some chemicals with a high molecular weight and a low vapor pressure can take a year or longer to completely evaporate, most will evaporate over a period on the order of a month or shorter. To avoid complex calculations to handle a small number of chemicals, it is currently assumed that all chemicals evaporate within a year; under this assumption, the calculation for the time-integrated concentration that was given in Section 8.2.1 applies equally here.

The peak concentration for this case will occur at the end of the application period or some time thereafter. The calculation for the peak concentration involves the amount of product used (m), the weight fraction of the chemical in the product (w), the duration of product use (q), the loss rate (k), the volume of the indoor environment (v), and the rate of decline in chemical emissions (r). Intermediate calculations are required for the emission rate (s) and the indoor concentration (C) at the end of the application period (see Appendix H, p. 10), and for the time (u) at which the maximum indoor concentration occurs (see Appendix H, bottom of p. 11 and p. 12):

$$s = \frac{m \cdot w}{q \cdot v} \cdot (1 - e^{-r \cdot q})$$

$$c = \frac{m \cdot w}{q \cdot v} \cdot r \cdot \left(\frac{1}{r \cdot k} + \frac{e^{-r \cdot q}}{r \cdot (r - k)} - \frac{e^{-k \cdot q}}{k \cdot (r - k)} \right)$$

$$u = \frac{-1}{r \cdot k} \cdot \ln \left(\frac{k \cdot [s + (r - k) \cdot c]}{r \cdot s} \right)$$

The peak concentration is then calculated as

$$C_{peak} = \frac{s + (r - k) \cdot c}{r - k} \cdot e^{-k \cdot u} - \frac{s}{r - k} \cdot e^{-r \cdot u}$$

The time-integrated concentration is calculated in the same manner as for case 1. As in the previous cases, both the peak and the time-integrated concentration are multiplied by 1,000, to convert from grams to milligrams, and by the number of product-use episodes per year, to provide an annual perspective. In a limited number of cases either the initial emission rate -- s(o), in μg/h per gram of product applied -- or this initial rate and the rate of decline (r) in the emission rate over time are available in the SRD. As described in Section 8.2.1, the expression [s(o)·m·q]/1,000,000 is substituted for m·w in the above equations when only s(o) is available, and the expression [s(o)·m/r]/1,000,000 is substituted when both s(o) and r are available.

It is possible for the parameters r and k to be equal; in this case, the above expressions for c, u, and C_{peak} are undefined. Solutions for this parameters-equal case, given in Appendix H (p. 10 and p. 12) but not summarized here, are also used by the program as needed.

8.2.4 Case 4: Product or Material Placed Indoors

This case can be viewed as an instantaneous application with an exponentially declining emission rate (see Appendix H, p. 15). Currently there are no products classified under this case, but there may be in the future. Calculations for a product involve the quantity used (m), the weight fraction (w), the duration of use (q), the loss rate (k), the volume of the environment (v), the initial emission rate [s(o)], and the rate of decline in the emission rate over time (r). The time-varying emission rate for a specific chemical, s(t), can be described by the following equation:

$$s(t) = s(o) \cdot e^{-r \cdot t}$$

where:

s(o) is in μg/h (after multiplication by the amount of product used, in grams).

The value for r is used directly, if available in SRD, or is derived from the assumption that 99 percent of the chemical evaporates over the duration of product use:

$$r = \frac{-\ln(0.01)}{q}$$

where 0.01 is the fraction of the product remaining at the end of product use. Thus, the same value of r is assumed for all chemicals, regardless of volatility. If a value of zero is found for q in the PRODUCT-ENVIRONMENT file, then this value is reset to 720 hours (one month). Neglecting the small amount of product remaining at the end of product use, the mass of a chemical in the product that is released to the indoor air over the duration of use is equal to the quantity used times the weight fraction, or m·w. The same mass can be obtained by integrating s(t) from zero to infinity; the value of this integral is s(o)/r, leading to the relationship

$$s(o) = m \cdot w \cdot r$$

The above equation provides an estimate for s(o) in units of g/h. If a value for s(o) is available in the SRD, then this value has units of μg/h (after multiplication by the amount of product used) and is therefore

