Exposure and Fate Assessment Screening Tool (E-FAST)

Version 2.0

Documentation Manual

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ACKNOWLEDGMENTS AND DISCLAIMER

To comply with the accessibility requirements of Section 508 of the Rehabilitation Act Amendments, the text, Figures, Tables, and Equations in this Manual are now accessible via the assistive technology reader.

TABLE OF CONTENTS

1.0 INTRODUCTION 1-1

1.1 Installing E-FAST V2.0 1-2
1.2 Running E-FAST V2.0 1-5
1.3 Saving, Printing, and Revising E-FAST V2.0 Results 1-7
1.3.1 *Saving Results* 1-7
1.3.2 *Printing Results* 1-8
1.3.3 *Revising Results* 1-8

2.0 PHYSICAL-CHEMICAL PROPERTIES AND FATE 2-1

3.0 MODELS FOR SCREENING-LEVEL EXPOSURE ESTIMATES 3-1

3.1 General Population and Ecological Exposure from Industrial Releases 3-3
3.1.1 Release Information Page 3-3
3.1.1.1 *Surface Water Releases* 3-6
3.1.1.2 *Landfill Releases* 3-10
3.1.1.3 *Ambient Air Releases* 3-10
3.1.2 Exposure Factors Page 3-13
3.1.3 Environmental Release Results Page 3-18
3.1.4 Rivers Results Page 3-18
3.1.4.1 *Rivers Results Page – General Site Information* 3-20
3.1.4.2 *Rivers Results Page – Drinking Water Information* 3-22
3.1.4.3 *Rivers Results Page – Fish Ingestion Information* 3-24
3.1.4.4 *Rivers Results Page – Endangered Species* 3-26
3.1.5 SIC Code Results Page 3-27
3.1.5.1 *SIC Code Results Page – General SIC Code Information* 3-29
3.1.5.2 *SIC Code Results Page – Drinking Water Information* 3-30
3.1.5.3 *SIC Code Results Page – Fish Ingestion Information* 3-31
3.1.6 Lakes Results Page 3-32
3.1.6.1 *Lakes Results Page – General Lake Information* 3-33
3.1.6.2 *Lakes Results Page – Fish Ingestion Information* 3-34
3.1.6.3 *Lakes Results Page – Endangered Species* 3-36
3.1.7 Landfill Results Page 3-36
3.1.8 Inhalation Results Page 3-40
3.1.8.1 *Inhalation Results Page – Inhalation Exposure Estimates* 3-41
3.1.8.2 *Inhalation Results Page – Release Information* 3-48
3.1.8.3 *Inhalation Results Page – Meteorological/Terrain and Downwash Information* 3-49
3.1.8.4 *Inhalation Results Page – SCREEN3 Model Results* 3-50
3.1.9 PDM Site-Specific Results Page 3-51
3.1.10 PDM SIC Code Results Page 3-54
3.2 Down-the-Drain 3-57
3.2.1 Consumer Disposal Inputs Page 3-57
3.2.2 Disposal Results Page 3-58
3.2.2.1 *Disposal Results Page – Concentrations* 3-60
3.2.2.2 *Disposal Results Page – PDM Information* 3-61
3.2.2.3 *Disposal Results Page – Drinking Water Information* 3-63
3.2.2.4 *Disposal Results Page – Fish Ingestion Information* 3-66

TABLE OF CONTENTS (Continued)

3.3 Consumer Exposure Module (CEM) 3-69
3.3.1 Introduction Page 3-69
3.3.2 Scenario Page 3-70
3.3.2.1 *Generic Consumer Product Scenarios* 3-71
3.3.2.2 *User-Defined Scenario* 3-76
3.3.2.3 *Exposed Population* 3-78
3.3.3 Inhalation Input Page 3-78
3.3.4 Day of Use Input Page 3-80
3.3.5 Days After Use (Non-Use Days) Input Page 3-81
3.3.6 Dermal Input Page 3-82
3.3.7 Estimation of Indoor Air Concentrations 3-85
3.3.7.1 *Pollutant Mass Balance* 3-86
3.3.7.2 *Air Mass Balance* 3-86
3.3.8 Estimation of Consumer Exposures 3-90
3.3.8.1 *Estimation of Inhalation Exposures* 3-92
3.3.8.2 *Estimation of Dermal Exposures* 3-95
3.4 Probabilistic Dilution Model (Stand-alone PDM) 3-97
3.4.1 PDM Site-Specific Page 3-98
3.4.2 PDM SIC Code Results Page 3-100

4.0 REFERENCES 4-1

Appendix A Definitions for Physical-Chemical/Fate Properties A-1

Appendix B Surface Water Discharge Information Organization and Sources B-1

Appendix C Statistical Framework of Probabilistic Dilution Model (PDM) C-1

Appendix D Issues Pertaining to Inhalation Exposure Estimation Conducted in CEM D-1

LIST OF TABLES

Table 2-1. Physical-Chemical Properties Required for Modeling in E-FAST V2.0 2-2
Table 3-1. Default Values for Select Input Parameters to SCREEN3 3-12
Table 3-2. Default Exposure Parameter Values Used in E-FAST V2.0 3-15
Table 3-3. Default Surface Area/Body Weight (SA/BW) Ratios Used in CEM Module for Bar Soap 3-74

LIST OF FIGURES

Figure 1-1. E-FAST V2.0 Welcome Screen 1-3
Figure 1-2. Customer Information Screen 1-3
Figure 1-3. Destination Folder Screen 1-4
Figure 1-4. Ready to Install Screen 1-4
Figure 1-5. Installing EFAST2 Screen 1-5
Figure 1-6. Installation Completed Screen 1-5
Figure 1-7. E-FAST V2.0 Introductory Screen 1-6
Figure 1-8. E-FAST V2.0 Model Schematic 1-6
Figure 1-9. Change the Data Drive Screen 1-8

LIST OF FIGURES (Continued)

Figure 2-1. PChem/Fate Inputs Screen 2-1

Figure 3-1. Screening Level Main Page 3-1
Figure 3-2. General Release Information Page 3-4
Figure 3-2a. General Release Information Page – Surface Water 3-5
Figure 3-2b. General Release Information Page – Landfill 3-5
Figure 3-2c. General Release Information Page – Ambient Air 3-6
Figure 3-3. Select a Facility Screen 3-8
Figure 3-4. Select an SIC Code Screen 3-10
Figure 3-5. SCREEN3 – Release Information 3-11
Figure 3-6. SCREEN3 – Meteorological and Terrain Information 3-12
Figure 3-7. SCREEN3 – Downwash Information 3-13
Figure 3-8. Exposure Factors Page 3-14
Figure 3-9. Environmental Release Results Page 3-18
Figure 3-10. Rivers Results Page – Aquatic Exposure Estimates - Surface Water 3-20
Figure 3-11. Rivers Results Page – Drinking Water Exposure Estimates 3-23
Figure 3-12. Rivers Results Page – Fish Ingestion Exposure Estimates 3-25
Figure 3-13. Rivers Results Page – Endangered Species 3-27
Figure 3-14. SIC Code Results Page – Aquatic Exposure Estimates - Surface Water 3-28
Figure 3-15. SIC Code Results Page – Drinking Water Exposure Estimates 3-30
Figure 3-16. SIC Code Results Page – Fish Ingestion Exposure Estimates 3-31
Figure 3-17. Lakes Results Page – Dilution Factors and Water Concentrations 3-33
Figure 3-18. Lakes Results Page – Fish Ingestion Exposure Estimates 3-35
Figure 3-19. Landfill Results Page – Landfill Exposure Estimates 3-37
Figure 3-20. Inhalation Results Page – Inhalation Exposure Estimates 3-41
Figure 3-21. Inhalation Results Page – Release Information 3-49
Figure 3-22. Inhalation Results Page – Meteorological/Terrain and Downwash Information 3-50
Figure 3-23. Inhalation Results Page – SCREEN3 Model Results 3-51
Figure 3-24. PDM Site-Specific Results Page 3-52
Figure 3-25. PDM SIC Code Results Page 3-55
Figure 3-26. Consumer Disposal Inputs Page – Selecting PDM 3-58
Figure 3-27. Disposal Results Page – Aquatic Exposure Estimates - Surface Water 3-59
Figure 3-28. Disposal Results Page – PDM Disposal Exposure Estimates 3-62
Figure 3-29. Disposal Results Page – Drinking Water Exposure Estimates 3-64
Figure 3-30. Disposal Results Page – Fish Ingestion Exposure Estimates 3-66
Figure 3-31. CEM Introduction Page 3-70
Figure 3-32. Scenario Page 3-71
Figure 3-33. User-Defined Scenario Description Screen 3-76
Figure 3-34. Inhalation Input Page 3-79
Figure 3-35. Day of Use Input Page 3-80
Figure 3-36. Days After Use (Non-Use Days) Input Page 3-82
Figure 3-37. Dermal Input Page 3-83
Figure 3-38. CEM Inputs 3-90
Figure 3-39. CEM Inhalation Exposure Estimates 3-91
Figure 3-40. CEM Dermal Exposure Estimates 3-91
Figure 3-41. PDM Site-Specific Results Page (Stand-alone) 3-97
Figure 3-42. PDM SIC Code Results Page (Stand-alone) 3-100

1.0 INTRODUCTION

The Exposure and Fate Assessment Screening Tool, Version 2.0, also known as E-FAST V2.0, is a screening-level computer tool that allows users to estimate chemical concentrations in water to which aquatic life may be exposed, as well as generate human inhalation, drinking water ingestion, and fish ingestion exposures resulting from chemical releases to air, water, and land. In addition, E-FAST V2.0 identifies endangered species in the vicinity of releases at known locations—"site-specific" releases. E-FAST V2.0 also may be used to assess inhalation and dermal exposures to chemicals that may result from the use of certain types of consumer products. The exposed populations assessed by the model are either some segment of the general population or consumers. Worker exposures are not assessed in this model. The exposure scenarios in E-FAST V2.0 contain default exposure parameter values that allow the exposures to be estimated with minimal data entry. Because E-FAST V2.0 incorporates defaults of either a combination of upper percentile and mean exposure parametric values or all upper percentile parametric values, the exposure/dose estimates are considered to be high-end estimates.

E-FAST V2.0 was developed to support U.S. Environmental Protection Agency (EPA) assessments of potential exposures to chemicals. Screening-level models are rarely if ever used as the sole justification for regulatory decision-making at EPA. Additional data and more rigorous tools are used to improve the estimates of exposures and risks for such decisions. Thus, the model's results may not accurately reflect all of the information and data used by EPA to make a regulatory decision on a chemical.

When Should I Use the Model?

E-FAST V2.0 is appropriate for use as a screening tool to assess potential exposures from chemical discharges to air (stack or fugitive releases), surface water, or land. E-FAST V2.0 can also be used to estimate potential inhalation and dermal exposures to consumer products, such as hard surface cleaners, soaps, air fresheners, paints, gasoline, and motor oil.

When Is It Not Appropriate To Use the Model?

E-FAST V2.0 is characterized by EPA as a "screening model." Screening model results are intended to be conservative, meaning that predicted concentrations and exposures are likely to be at the high end of or higher than concentrations that might actually be occurring in a real-world setting. If an exposure estimated by a screening model results in an unacceptably high health risk, then an appropriate next step in the assessment process would be to refine the parameter input or perform the assessment with different and perhaps more complex models. Another response might be to consider monitoring to gather actual emissions data that can be used to estimate exposure.

E-FAST V2.0 does not estimate physical-chemical properties, environmental fate parameters, or environmental releases. If measured physical-chemical and environmental fate data do not exist, software available from EPA or commercially available estimation software can be used to estimate these properties. The exposures estimated by E-FAST V2.0 reflect the amounts of chemical inhaled, ingested, or on the surface of the skin. In general, E-FAST V2.0 does not estimate chemical absorption; however, the Consumer Exposure Module (CEM) (See Section 3.3) does contain the option to estimate an absorbed dermal dose if permeability coefficient data are available.

How Does E-FAST V2.0 Relate to Previous Versions of E-FAST Developed by OPPT?

E-FAST V2.0 replaces E-FAST beta and incorporates revisions based on internal and external peer review. Revisions include an update of data sources, enhanced programming capabilities, and improved user-friendliness, including an option to save in Corel® WordPerfect or Microsoft® Word formats.

Potential Average Daily Dose (ADD_{POT}) and Average Daily Concentration (ADC_{POT}) values are not estimated in E-FAST V2.0 because averaging times for non-cancer chronic or subchronic effects vary by effect. In these cases, it is suggested that the averaging times should be determined on a case-by-case basis via communication between the exposure assessor and hazard assessor. When the appropriate averaging times have been determined, potential ADD and ADC values may be estimated by substituting those averaging times for the lifetime averaging time in the potential Lifetime Average Daily Dose ($LADD_{POT}$) and Lifetime Average Daily Concentration ($LADC_{POT}$) equations.

E-FAST V2.0 March 2007 differs from E-FAST V2.0 April 2006 in that an error in the landfill calculation was corrected - this correction is reflected in Figure 3-19.

How Do I Get Started Using E-FAST V2.0?

To run E-FAST V2.0, your computer system should meet the following requirements:

- An IBM-compatible computer with a Pentium processor or higher
- Windows 95 or higher operating system
- 32 MB or higher of RAM (64 MB recommended)
- 85 MB of hard disk space

Also, E-FAST V2.0 was designed for a computer monitor with a minimum 800 × 600 screen resolution for maximum user-friendliness.

1.1 Installing E-FAST V2.0

To install E-FAST V2.0, download the installation file from EPA's Office of Pollution Prevention and Toxics (OPPT) website (http://www.epa.gov/oppt/exposure). After downloading is complete, run the installation program (self-extracting zip file). The install program begins with a window that indicates that the computer is performing certain functions such as checking, configuring, and preparing to install E-FAST V2.0. This screen requires no user input. In the E-FAST V2.0 Welcome screen (shown in Figure 1-1), select "Next" to display the Customer Information screen and enter your user name and the company name (Figure 1-2). After you have entered this information, click on "Next" to continue.

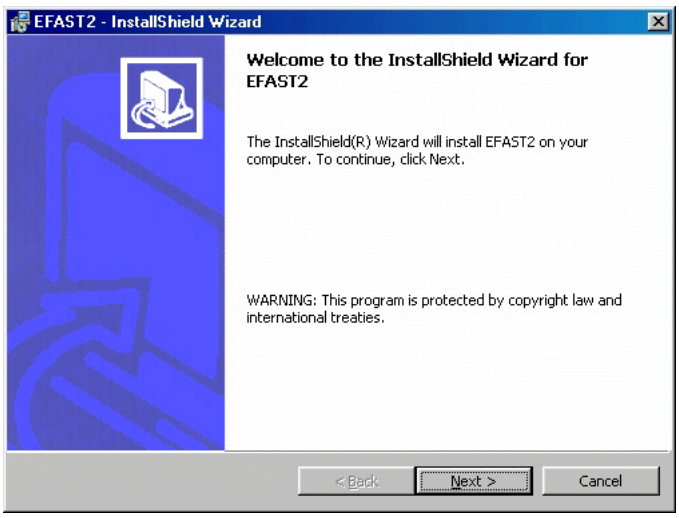

Figure 1-1. E-FAST V2.0 Welcome Screen

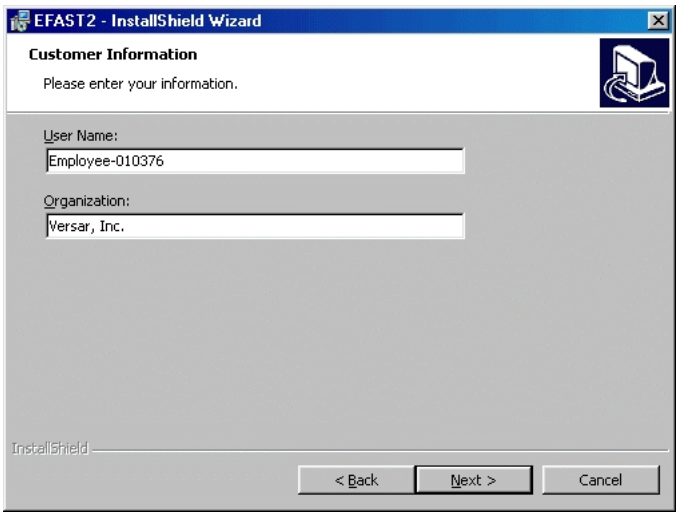

Figure 1-2. Customer Information Screen

The next screen, Destination Folder (Figure 1-3), allows you to install the program under the default directory shown on the screen or in another directory. If you wish to install E-FAST V2.0 in the default directory, and your computer already contains a directory named C:\Program Files\EFAST2, it should be removed or renamed prior to installing E-FAST V2.0. To install E-FAST V2.0 in a different directory, click the "Browse" button and select the desired directory and path, then select "Next." Note that the name of the Program Folder in the Windows® Start Menu will be "EFAST 2.0" and cannot be changed during the installation of the model.

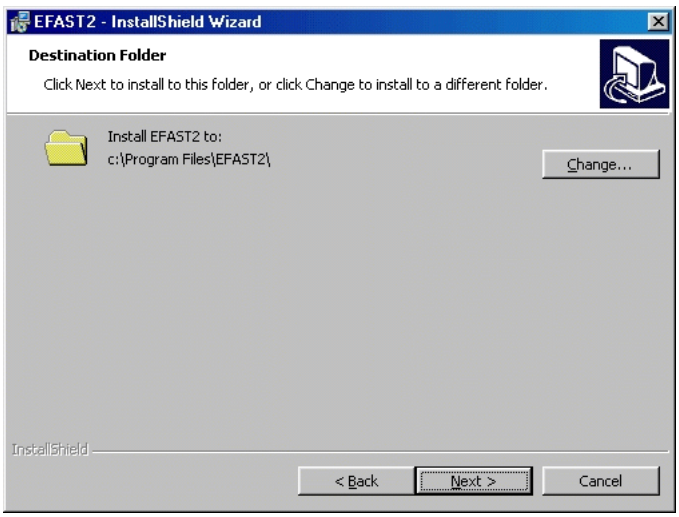

Figure 1-3. Destination Folder Screen

E-FAST V2.0 is ready to install the program files on your computer. Figure 1-4 shows the information you have entered so far. If you need to modify anything, click on the "Back" button to make the necessary changes. Otherwise, click on the "Install" button to begin the installation. The Installing EFAST2 screen, shown in Figure 1-5, will automatically disappear once the necessary files have been installed.

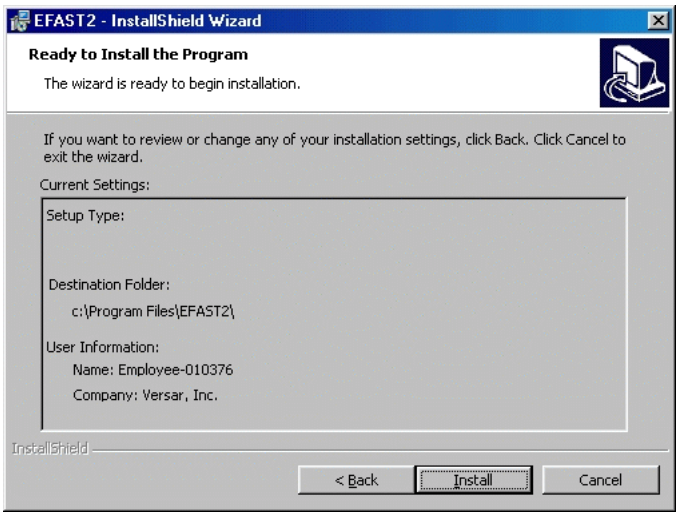

Figure 1-4. Ready to Install Screen

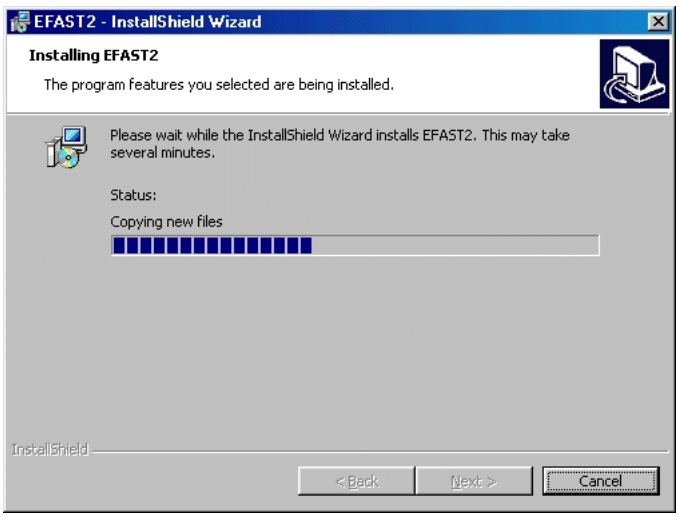

Figure 1-5. Installing EFAST2 Screen

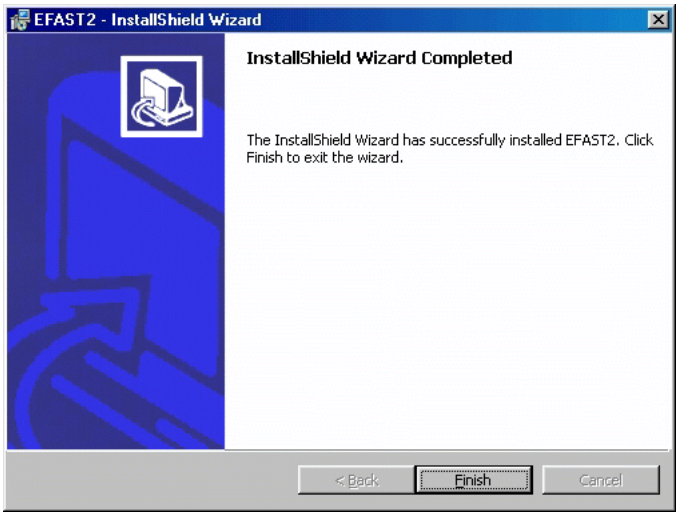

Figure 1-6. Installation Completed Screen

Figure 1-6 shows the final screen for the E-FAST V2.0 installation program. Click on the "Finish" button to complete the process.

1.2 Running E-FAST V2.0

After installing E-FAST V2.0, open it by clicking on the "Start" button on the Windows taskbar at the bottom of the screen and selecting the E-FAST V2.0 under the Programs listing. The E-FAST V2.0 Introductory screen (Figure 1-7) shows E-FAST V2.0's three major components, which are accessible from the E-FAST V2.0 Introductory screen. Figure 1-8 shows a schematic of how each component interacts with the numerous models E-FAST V2.0 uses to calculate exposure.

Figure 1-7. E-FAST V2.0 Introductory Screen

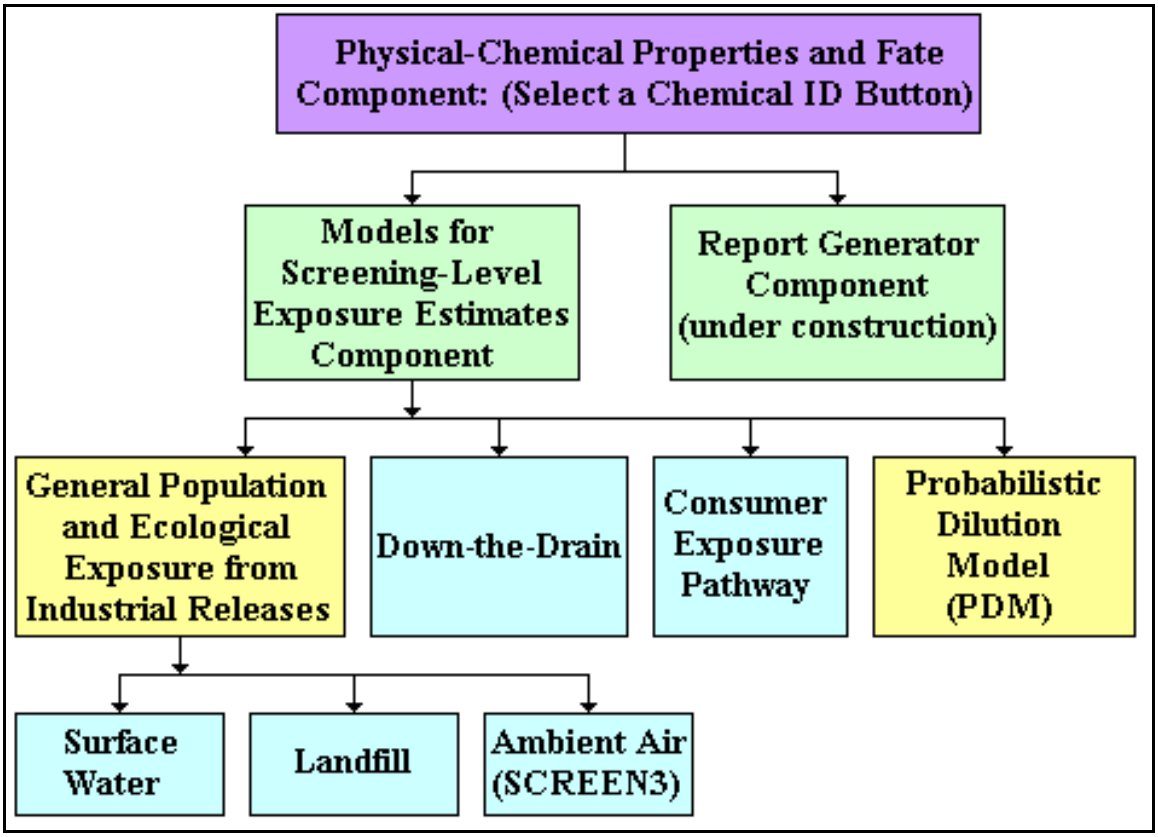

Figure 1-8. E-FAST V2.0 Model Schematic

The three components that make up E-FAST V2.0 are briefly described below:

1. **Physical-Chemical Properties and Fate Component**. This component of E-FAST V2.0 defines the physical-chemical properties you will need for use with the other modeling components. You cannot access the other components of E-FAST V2.0 without first going to this component. To access it, click on the bar, "Select a Chemical ID and modify its physical-chemical and fate properties before continuing to any module" on the E-FAST V2.0 Introductory screen. This will take you to the PChem/Fate Inputs screen (Figure 2-1), where the program will define the physical-chemical properties needed for the other modeling modules. See Section 2.0 for a more detailed description of this model component. After filling in the required information and clicking on "Select This Chemical ID," you will be returned to the E-FAST V2.0 Introductory screen, where you may select another model component.

2. **Models for Screening-Level Exposure Estimates Component**. This component provides modeled, screening-level estimates of the concentrations and the potential doses of chemicals released to air, surface water, and landfills, and from consumer products. The estimates are designed to be conservative (i.e., to use high-end estimates of exposure or even to overestimate exposure). A detailed description of the exposure and fate modeling process is presented in Section 3.0.

3. **Report Generator Component**. A future capability of E-FAST V2.0 will be the addition of an exposure summary report generator. EPA envisions that the report generator would assist the assessor in completing summary exposure reporting formats such as the formats that are currently under development within the Organization for Economic Cooperation and Development (OECD). If the assessor had monitoring data for an exposure scenario (EPA's preference), the report generator would prompt the user for an exposure estimate based upon that data as well as other relevant information associated with the monitoring data (e.g., the objective of the monitoring study, a brief description of the study design, etc.). If the assessor did not have monitoring data, the report generator would be linked to the E-FAST V2.0 exposure models and many of the exposure summary report entries would be filled in by E-FAST V2.0.

E-FAST V2.0 also provides on-screen guidance to assist users with questions they may have while running the model. You can access the on-screen guidance by clicking on the "Help" button found on most data entry screens.

1.3 Saving, Printing, and Revising E-FAST V2.0 Results

1.3.1 Saving Results

The **Change Data Drive** menu at the upper left-hand corner of the Introductory screen (Figure 1-7) allows you to change the directory to which model results are saved. By default, results are written to C:\Program Files\EFAST2\results. To change this directory, click on the bar "Change the Data Drive." A pop-up window (Figure 1-9) will guide you through the process of selecting a new directory. Click on **Save changes** to save the new directory.