divided by 1,000,000 to convert to g/h. Given these values for s(o) and r, the peak concentration is calculated as

$$C_{peak} = \frac{s(o)}{v \cdot r} \cdot \left(\frac{r}{k}\right)^{\frac{k}{k-r}}$$

and the time-integrated concentration is calculated as

$$C_{int} = \frac{s(o)}{v \cdot (r-k)} \cdot \left[\frac{1}{r} \cdot (e^{-r \cdot t2} - e^{-r \cdot t1}) - \frac{1}{k} \cdot (e^{-k \cdot t2} - e^{-k \cdot t1})\right]$$

where t1 is the beginning of the integration period (0 hours) and t2 is the end of the integration period (8760 hours). As with the other cases for products, the values for C_{peak} and C_{int} are multiplied by 1,000, to convert from grams to milligrams, and by the number of usage episodes per year, to provide an annual perspective. Solutions for the case where r = k (see Appendix H, p. 15) are also used by the program as needed.

The calculations for a material placed in an environment are similar to those given above, but involve different values for s(o), r, t1 and t2. The value for r is used directly, if available in the SRD, or is derived from the assumption that 99 percent of the chemical mass will be released from the material over a period of 5 years (43,800 hours), leading to the relationship

$$r = \frac{-\ln(0.01)}{43,800}$$

The value for the initial emission rate is provided in the MATERIAL-ENVIRONMENT file, in units of µg/h per unit of material (e.g., m² of carpeting). This value is divided by 1,000 to convert to mg/h per unit of material and then multiplied by the loading rate (number of material units per m³ of volume) and the indoor volume (m³) to derive an initial emission rate, s(o), in mg/h.

The program calculates two values for both the peak and the time-integrated concentration, one assuming a short duration since installation (currently set at 30 days) and one assuming a longer duration since installation (currently set at 2 years). The resultant values are weighted by the fraction of buildings assumed to be represented by these durations (see Section 5.2) to obtain final peak and integrated values. The equation

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for the time-integrated concentration is the same as that above for products, except that t1 is equal to 720 hours for the short duration since installation and 17,520 hours for the longer duration. Since the integration is over a period of one year, the value for t2 in either case is the sum of t1 plus 8,760 hours. Because the material has been emitting for some time, in either case, at the start of the period of assumed exposure, the peak concentration is that occurring at the start of the integration period:

$$C_{peak} = \frac{s(o)}{v \cdot (r - k)} \cdot (e^{-k \cdot t_1} - e^{-r \cdot t_1})$$

8.3   Environment Weights

Weights assigned to each environment, which are used in calculating the total score for each chemical in a product or material (see Section 8.1), reflect the relative share of full-time-equivalent (FTE) exposures associated with the environment. An FTE exposure equates to one individual spending 100 percent of his or her time in the environment over the course of a year. For example, two people who both spend 50 percent of their time in the residence are equivalent to one FTE residential exposure.

The numerator for calculating the weight for an environment is obtained by multiplying together the following three quantities:

! Number of buildings (Replication Factor in the ENVIRONMENT file);

! Size of each population in the building (from the PEOPLE ENVIRONMENT file); and

! Average fraction of time spent by each population in the building (from the PEOPLE-ENVIRONMENT file).

The denominator is simply the sum of the numerator values across all environments. Thus, the weights sum to unity when added across environments. More specifically, the weight that is calculated for each environment can be expressed as follows:

$$w_i = \frac{NB_i \cdot (\sum_{j=1}^{n} SP_{ij} \cdot FT_{ij})}{\sum_{i=1}^{m} NB_i \cdot (\sum_{j=1}^{n} SP_{ij} \cdot FT_{ij})}$$

where:

        w is the weight

        NB is the number of buildings associated with the environment

        SP is the size of the population per building

        FB is the fraction of buildings in which the product or material is used

        I is a subscript denoting different types of environments

        j is a subscript denoting different populations that occupy an environment

        m is the number of environments selected by the user when ranking products

        n is the number of populations occupying each environment (1 or 2).

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