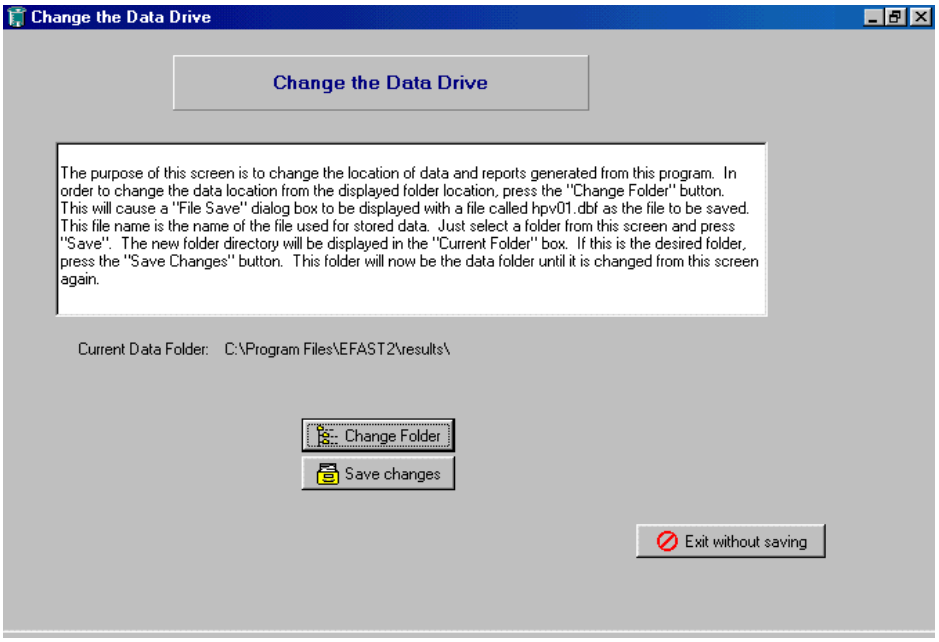

Figure 1-9. Change the Data Drive Screen

1.3.2 Printing Results

Although the Report Generator is not yet functional, E-FAST V2.0 has two options for printing. Single results pages may be printed by clicking on the "Print Page" button on the right-hand side of each results screen with the exception of CEM (Printing results screens from CEM is accomplished by using pull-down menus.); this will send the information displayed on the screen to the printer. When the model is run, results for each scenario are written to a file in the folder specified using the procedure in Section 1.3.1. The user may specify to save outputs in Corel® WordPerfect or Microsoft® Word formats (see Section 3.0). E-FAST V2.0 uses components of Microsoft® Word to generate outputs in Word format. If the user does not have Microsoft® Word, this option is not available to the user.

1.3.3 Revising Results

After a user has completed a model run, the results are saved in the directory selected by the user as described above in Section 1.3.1. To recall a model run for whatever reason (e.g., to modify, add, or delete information), click on the "Select a Chemical ID and modify its physical-chemical and fate properties before continuing to any module" bar, as described in Section 1.2. Once at the P-Chem/Fate input screen, rather than entering a new Chemical ID, use the pull-down menu to select a previous model run. As the user proceeds through the various modules, all of the previous inputs will be displayed, and can be modified by the user. Additional scenarios can be added to the model run as well.

2.0 PHYSICAL-CHEMICAL PROPERTIES AND FATE

The PChem/Fate Inputs screen (Figure 2-1) prompts you to select the desired modeling modules and Chemical ID (e.g., CAS number) for the chemical of interest. Note that only one chemical of interest may be selected for each model run. The Chemical ID will be used throughout the execution of the E-FAST V2.0 program. The modeling modules you can select include General Population and Ecological Exposure from Industrial Releases, including surface water, landfill, and ambient air releases; Down-the-Drain; Consumer Exposure Pathway; and the Probabilistic Dilution Model (PDM). The Chemical ID combination list box contains a list of all Chemical IDs that have been entered since the model was first installed. You may select one of these Chemical IDs or enter a new ID by typing it into the combination list box. If you select a pre-existing ID, E-FAST V2.0 will fill in the properties that were used the last time that Chemical ID was modeled. Otherwise, the fields for physical-chemical properties and fate will be blank.

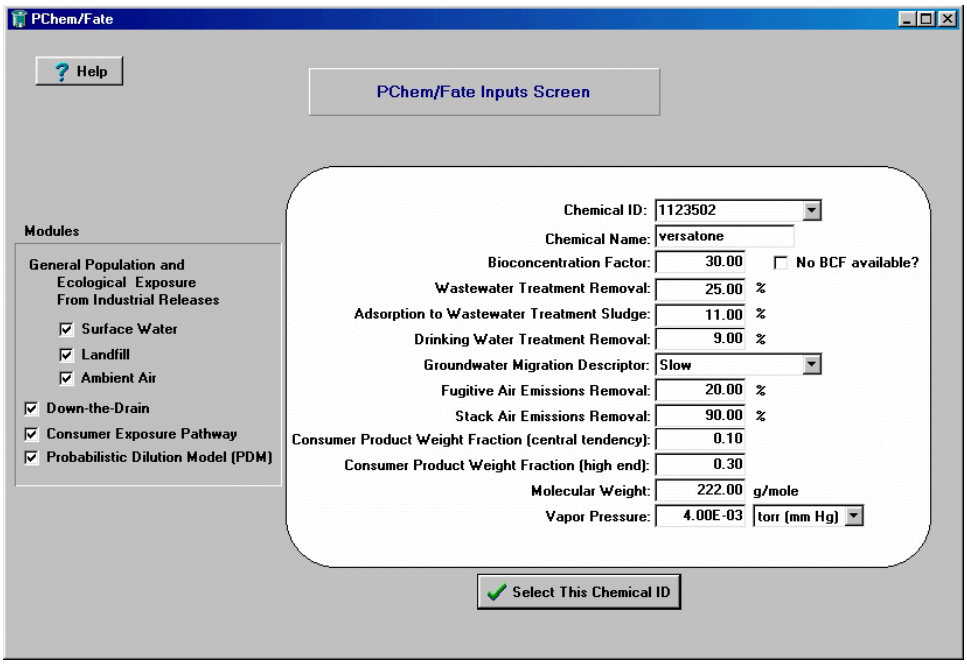

Figure 2-1. PChem/Fate Inputs Screen

After selecting a Chemical ID or entering a new one, you may select the media and the exposure pathway you wish to model by clicking on the appropriate checkboxes on the left-hand side of the screen. The fields that appear at the center of the screen depend on the status of the checkboxes; you will only be prompted for physical-chemical properties that are required for the models you have chosen to run. Depending on the modules you selected, you must enter some or all of the following relevant physical-chemical properties, in the appropriate units and in the adjacent blanks on the screen: the bioconcentration factor (BCF) of the chemical, if known (unitless); the wastewater treatment removal percentage for the chemical (%); the adsorption in wastewater treatment of the chemical to sludge (%); the drinking water treatment removal percentage for the chemical (%); the groundwater migration descriptor of the chemical (unitless); the removal rates for fugitive and stack air emissions (%); the weight fraction of the chemical in consumer products (Central Tendency and High-End - e.g., median and 90th percentile, respectively); the molecular weight of the chemical (g/mol); and the vapor pressure of the chemical (torr, atm, mb, or Pa, which you may select from a drop-down list). Definitions of these terms are provided in Appendix A.

Table 2-1 shows the available modules and the physical-chemical and fate properties you are asked to provide.

Table 2-1. Physical-Chemical Properties Required for Modeling in E-FAST V2.0

	Surface Water	Landfill	Ambient Air	Down the Drain	Consumer Exposure Pathway	Probabilistic Dilution Model (PDM)
Chemical Name/Chemical ID	✔	✔	✔	✔	✔	✔
Bioconcentration Factor	✔			✔		
Wastewater Treatment Removal	✔			✔		✔
Adsorption to Wastewater Treatment Sludge	✔	✔				
Drinking Water Treatment Removal	✔	✔				
Groundwater Migration Descriptor		✔				
Fugitive Air Emissions Removal			✔			
Stack Air Emissions Removal			✔			
Consumer Product Weight Fraction (Central Tendency)					✔	
Consumer Product Weight Fraction (High-End)					✔	
Molecular Weight					✔	
Vapor Pressure					✔	

The model inputs that are requested of you as you move forward through the input screens depend on which models have been selected on this screen. For example, if you do not mark the Surface Water checkbox, you will not be prompted to enter surface water releases. For the sake of clarity, the instructions and screen images in Section 3.0 assume that all six checkboxes are selected. If this is not the case for you, your input screens will appear slightly different, but the instructions that relate to the models you are interested in will remain the same.

Once you have put a checkmark beside all desired modules and entered all required values, click on “Select this Chemical ID” to return to the E-FAST V2.0 Introductory screen (Figure 1-7). You may now proceed to the Models for Screening-Level Exposure Estimates component of E-FAST V2.0.

3.0 MODELS FOR SCREENING-LEVEL EXPOSURE ESTIMATES

After you have selected the Chemical ID for the chemical of interest, you can click on "Models for Screening-Level Exposure Estimates." The Screening Level Main page will appear (see Figure 3-1).

Figure 3-1. Screening Level Main Page

The Screening Level Main page consists of four exposure assessment modules, which you can open by clicking on the appropriate button:

- **General Population and Ecological Exposure from Industrial Releases** — addresses human exposures resulting from facility releases to air, water, and land. Incorporates the Probabilistic Dilution Model (PDM) to address aquatic and ecological exposures and risks from releases to water. Also identifies endangered animal species near site-specific water releases. See Section 3.1.

- **Down-the-Drain** — addresses human and aquatic ecological exposures and risks resulting from chemical releases in household wastewater. See Section 3.2.

- **Consumer Exposure Pathway** — addresses various consumer exposure pathways (i.e., dermal and inhalation) using CEM. The model calculates exposure resulting from consumer use. See Section 3.3.

- **Probabilistic Dilution Model (PDM)** — addresses aquatic ecological exposures and risks. PDM is used by the General Population and Ecological Exposure from Industrial Releases, and Down-the-Drain modules to calculate concentrations and to predict the number of days per year a chemical's concentration of concern (COC) in an ambient water body will be exceeded by the

discharge from a facility. This module allows the user to run the model independently of the release scenarios that are used in those modules. See Section 3.4.

In addition to the four modules, this screen contains a box where you may select the exposed population for which the model will estimate concentrations and exposures. The default selection is for adults, but the user may also select youths (children 13-19 years), children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years old, or infants less than one year old. To the right is a box marked "Select Document Report Format," where you may select the word processing format in which model output files will be saved. At the bottom of the screen is a button marked "Return to E-FAST2 Main Page," which you may click if you want to return to the E-FAST V2.0 startup screen.

3.1 General Population and Ecological Exposure from Industrial Releases

The General Population and Ecological Exposure from Industrial Releases module was developed by OPPT as a software program to generate estimates of chemical concentrations in surface waters to which aquatic life may be exposed and estimates of human inhalation, drinking water, and fish ingestion exposures resulting from chemical releases to water, land, and air.

The General Population and Ecological Exposure from Industrial Releases screen consists of two pages: the Release Information page and the Exposure Factors page. Each page appears as a tab at the top of the screen. When you first access this module, only the Release Information page is present. After entering the required data for all environmental releases, as described below, the Exposure Factors page appears; the Release Information page is hidden and can be accessed by clicking on the Release Information tab at the top of the screen.

The following text describes, in outline form, the data entry procedure that is described in this section:

1. Release Information Page
   For each release activity:
   - Enter number of sites
   - Select and Enter surface water, landfill, and/or ambient air releases
   - Click “next release activity” button and repeat above steps until all release activities are entered

2. Click “Release activities completed...” button

3. Exposure Factors Page
   - Enter exposure factors

4. Click “Calculate, save results...” button to run model

3.1.1 Release Information Page

The Release Information page presents three sub-pages labeled “General Release Info,” and “Select a Facility,” or “Select an SIC code.” The “General Release Info” sub-page is the main page for entering release data. The other two are secondary pages used to specify a facility or industrial category for surface water releases, and are discussed in Section 3.1.1.1. On the General Release Information page (Figure 3-2), you may enter releases to the environment for any number of release activities; a release activity is defined as an industrial or commercial process that causes a chemical to enter the environment through the air, surface water, and/or groundwater (i.e., landfill). The tabs for entering this information are displayed when the appropriate box is selected from the white bar near the middle of the page. The box in the upper left-hand corner of the page lists all the release activities that have been entered; when you first encounter this page, there will be one item in this box (the release that you are currently entering). As you specify additional release activities, they will appear in this box; you may revisit an earlier entry by clicking once on an item in the list. Below this box is a text field where you may enter an identifying word or phrase for the release activity (i.e., “Manufacturing” or “Processing”). Below that is a numerical text field where you must enter the number of sites to which the releases on this page are applicable.

To develop exposure doses, you must provide the estimated disposal release amounts. To enter release information, first select the box or boxes located next to Surface Water, Landfill, or Ambient Air in the white bar on the General Release Information page. For each box you select, a tab displaying the applicable model inputs will appear (Figures 3-2a, b, and c.). To enter chemical releases, select each tab in sequence and enter the amount of the release. Note that the units of these releases are on a per site basis. Each disposal release option has a check box that allows you to omit dose calculations for that particular release. You may choose this option if you have a release that is below a threshold of concern, and you would like the release to be reported in the model output even though you do not need dose calculations. Remarks about any of the releases may be entered in the text field at the lower left-hand corner of the page. A more detailed description of the entry fields for surface water, landfill, and ambient air releases may be found in Sections 3.1.1.1, 3.1.1.2, and 3.1.1.3, respectively.

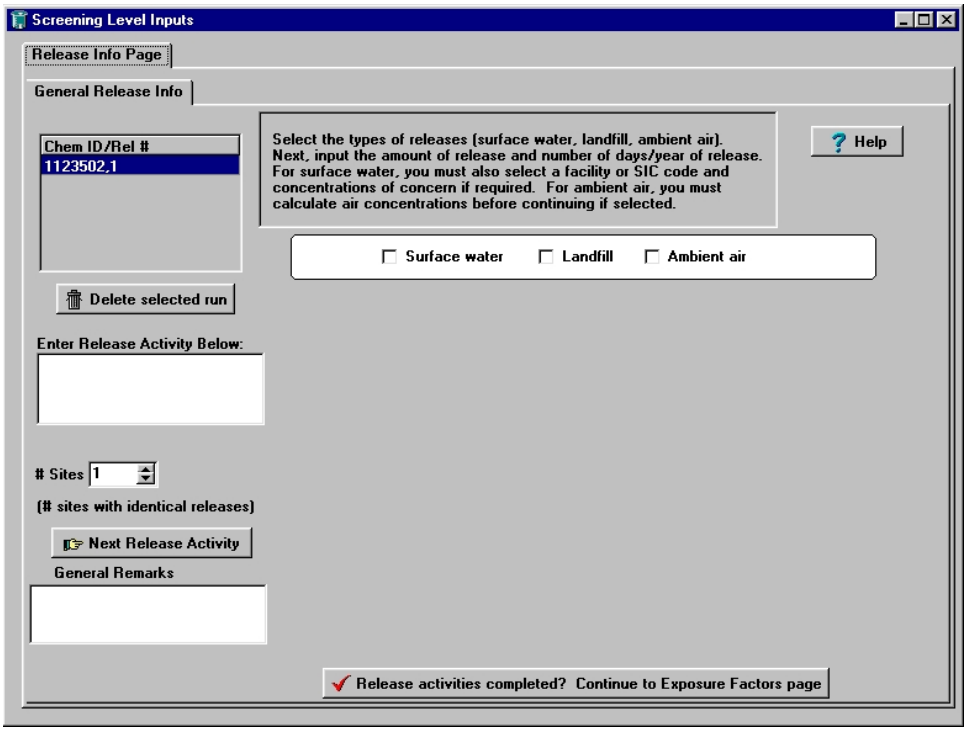

Figure 3-2. General Release Information Page

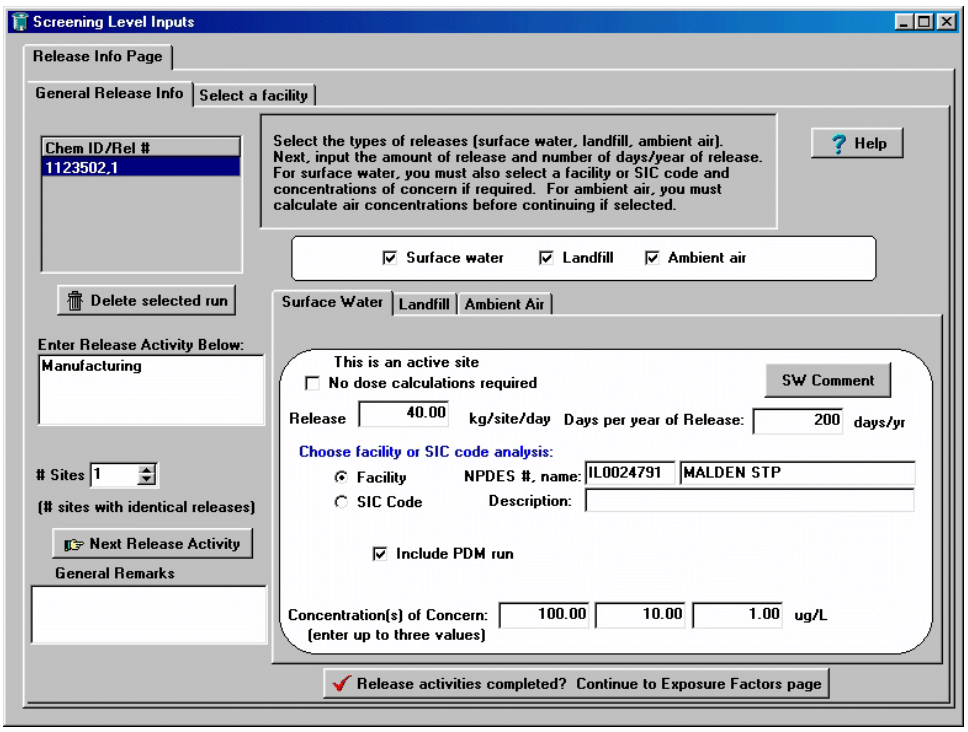

Figure 3-2a. General Release Information Page – Surface Water

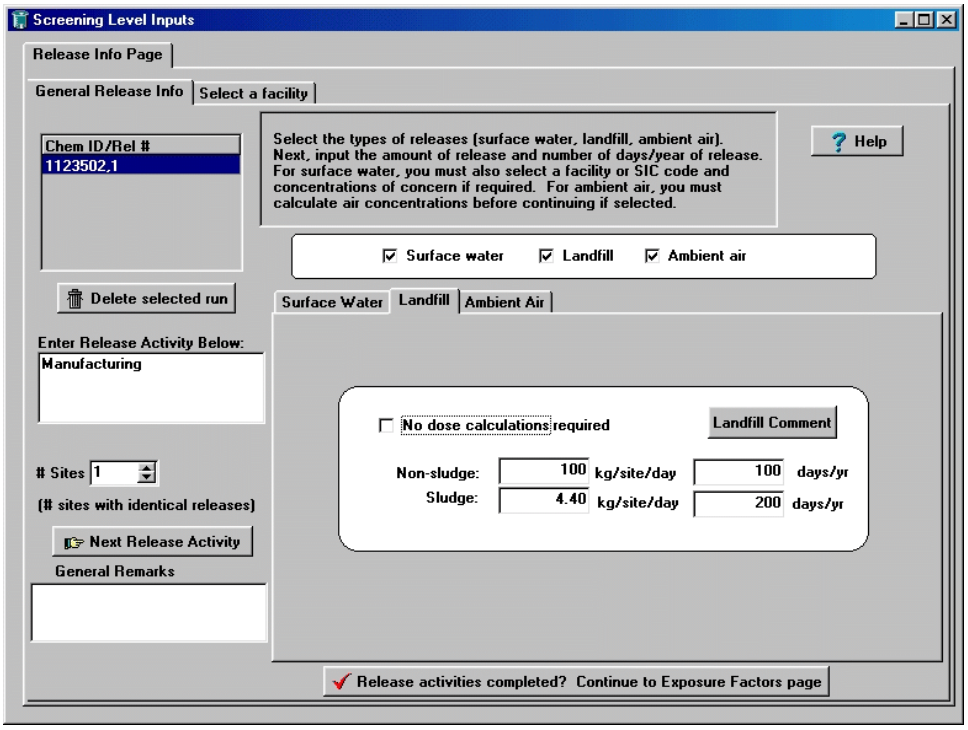

Figure 3-2b. General Release Information Page – Landfill

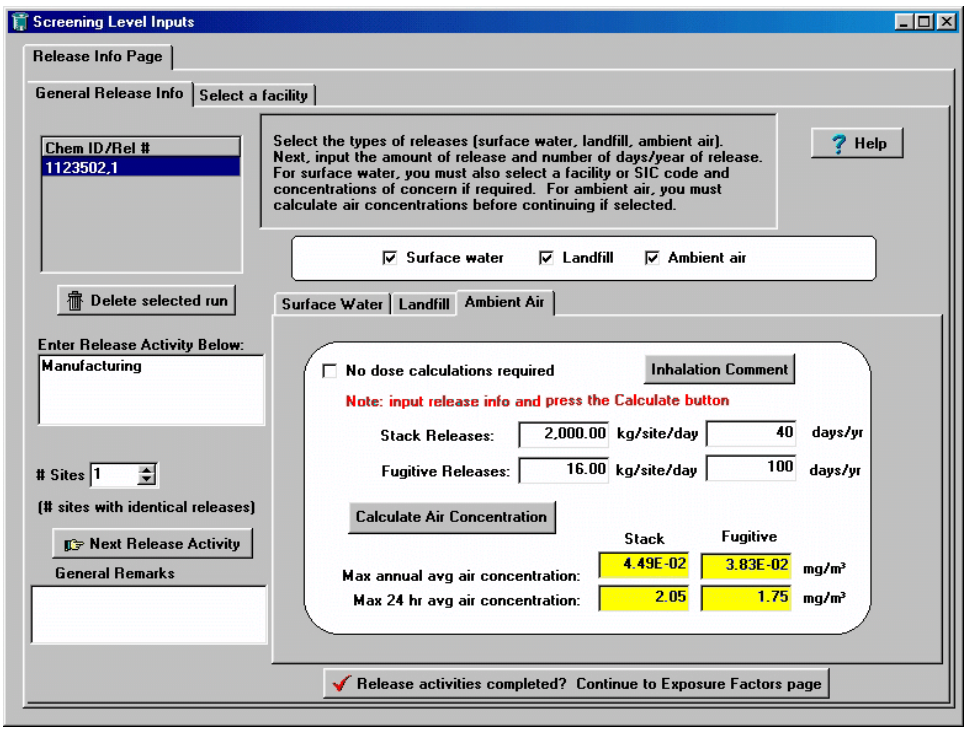

Figure 3-2c. General Release Information Page – Ambient Air

Once all the information for a release activity is entered, you may enter another release activity by clicking the "Next Release Activity" button. If you have finished entering release activities, click on the "Release activities completed? Continue to Exposure Factors page" button to continue to the Exposure Factors page (Section 3.1.2).

3.1.1.1 *Surface Water Releases*

In the Surface Water tab of the General Release Information page (Figure 3-2a), you may enter a release amount (kg/site/day) and frequency of discharge (days/year). The model requires flow data for the body of water receiving the discharge. If the site is a known facility with a known National Pollutant Discharge Elimination System (NPDES) number, E-FAST V2.0 can access the required flow data for the site. If there are multiple sites or a single site without any available flow data, E-FAST V2.0 will use flow data based on typical values for the Standard Industrial Classification (SIC) code of the industry producing the discharge. These two options are labeled on the page as "Facility" and "SIC Code." The NPDES number and SIC code options are described in more detail below.

You may also choose whether or not to run PDM for any given surface water release by checking or unchecking the "Include PDM run" box. If you choose to run PDM, you may select either an average or a high-end PDM analysis. PDM predicts the number of days per year a facility's discharge will exceed a chemical's concentration of concern (COC) in a specific stream or river. The COC values specific to your analysis are entered on the General Release Information page. You may enter up to three COC values; this may be useful if the chemical you are assessing has an uncertain COC. If the discharge is at a known site, a PDM analysis can be performed on a reach with measured flow data from a U.S. Geological Survey (USGS) gaging station or a reach with only estimated flow values. If the reach has a gaging station, PDM will use the ranked measured daily flow values from EPA's STORET Daily Flow Statistical

File (Appendix B) to determine the frequency of exceedence. If only estimated flow data are available from EPA's Gage File (Appendix B), the frequency of exceedence is estimated using a stochastic procedure developed by Di Toro (1984) that uses the means and coefficients of variation of stream flow, effluent flow, and effluent concentration (Appendix C). The streamflow coefficient of variation is estimated using the mean flow, 7Q10 flow (i.e., 7 consecutive days of lowest flow over a 10-year period), and empirically-derived coefficients specific to each watershed. Days of exceedence are calculated for each of the COC values specified on the General Release Information Page. PDM can also base its calculation on generic, SIC code-based scenarios. When you choose to run PDM within the "General Population and Ecological Exposure from Industrial Releases" module or the "Down-the-Drain" module (Sections 3.1 and 3.2, respectively), the setup and execution of PDM is carried out by E-FAST V2.0 using your data; no additional input is required on your part. You may also run PDM as a stand-alone model; see Section 3.4.

In addition, if the percent adsorption to wastewater treatment sludge was entered in the PChem/Fate Inputs screen, a sludge value is calculated. The value is calculated by multiplying the amount of chemical release to water by the percent adsorbed. The percent adsorbed must be less than or equal to the wastewater treatment removal. The calculated sludge value is used in estimating exposures to landfill releases.

You may add a comment to the surface water release by clicking on the "SW comment" button, typing in the dialog box that appears, and clicking "OK." The text will appear in the output file.

Select a Facility

If a release activity takes place at a known location, you may select "Facility" in the Surface Water section of the General Release Information page and search for site-specific flow data on the "Select a Facility" page, which can be accessed by clicking on the tab to the right of the tab for the General Release Information page. E-FAST V2.0 contains facility and stream data from various EPA water-related information systems (See Appendix B). Lists of NPDES numbers, facility names, SIC codes, and reach numbers can be searched using search substrings. (Under the Clean Water Act, discharges of chemicals to surface waters are required to obtain a permit. A NPDES permit number is a unique nine-character code, beginning with the two-letter state abbreviation. E-FAST V2.0 only contains NPDES numbers for permitted facilities in the format IL*xxxxxxx*, where the first two letters are a state abbreviation and *x* is numeric. NPDES numbers for general permits and nonpermitted facilities are not included.) To search for a facility, fill in the two fields that appear in the following message at the center of the screen: "Locate facilities where this field [select NPDES, Facility name, SIC code, or Reach number from the drop-down menu] has the following substring [type in the State abbreviation for NPDES, first letters of the facility name, first digits of the SIC code, or numbers at the beginning of the reach number]." Be sure to follow the acceptable NPDES format as described above. If you are searching by facility name or SIC code, you may restrict the search to a single state or EPA region by clicking the appropriate button and selecting the state or region from the drop-down menu on the left-hand side of the screen.

For example, entering AR will produce a listing of all NPDES numbers in the State of Arkansas. Entering a substring of AR000058 will yield a list of NPDES numbers ranging from AR0000580 to AR0000589. To search facility names, select "Facility name" in the first field, then enter "Alc" to get a list of all facility names beginning with those letters. For SIC code searches, entering a substring of 27 will yield a listing of four-digit SIC codes that begin with 27. Reach numbers are unique 11-digit

numbers used to identify surface water bodies and can be searched using the first few digits. Reach numbers consist of the following information:

02*xxxxxxxxx*	Region
*xx*03*xxxxxxx*	Subregion
*xxxx*04*xxxxx*	Accounting unit
*xxxxxx*06*xxx*	Cataloging unit
*xxxxxxxx*011	Segment number

The region number is one of 21 regions, or major river drainage basins, within the United States and Puerto Rico. Each region contains subregions, accounting units, cataloging units, and segment numbers based on the number of surface water bodies.

Conduct the search by selecting the "Perform search for facilities" button. E-FAST V2.0 will display the facilities matching the search strings as shown in Figure 3-3. Select the facility of interest by double-clicking; you will then be returned to the General Release Information screen.

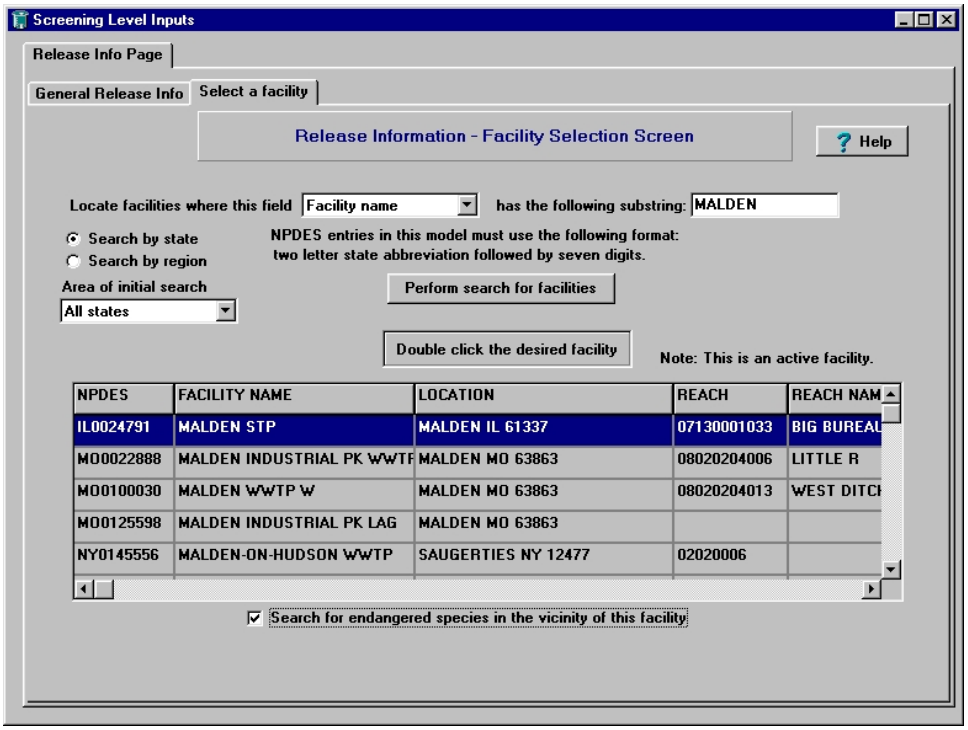

Figure 3-3. Select a Facility Screen

You may also choose to search for a list of endangered species in the vicinity of the facility. E-FAST V2.0 contains a database of endangered species obtained from EPA's Endangered Species Protection Program Database (U.S. EPA, 2004). By selecting this search query, the presence of endangered species in the vicinity of industrial discharges to surface water can be identified. The location of endangered species is correlated with the facility location using Federal Information Processing Standards (FIPS) state and county codes. The endangered species information presented include common name, taxonomic group, listing action and known occurrence.

Select an SIC Code

The Standard Industrial Classification (SIC) system was developed by the U.S. Government in order to provide agencies with a uniform framework for organizing economic, engineering, and scientific data for a wide range of economic activities. These activities include agriculture, mining, manufacturing, construction, utilities, retail trade, and finance. Under the SIC system, every establishment, defined as a single economic production unit such as a factory, a mill, or a mine, is assigned a four-digit numerical code. The system is structured in such a way that the first one or two digits are used as a broad classification and the full four digits are used for more detailed recordkeeping. The SIC system has been periodically revised since its inception to reflect the economy's changing industrial composition and organization. The classification system currently used by E-FAST V2.0 is based on the 1987 SIC system and includes facilities in 36 industrial categories. In 1998, the U.S. Office of Management and Budget (OMB) initiated efforts to replace the SIC system with the North American Industry Classification System (NAICS), which identifies industries using a six-digit code rather than the four-digit SIC code (U.S. OMB, 1998). The longer code accommodates the larger number of sectors and allows more flexibility in designating subsectors. This six-digit code is a major revision that not only provides for newer industries, but also reorganizes the categories on a production/process-oriented basis (SIC used a mixture of production-based and market-based categories). The NAICS codes do not directly correspond to the SIC codes because some SIC codes were split into multiple NAICS codes, and the NAICS system has 20 broad sectors, whereas the SIC system had 10. Currently, the EPA water-related information systems used in E-FAST V2.0 do not associate their data with the NAICS codes. When these databases are updated, E-FAST V2.0 will be updated to search on the basis of NAICS codes. Although the NAICS codes are now readily available and it is possible to identify a NAICS code for a particular facility, E-FAST V2.0 does not use NAICS codes. Because there are 27,247 direct discharging facilities reported in E-FAST V2.0, it is not practical to contact each facility to acquire its NAICS code. (Direct discharge refers to the discharge of pollutant(s) directly to surface waters of the United States under the NPDES permit program.) According to representatives from the EPA, the NAICS codes will not be put into the EPA water-related information systems used in E-FAST V2.0 until the EPA begins to modernize their systems, which is not scheduled to be done in the immediate future. However, a list of facilities' SIC codes and their corresponding NAICS codes is currently available through the NAICS Association's website at http://www.naics.com.

Within E-FAST V2.0, the full four-digit SIC codes are used to classify establishments that discharge wastewater. E-FAST V2.0 provides receiving stream flows and dilution factors for direct dischargers in selected SIC codes (i.e., 10th and 50th percentile). The harmonic mean, 30Q5, 7Q10, and 1Q10 flow statistics are provided (See Section 3.1.4.1 for definitions of these flows). You can select such flow data when the exact location of a discharger to surface water is not known, but the nature of the discharge facility is known (e.g., a paper mill, an electroplater, etc., as shown in Figure 3-4). In the Surface Water section of the General Release Information page, click the "SIC code" button. The Select an SIC Code page will appear in the foreground and the General Release Information page will be hidden. If necessary, you can alternate between the two pages by clicking on the tabs at the top of the screen. The Select an SIC Code page presents a list of industrial categories. Double click on the one that best fits the release activity you are modeling. You will then be returned to the General Release Information page.

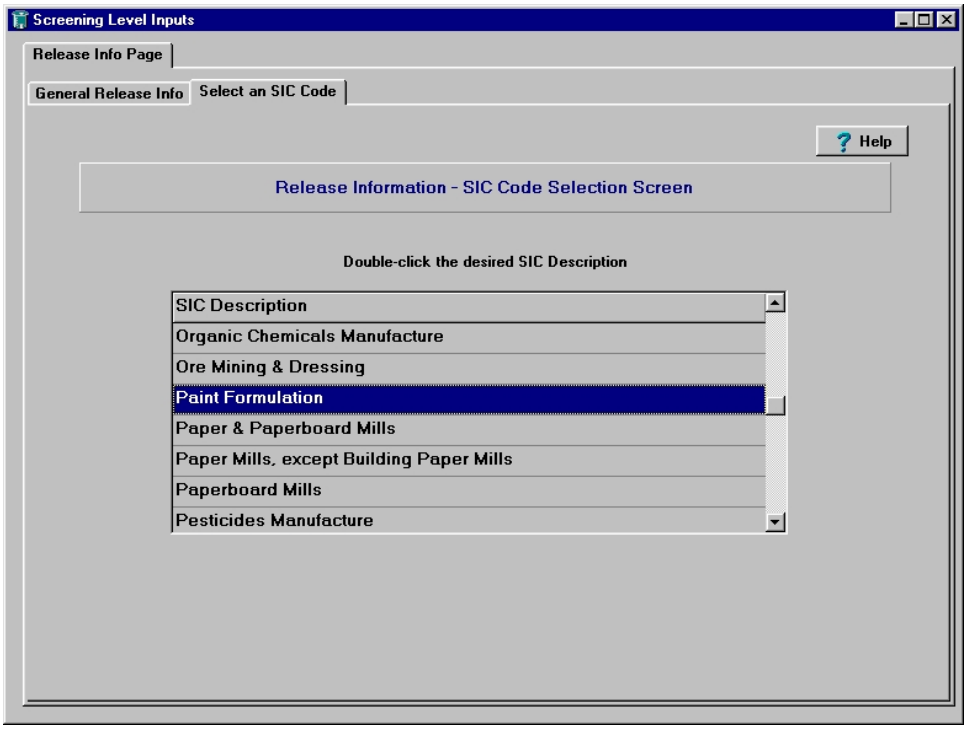

Figure 3-4. Select an SIC Code Screen

3.1.1.2 *Landfill Releases*

If you checked "Landfill Releases" on the General Release Information page (Figure 3-2), you may enter the amount of a chemical sent to a landfill (kg/site/day) and frequency of discharge (days/year) (Figure 3-2b). E-FAST V2.0 has already calculated the sludge release for you, if you have entered a surface water release and the percent adsorption to wastewater releases in the PChem/Fate Inputs screen. Note, however, that if you change the adsorption percentage after the model fills in the sludge release, the release amount will not automatically update. To generate a new sludge release using the updated adsorption value, you must re-enter the water release.

As with surface water releases, you may add a comment to the landfill release by clicking on the "Landfill Comment" button, typing in the dialog box that appears, and clicking "OK." The text will appear in the output file.

3.1.1.3 *Ambient Air Releases*

The Ambient Air tab of the General Release Information page (Figure 3-2c) contains two input lines for release to air: one for stack releases and one for fugitive releases. Stack releases include, but are not limited to, incineration. To model releases, enter the stack and/or fugitive release amounts and the corresponding number of days per year. Click on the "Calculate Air Concentration" button. A new screen called E-FAST2 Downwind Concentration Predictor will appear, containing the release data you just entered, the stack and fugitive air emission removal rates you specified in the PChem/Fate Inputs screen (Section 2.0), and modeling parameters. You may edit the SCREEN3 parameters or use the default values. E-FAST V2.0 uses EPA's SCREEN3 Model (U.S. EPA, 1995a) to estimate the maximum 1-hour average air concentration for stack and fugitive air emission releases. The model is invoked twice for each

stack release and twice for each fugitive release– once for a 24-hour maximum and once for the maximum annual average. Each model run yields a maximum 1-hour average air concentration; conversion factors (see section 3.1.8) are used to translate the maximum 1-hour average air concentration into a maximum 24-hour or annual average air concentration. In E-FAST V2.0, SCREEN3 models stack emissions as point sources and fugitive emissions as area sources.

The modeling parameters for SCREEN3 are listed in the Release Information and Meteorological and Terrain Information tabs. The Release Information tab contains stack parameter data, such as the stack height, inside stack diameter, stack gas exit velocity, and stack gas temperature for stack releases, and fugitive parameter data, such as the release height, length of release opening, and width of release for fugitive releases. An example Release Information tab is shown in Figure 3-5.

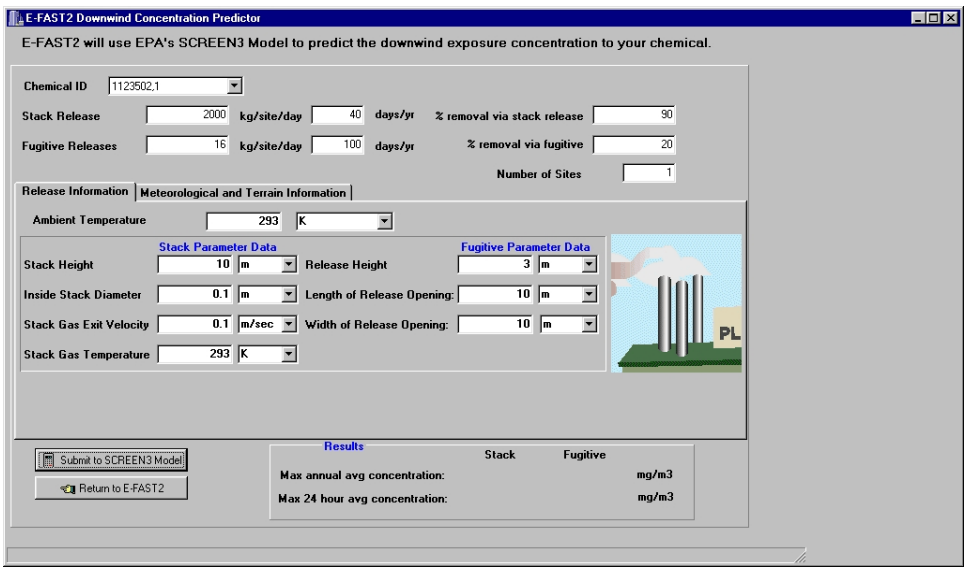

Figure 3-5. SCREEN3 – Release Information

The Meteorological and Terrain Information tab contains data concerning surrounding land use, terrain height, distance to the residence of interest, and meteorological class. All of these parameters, as well as ambient temperature, have default values (Table 3-1), but may be changed to conform to a known facility or location. An example Meteorological and Terrain Information tab is shown in Figure 3-6.

Table 3-1. Default Values[1] for Select Input Parameters to SCREEN3

Parameter	Stack	Fugitive
Stack / Release Height	10 m	3 m
Inside Stack Diameter	0.1 m	NA
Stack Gas Exit Velocity	0.1 m/s	NA
Stack Gas Temperature	20°C (293 K)	NA
Ambient Temperature	20°C (293 K)	NA
Length of Release Opening	NA	10 m
Width of Release Opening	NA	10 m
Surrounding Land Use	Rural	Rural
Meteorological Class	Full	Full
Terrain Height	0 m	0 m
Distance to Residence	100 m	100 m

[1]Source: Personal Communication from Lynn Delpire, EPA, OPPT, to Conrad Flessner, EPA, OPPT, May 2002. These default values were selected to generate conservative concentrations.

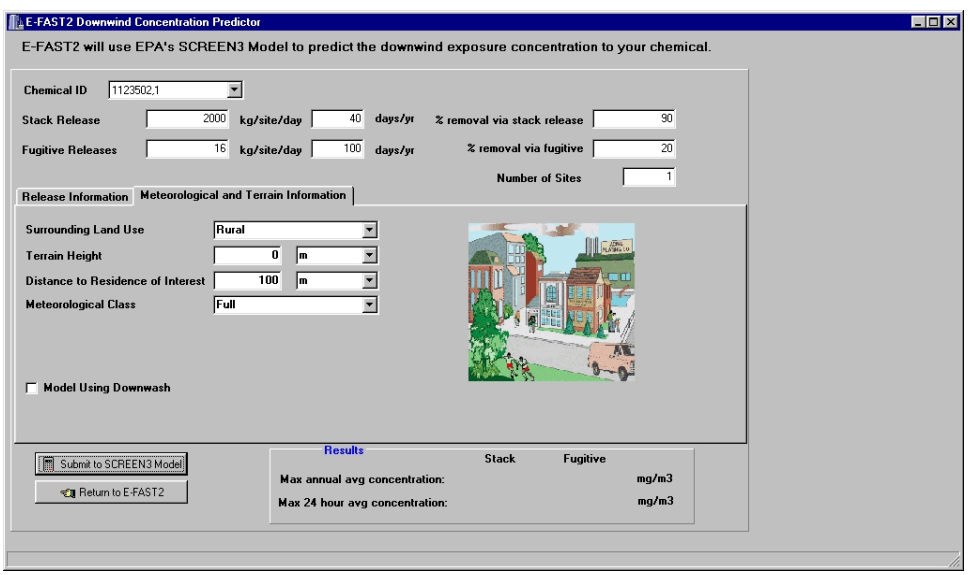

Figure 3-6. SCREEN3 – Meteorological and Terrain Information

In the Meteorological and Terrain Information tab, you can mark the checkbox for "Model Using Downwash" if the stack emissions are affected by the building's dimensions. Checking this box produces a third tab, Downwash Information, which collects information on the dimensions of the building (default: 100m x 100m x 10m). An example Downwash Information tab is shown in Figure 3-7.

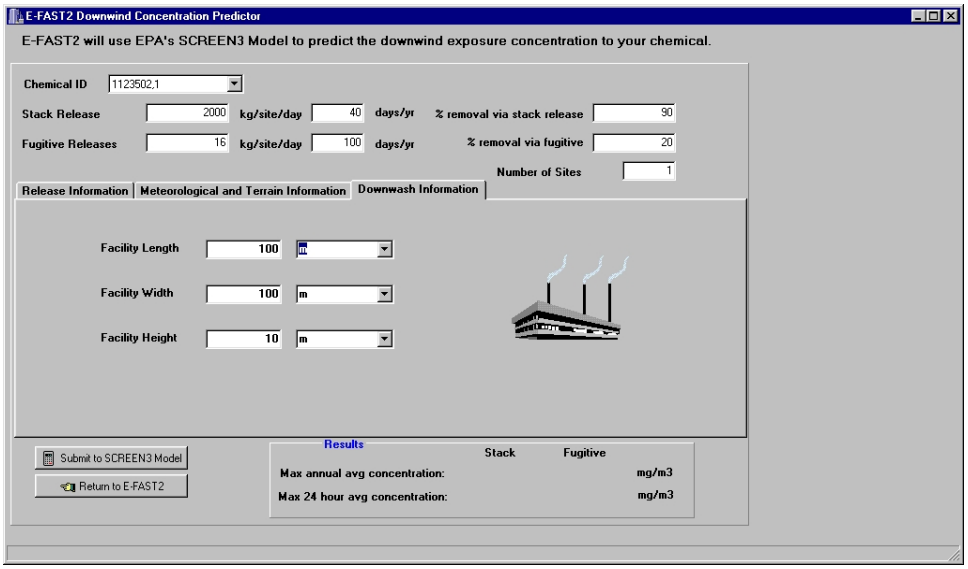

Figure 3-7. SCREEN3 – Downwash Information

Once you have entered all of this information, click on the "Submit to SCREEN3 Model" button to calculate the maximum annual and maximum 24-hour air concentrations. In a few seconds, the concentrations will appear in the yellow text fields in the lower right-hand corner of the screen. Click on the "Return to E-FAST2" button to exit SCREEN3. The air concentrations will now appear in the yellow text fields at the bottom of the Ambient Air section of the General Release Information page.

3.1.2 Exposure Factors Page

When all environmental releases have been entered and you click on the button "Release activities completed? Continue to Exposure Factors page," you will be taken to the Exposure Factors page. This page appears as a tab next to the Release Information page, and you may switch back and forth between these pages by clicking on the tabs at the top of the window. In order to calculate exposures and doses, E-FAST V2.0 requires exposure parameters for body weight, intake rates, and other exposure characteristics. The model provides default values for each of these parameters for six age classifications (adults, youths (children 13-19 years), children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years old, and infants less than one year old) and two exposure types (acute and chronic for adults; acute only for children and infants), where appropriate. Figure 3-8 shows an example of the Exposure Factors page. The values that appear on this screen will vary depending on the age group you selected on the Screening Level Main page (See Section 3.0). Most of these default values are conservative and are the recommended values in EPA's *Exposure Factors Handbook* (U.S. EPA, 1997). You can change these default values. The E-FAST V2.0 default exposure parameter values are presented in Table 3-2.

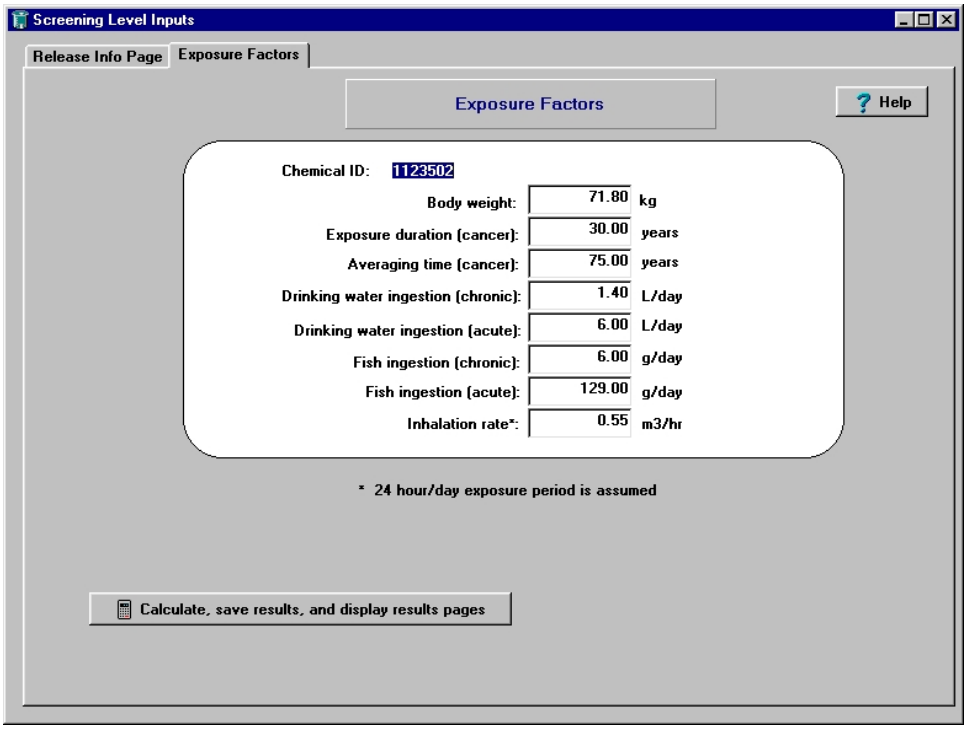

Figure 3-8. Exposure Factors Page

To perform all calculations and display the appropriate results pages, select the "Calculate, save results, and display results pages" button. You will see a progress bar move across the screen as exposures are calculated and written to disk. When the calculations are done, a dialog box will notify you that the output file has been saved to your default data drive. Click "OK." The model results are then displayed in a series of tabs, starting with Environmental Releases. The tabs that follow will vary depending on the types of releases being modeled. The tabs that may appear include Rivers (See Section 3.1.4), SIC Code (See Section 3.1.5), Lakes (See Section 3.1.6), Landfill (See Section 3.1.7), Inhalation (See Section 3.1.8), PDM Site-Specific (See Section 3.1.9), and PDM SIC Code (See Section 3.1.10).

Table 3-2. Default Exposure Parameter Values Used in E-FAST V2.0

Exposure Parameter	Population (years)	Exposure Type	Default Value	Source	Comment
Body Weight (BW)	Adult	All	71.8 kg	U.S. EPA (1997)	Mean adult body weight (EFH Table 7-11).
	Youth (age 13-19)	All	60.2 kg	U.S. EPA (1997)	Average of mean body weights for youth ages 13-19 years (EFH Table 7-3).
	Child (age 6-12)	All	32.8 kg	U.S. EPA (1997)	Average of mean body weights for children ages 6-12 years (EFH Table 7-3).
	Small Child (age 3-5)	All	17.5 kg	U.S. EPA (1997)	Average of mean body weights for children ages 3-5 years (EFH Table 7-3).
	Infant (age 1-2)	All	12.3 kg	U.S. EPA (1997)	Average of mean body weights for children ages 1-2 years (EFH Table 7-3).
	Infant (age <1)	All	9.1 kg	U.S. EPA (1997)	Mean body weights for children 6-11 months (EFH Table 7-3).
Drinking Water Intake (IR_{dw})	Adult	Chronic	1.4 L/day	U.S. EPA (1997)	Mean adult ingestion rate (EFH Table 3-30).
	Adult	Acute	6 L/day	U.S. EPA (1997)	Ingestion rate for active adults in temperate climates (EFH Table 3-30).
	Youth (age 13-19)	Acute	2 L/day	U.S. EPA (1997)	95th percentile ingestion rate for children ages 11-19 years (EFH Table 3-30).
	Child (age 6-12)	Acute	1.75 L/day	U.S. EPA	Average of values for youth (age 13-19 years) and Child (age 3-5 years). EFH does not recommend a rate for age 6-12.
	Small Child (age 3-5)	Acute	1.5 L/day	U.S. EPA (1997)	90th percentile ingestion rate for children ages 3-5 years (EFH Table 3-30).
	Infant (age 1-2)	Acute	1.5 L/day	U.S. EPA (1997)	90th percentile ingestion rate for children ages < 3 years (EFH Table 3-30).
	Infant (age < 1)	Acute	0.76 L/day	U.S. EPA (1997)	95th percentile ingestion rate for children ages < 1 years (EFH Table 3-30).

Table 3-2. Default Exposure Parameter Values Used in E-FAST V2.0 (Cont'd)

Exposure Parameter	Population (years)	Exposure Type	Default Value	Source	Comment
Inhalation Rate (InhR)	Adult	Chronic	13.3 m^3/day	U.S. EPA (1997)	For general population exposure, average of adult male and female means (EFH Table 5-23); equivalent to 0.55 m^3/hr.
	Adult	Acute	see comment	U.S. EPA (1997)	For consumer exposures: 1.0 m^3/hr during product use (based on light activity level) and 0.55 m^3/hr after product use; for general population exposure, 0.55 m^3/hr or 13.3 m^3/day, assuming exposure period of 24 hr/day (EFH Table 5-23).
	Youth (age 13-19)	Acute	14.0 m^3/day	U.S. EPA (1997)	For consumer and general population exposures: Average of mean long-term values for males and females age groups 12-14 years and 15-18 years (EFH Table 5-23); equivalent to 0.58 m^3/hr.
	Child (age 6-12)	Acute	12.3 m^3/day	U.S. EPA (1997)	For consumer and general population exposures: Average of mean long-term values for males and females age groups 6-8 years and 9-11 years (EFH Table 5-23); equivalent to 0.51 m^3/hr.
	Small Child (age 3-5)	Acute	8.3 m^3/day	U.S. EPA (1997)	For consumer and general population exposure: Mean long-term value for age group 3-5 years (EFH Table 5-23); equivalent to 0.35 m^3/hr.
	Infant (age 1-2)	Acute	6.8 m^3/day	U.S. EPA (1997)	For consumer and general population exposures: Mean long-term value for age groups 1-2 year (EFH Table 5-23); equivalent to 0.28 m^3/hr.
	Infant (age < 1)	Acute	4.5 m^3/day	U.S. EPA (1997)	For consumer and general population exposure: Mean long-term value for infants (<1 year) (EFH Table 5-23); equivalent to 0.19 m^3/hr.
Fish Ingestion Rate (IR_{fish})	Adult	Chronic	6.0 g/day	U.S. EPA (1997)	Long-term general population average ingestion of freshwater/estuarine fish (EFH Table 10-81).
	Adult	Acute	129 g/day	U.S. EPA (1997)	Mean serving size for general population (EFH Table 10-82).
	Youth (age 13-19)	Acute	118 g/day	U.S. EPA (1997)	Average of mean 1-day intakes for males and females ages 12-19 years, consumers only (EFH Table 10-46).
	Child (age 6-12)	Acute	89 g/day	U.S. EPA (1997)	Average of mean 1-day intakes for males and females ages 6-11 years, consumers only (EFH Table 10-46).
	Small Child (age 3-5)	Acute	67 g/day	U.S. EPA (1997)	Average of mean 1-day intakes for ages # 5, consumers only (EFH Table 10-46).

Table 3-2. Default Exposure Parameter Values Used in E-FAST V2.0 (Cont'd)

Exposure Parameter	Population (years)	Exposure Type	Default Value	Source	Comment
	Infant (age 1-2)	Acute	52 g/day	U.S. EPA (1997)	Mean quantity of fish consumed per eating occasion for ages 1-2 years, consumer only (EFH Table 10-45).
	Infant (age < 1)	Acute	NA	NA	NA
Exposure Duration (ED)	Adult	Chronic	30 years	U.S. EPA (1997)	For ambient exposures (air, water, and fish ingestion): 95th percentile residential occupancy value (EFH Table 15-176).
	Adult	Chronic	57 years	-	For consumer exposures: Active usage of consumer products during years 18 to 75.
	Adult	Acute	1 day	-	Assumed 1 day exposure for acute scenarios.
	Youth (age 13-19)	Acute	1 day	-	Assumed 1 day exposure for acute scenarios.
	Child (age 6-12)	Acute	1 day	-	Assumed 1 day exposure for acute scenarios.
	Small Child (age 3-5)	Acute	1 day	-	Assumed 1 day exposure for acute scenarios.
	Infant (age 1-2)	Acute	1 day	-	Assumed 1 day exposure for acute scenarios.
	Infant (age < 1)	Acute	1 day	-	Assumed 1 day exposure for acute scenarios.
Carcinogenic Averaging Time (AT)	Adult	NA	75 years	U.S. EPA (1997)	Average life expectancy of general population (EFH page 8-1).
Acute Averaging Time (AT)	All	Acute	1 day	-	Assumed 1 day exposure for acute scenarios.

EFH = *Exposure Factors Handbook* (U.S. EPA, 1997)

3.1.3 Environmental Release Results Page

The Environmental Release Results page (Figure 3-9) presents the calculated total potential (i.e., before treatment) environmental releases for each site release to surface water, to landfills (non-sludge/sludge), in stack emissions, and in fugitive emissions. The box in the upper left-hand corner shows all of the release activities you entered on the General Release Information page; you can click on any release activity to view the results for that activity. In the output fields highlighted in yellow, the total releases (kg/year) are calculated by multiplying the per site release rate (kg/site/day), the release days per year (days/year), and the number of sites. A "Print Page" button at the lower right-hand corner may be used to generate a hard copy of the data on the screen.

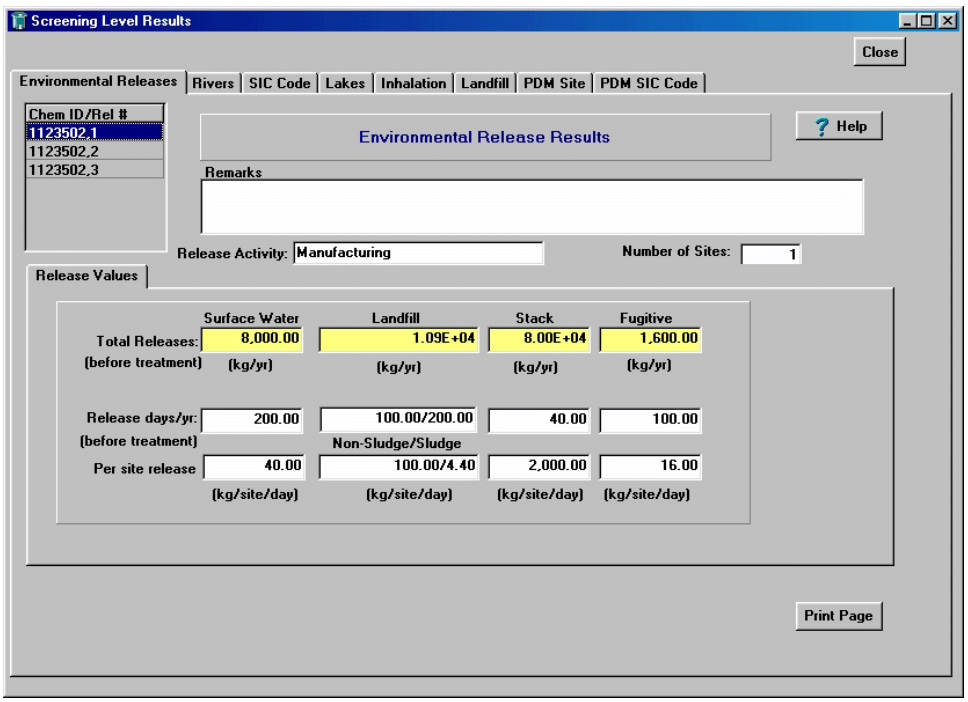

Figure 3-9. Environmental Release Results Page

3.1.4 Rivers Results Page

Figure 3-10 shows an example Rivers Results page. The box in the upper left-hand corner shows all of the release activities that included discharges to rivers; you can click on any release activity to view the results for that activity. The following are short descriptions of the fields listed in the upper half of this page:

- **Release Activity** — can be manufacturing, processing, industrial use, or other. This was entered in a text field on the left-hand side of the General Release Information page (Figure 3-2).

- **Facility Name, Location, NPDES, Reach Number, Reach Name** — information on the discharging facility extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Facility on Reach?** — indicates whether the facility discharges to the identified reach, discharges to a tributary stream, or if the discharge point is unknown.

- **Exposed Population** — can be adults, youths 13 to 19 years, children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years, or infants less than one year old. This was entered on the Screening Level Main page (Figure 3-1).

- **Discharge Type —** indicates whether the facility is a direct discharger that discharges treated wastewater directly to a surface water body or an indirect discharger that discharges wastewater to a POTW for treatment.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release Days** — number of days per year that the chemical is discharged, as entered on the General Release Information page.

- **Pretreatment Release** — rate of release of the chemical by the facility to a wastewater treatment facility (kg/site/day), as entered on the General Release Information page.

- **Post-treatment Release** — rate of release of the chemical after treatment by a wastewater treatment facility. The post-treatment release amount is equal to the pretreatment release reduced by the wastewater treatment removal percentage.

- **Bioconcentration Factor —** indicates the tendency of the chemical to accumulate in living organisms. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

In addition to these fields, the top portion of the Rivers results page displays a "Print Page" button that may be used to generate a hard copy of the data on the screen. The hard copy includes the data in all of the tabs in the lower portion of the screen (General Site Information, Drinking Water Information, Fish Ingestion Information, and Endangered Species), so there is no need to click the "Print Page" button for each of these tabs.

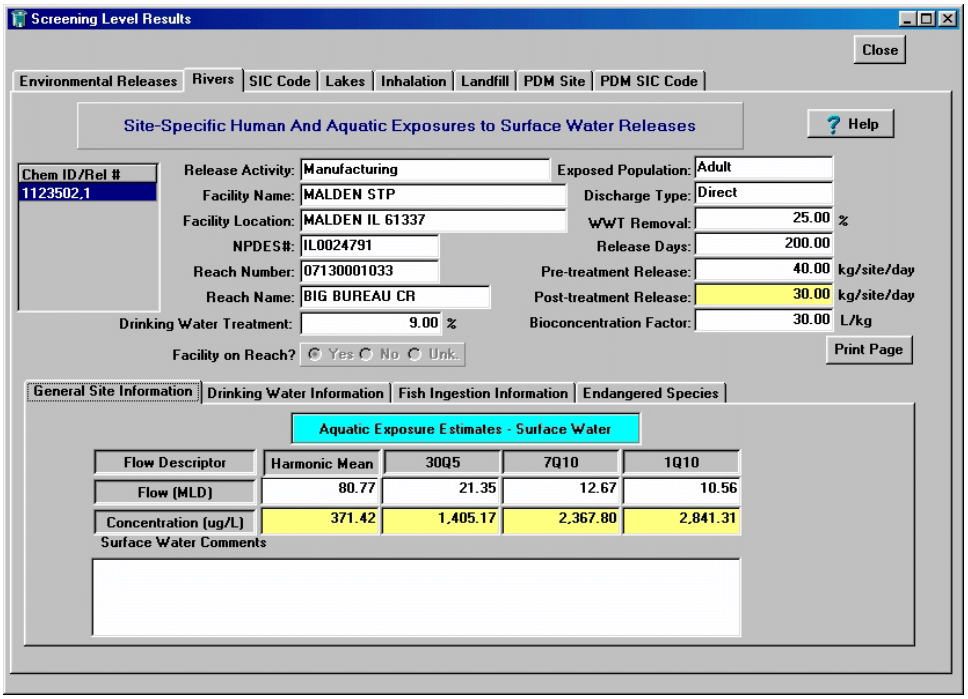

Figure 3-10. Rivers Results Page – Aquatic Exposure Estimates - Surface Water

Four tabs located in the lower half of the page allow you to view General Site Information, Drinking Water Information, Fish Ingestion Information, and Endangered Species.

3.1.4.1 *Rivers Results Page – General Site Information*

Site-specific surface water concentrations are calculated from estimated arithmetic mean and 7Q10 stream flows obtained from an EPA database (See Appendix B). Harmonic mean, 30Q5, and 1Q10 flows are calculated from the 7Q10 flows and arithmetic mean flows. The units of flow are million liters per day (MLD). The estimated chemical concentrations are presented for each flow rate. The following are short definitions of the flows displayed in the lower half of the screen.

- **Harmonic Mean Flow ($SF_{harmonic}$)** — inverse mean of reciprocal daily arithmetic mean flow values. In other words, harmonic mean (H) is defined as $H = n/[(1/x_1) + (1/x_2) +...+ (1/x_n)]$ where x is a particular number in a group of measured values and n is the number of measurements in the series. These flows are used to generate estimates of chronic human exposures via drinking water and fish ingestion.

- **30Q5 Flow (SF_{30Q5})** — 30 consecutive days of lowest flow over a 5-year period. These flows are used to determine acute human exposures via drinking water.

- **7Q10 Flow (SF_{7Q10})** — 7 consecutive days of lowest flow over a 10-year period. These flows are used to calculate estimates of chronic surface water concentrations to compare with the COCs for aquatic life.

- **1Q10 Flow (SF_{1Q10})** — single day of lowest flow over a 10-year period. These flows are used to calculate estimates of acute surface water concentrations to compare with the COCs for aquatic life.

At the bottom of the page is a text box containing any comments entered by clicking on "SW comment" on the General Release Information page (See Section 3.1.1.1).

Estimation of Surface Water Exposure Concentrations in Rivers and Streams

E-FAST V2.0 uses the following equation to calculate surface water concentrations in free-flowing rivers and streams:

$$SWC = \frac{WWR \times CF1 \times \left(1 - \frac{WWT}{100}\right)}{SF \times CF2} \qquad \text{(Eq. 3-1)}$$

where:

SWC	=	Surface water concentration (parts per billion (ppb) or µg/L)
WWR	=	Chemical release to wastewater (kg/day)
WWT	=	Removal from wastewater treatment (%)
SF	=	Estimated flow of the receiving stream (MLD)
CF1	=	Conversion factor (10^9 µg/kg)
CF2	=	Conversion factor (10^6 L/day/MLD)

The amount of chemical released to wastewater and the estimated removal from wastewater treatment are input values to this equation. The conversion factor of 10^9 converts the chemical release from kg to µg. This value is then divided by the stream flow in MLD, which is converted to L/day (10^6 L/day/MLD). The results of this equation are chemical concentrations in units of µg/L. For very dilute aqueous solutions (such as surface water concentrations estimated by E-FAST V2.0), the units of µg/L and ppb can be considered equivalent.

This equation is valid for both site-specific and generic-release situations. Generic analyses using SIC codes can be performed when the locations of chemical releases are unknown or when there are no available streamflow data for the receiving stream.

E-FAST V2.0 calculates surface water concentrations for four streamflow conditions as shown in Equation 3-1. The equations used to estimate the harmonic mean, 30Q5, and 1Q10 flows from estimated arithmetic mean and 7Q10 flows also are presented below (Versar, 1992). The units for the arithmetic mean flow ($SF_{arithmetic}$) and the 7Q10 flow (SF_{7Q10}) used in these equations (Equations 3-2 through 3-4) are MLD. The factor 0.409 is used to convert MLD to units of cubic feet per second (cfs).

Harmonic mean stream flows are used to generate estimates of chronic human exposures via drinking water and fish ingestion.

$$SF_{harmonic}\ (MLD)\ \ 4\ 1.194 \times \frac{\left(0.409\ \frac{cfs}{MLD} \times SF_{arithmetic}\right)^{0.473} \times \left(0.409\ \frac{cfs}{MLD} \times SF_{7Q10}\right)^{0.552}}{0.409\ \frac{cfs}{MLD}} \qquad \text{(Eq. 3-2)}$$

SF_{30Q5} (30 consecutive days of lowest flow over a 5-year period) stream flows are used to generate estimates of acute human exposures via drinking water and fish ingestion.

$$SF_{30Q5}\ (MLD)\ \ 4\ 1.782 \times \frac{\left(0.409\ \frac{cfs}{MLD} \times SF_{7Q10}\right)^{0.966}}{0.409\ \frac{cfs}{MLD}} \qquad \text{(Eq. 3-3)}$$

SF_{7Q10} (7 consecutive days of lowest flow over a 10-year period) stream flows are used to generate estimates of exceedences of chronic COCs for aquatic life.

SF_{1Q10} (single day of lowest flow over a 10-year period) stream flows are used to determine if there are acute ecological concerns.

$$SF_{1Q10}\ (MLD)\ \ 4\ 0.843 \times \frac{\left(0.409\ \frac{cfs}{MLD} \times SF_{7Q10}\right)^{0.993}}{0.409\ \frac{cfs}{MLD}} \qquad \text{(Eq. 3-4)}$$

3.1.4.2 *Rivers Results Page – Drinking Water Information*

The Drinking Water Information tab (Figure 3-11) presents the acute and chronic exposure doses for individuals who ingest drinking water from streams and rivers that receive wastewater discharges containing the chemical of concern. The first column, “Exposure Types,” lists three different measurements of exposure. To the right of each, under the “Results” heading, is the corresponding exposure value. The subsequent columns contain exposure factors that were entered in the Exposure Factors page (See Section 3.1.2). The exposure types and exposure factors are defined below.

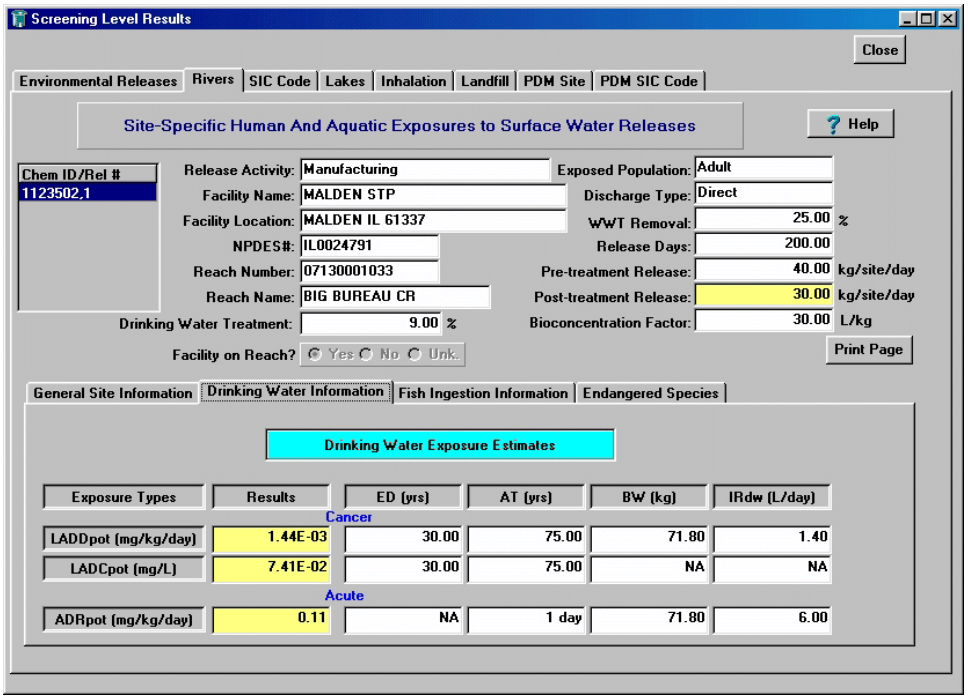

Figure 3-11. Rivers Results Page – Drinking Water Exposure Estimates

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from drinking water intake; calculated to represent chronic exposures to contaminated drinking water over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in drinking water; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from drinking water intake; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** — number of years a resident drinks contaminated water. E-FAST V2.0 uses a default value of 30 years; see Table 3-2.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Drinking Water Ingestion Rate (IR_{dw})** — used for calculating acute and chronic exposures.

Estimation of Drinking Water Potential Doses

To estimate how much of a given chemical a person will ingest through drinking water, E-FAST V2.0 uses the equations presented below. These equations convert an estimated surface water concentration to a drinking water exposure estimate. The surface water concentration (in µg/L) is

adjusted to account for any removal of the chemical during treatment of the drinking water and is then multiplied by the estimated drinking water ingestion rate in liters per day, the number of release days per year, and exposure duration in years. This product is then divided by body weight (in kg) and averaging time to yield the exposure dose in mg/kg/day.

$$ADR_{POT} = \frac{SWC \times \left(1 - \frac{DWT}{100}\right) \times IR_{dw} \times RD \times CF1}{BW \times AT} \qquad \text{(Eq. 3-5)}$$

$$LADD_{POT} = \frac{SWC \times \left(1 - \frac{DWT}{100}\right) \times IR_{dw} \times ED \times RD \times CF1}{BW \times AT \times CF2} \qquad \text{(Eq. 3-6)}$$

$$LADC_{POT} = \frac{SWC \times \left(1 - \frac{DWT}{100}\right) \times ED \times RD \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-7)}$$

where:

ADR_{POT}	=	Potential Acute Dose Rate (mg/kg/day)
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose (mg/kg/day)
$LADC_{POT}$	=	Potential Lifetime Average Daily Concentration in drinking water (mg/L)
SWC	=	Surface water concentration (ppb or µg/L)
DWT	=	Removal during drinking water treatment (%)
IR_{dw}	=	Drinking water intake rate (L/day)
RD	=	Release days (1 day for ADR_{POT}; days/yr for $LADD_{POT}$ and $LADC_{POT}$)
BW	=	Body weight (kg)
ED	=	Exposure duration (years for $LADC_{POT}$ and $LADD_{POT}$; see Table 3-2)
AT	=	Averaging time (years for $LADD_{POT}$ and $LADC_{POT}$; day for ADR_{POT})
CF1	=	Conversion factor (10^{-3} mg/µg)
CF2	=	Conversion factor (365 days/year)

The harmonic mean streamflow concentration is used to calculate the $LADD_{POT}$ and $LADC_{POT}$. The 30Q5 streamflow concentration is used to calculate the ADR_{POT}. This is consistent with EPA's OW guidance (U.S. EPA, 1991). The mean (central tendency) drinking water intake rate is used to calculate $LADD_{POT}$ and the high-end drinking water intake rate is used to calculate ADR_{POT}.

3.1.4.3 *Rivers Results Page – Fish Ingestion Information*

The Fish Ingestion Information tab (Figure 3-12) presents the exposure doses for individuals who ingest fish from streams and rivers that receive wastewater discharges containing the chemical of concern. The first column, "Exposure Types," lists three different measurements of exposure. To the right of each, under the "Results" heading, is the corresponding exposure value. The subsequent columns contain exposure factors that were entered in the Exposure Factors page (Section 3.1.2). The exposure types and exposure factors are defined below.

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from ingestion of fish tissue; calculated to represent chronic exposures to fish over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in ingested fish tissue; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from ingestion of fish tissue; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** — length of time the fish consumer is exposed.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Fish Ingestion Rate (IR_{fish})** — used for calculating acute and chronic exposures.

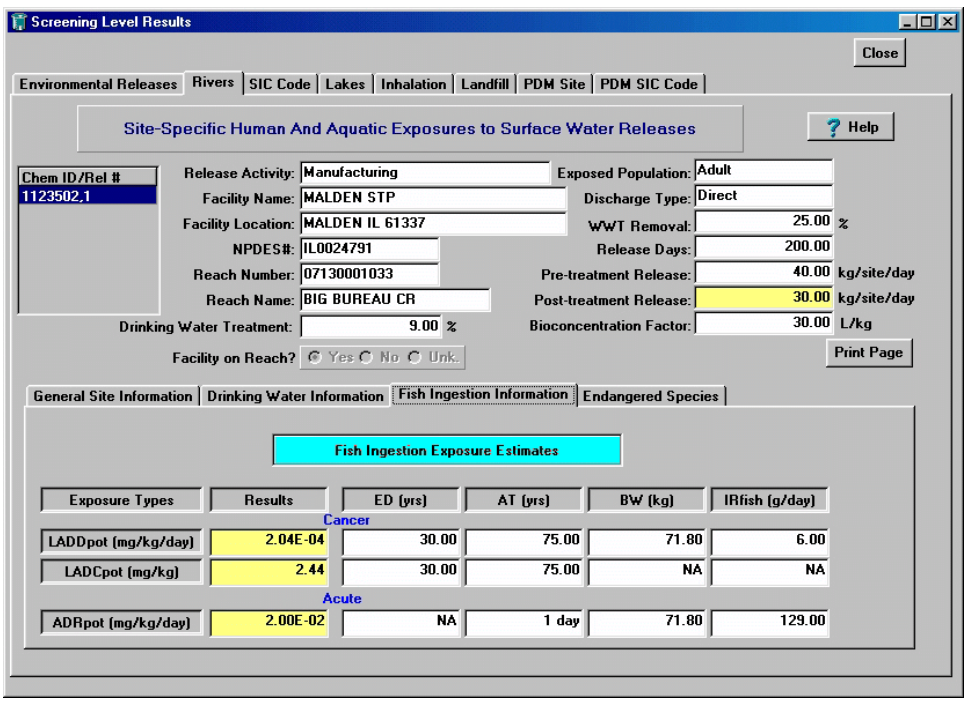

Figure 3-12. Rivers Results Page – Fish Ingestion Exposure Estimates

Estimation of Potential Doses via Fish Ingestion

To estimate how much of a given chemical a person will ingest through eating fish, E-FAST V2.0 uses Equations 3-8 through 3-10. These equations convert an estimated surface water concentration to a fish ingestion exposure estimate. The distinction between acute and chronic fish ingestion is made on the basis of daily ingestion rate. The mean long-term fish ingestion rate is used to calculate chronic

exposures and the mean serving size is used to calculate acute fish ingestion exposures for adults. This is in contrast to drinking water estimates, where the distinction between acute and chronic values is made on the basis of stream flows and on ingestion rates. The reason for this difference is that it takes time for chemical concentrations to accumulate in fish; therefore, the harmonic mean flow is used to calculate concentrations for both acute and chronic scenarios. It is not appropriate to use a very low streamflow value that occurs rarely as the basis for calculating a chemical residue in fish.

$$ADR_{POT} = \frac{SWC \times BCF \times IR_{fish} \times RD \times CF1}{BW \times AT} \qquad \text{(Eq. 3-8)}$$

$$LADD_{POT} = \frac{SWC \times BCF \times IR_{fish} \times ED \times RD \times CF1}{BW \times AT \times CF2} \qquad \text{(Eq. 3-9)}$$

$$LADC_{POT} = \frac{SWC \times BCF \times ED \times RD \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-10)}$$

where:

ADR_{POT}	=	Potential Acute Dose Rate (mg/kg/day)
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose (mg/kg/day)
$LADC_{POT}$	=	Potential Lifetime Average Daily Concentration in fish tissue (mg/kg)
SWC	=	Surface water concentration (ppb or µg/L)
BCF	=	Estimate of chemical's bioconcentration potential (L/kg)
IR_{fish}	=	Fish ingestion rate (kg/day)
RD	=	Release days (1 day for ADR_{POT}; days/yr for $LADD_{POT}$ and $LADC_{POT}$)
BW	=	Body weight (kg)
ED	=	Exposure duration (years for $LADC_{POT}$ and $LADD_{POT}$; see Table 3-2)
AT	=	Averaging time (years for $LADC_{POT}$ and $LADD_{POT}$; day for ADR_{POT})
CF1	=	Conversion factor (10^{-3} mg/µg)
CF2	=	Conversion factor (365 days/year)

3.1.4.4 *Rivers Results Page – Endangered Species*

The Endangered Species tab (Figure 3-13) presents the endangered species known (or possible) to exist in the vicinity of streams and rivers that receive wastewater discharges containing the chemical of concern. The location of endangered species is correlated with the facility location via FIPS State and county codes. The endangered species information is presented in six columns and includes common name, county and State, taxonomic group (e.g., mammals, birds, fish, plants, reptiles, amphibians, clams, etc.), listing action (listing, proposed, delisting), and known occurrence (true = known, false = possible). The data were obtained from EPA's Endangered Species Protection Program (ESPP) Databases (U.S. EPA, 2004). The ESPP is a cooperative effort between the U.S. Fish and Wildlife Service (FWS), EPA Regions, States, and pesticide users. ESPP is located in the Field and External Affairs Division (FEAD) of the Office of Pesticide Programs (OPP).

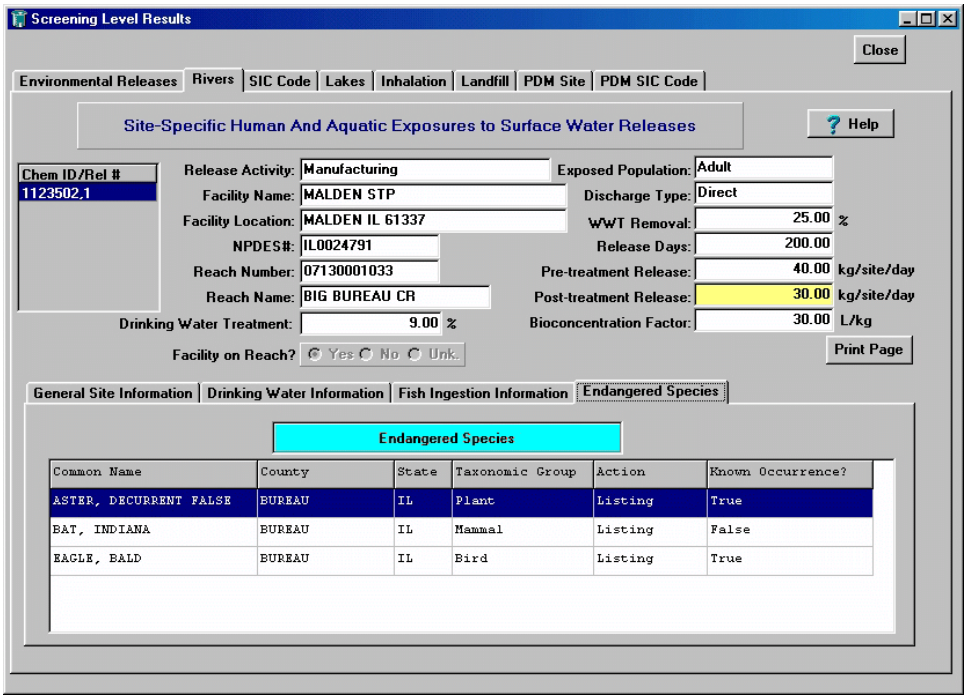

Figure 3-13. Rivers Results Page – Endangered Species

3.1.5 SIC Code Results Page

The SIC Code Results page (Figure 3-14) presents the releases, and drinking water and fish ingestion exposures for discharge activities that were entered using SIC codes (Section 3.1.1.1), as opposed to specific facilities. The exposure factors are derived from EPA's *Exposure Factors Handbook* (U.S. EPA, 1997). The box in the upper left-hand corner of the tab contains a list of every release activity that you elected to model using SIC codes; click on any of the release activities in the list to view the results for that activity.

The following are short descriptions of the fields listed in the upper half of this page. The values in the fields are those entered previously, as noted.

- **Release Activity** — can be manufacturing, processing, industrial use, or other. This was entered in a text field on the left-hand side of the General Release Information page (Figure 3-2).

- **SIC Code Description** — text description of the industry selected in the Select an SIC code page.

- **SIC Codes** — the 4-digit code or codes assigned to the industry selected.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release Days** — number of days per year that the chemical is discharged, as entered on the General Release Information page.

- **Bioconcentration Factor —** indicates the tendency of the chemical to accumulate in living organisms. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Exposed Population** — can be adults, youths 13 to 19 years, children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years, or infants less than one year old. This was entered on the Screening Level Main page (Figure 3-1).

- **Pretreatment Release** — rate of release of the chemical by the facility to a wastewater treatment facility (kg/site/day), as entered on the General Release Information page.

- **Post-treatment Release** — rate of release of the chemical after treatment by a wastewater treatment facility. The post-treatment release amount is equal to the pretreatment release reduced by the wastewater treatment removal percentage.

In addition to these fields, the top portion of the SIC Code results page displays a "Print Page" button that may be used to generate a hard copy of the data on the screen. The hard copy includes the data in all of the tabs in the lower portion of the screen (General SIC Code Information, Drinking Water Information, and Fish Ingestion Information), so there is no need to click the "Print Page" button for each of these tabs.

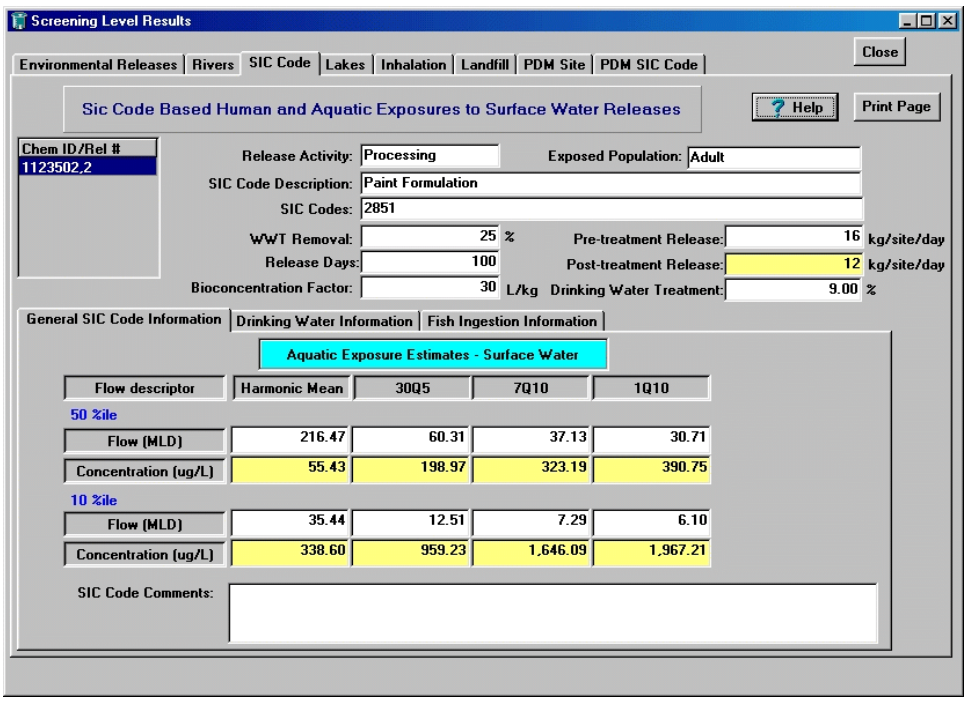

Figure 3-14. SIC Code Results Page – Aquatic Exposure Estimates - Surface Water

Three tabs located in the lower half of the page allow you to view three sets of results: General SIC Code Information, Drinking Water Information, and Fish Ingestion Information.

3.1.5.1 *SIC Code Results Page – General SIC Code Information*

The General SIC Code Information tab displays flow rates and concentrations, at both the 10th and 50th percentiles, under four flow conditions: harmonic mean, 30Q5, 7Q10, and 1Q10. SIC code-based surface water concentrations are calculated from the 10th and 50th percentile stream flows obtained from the Stream Dilution Factor Program (SDFP) for 36 industrial categories. (SDFP is a software program originally developed by the OW to obtain effluent and stream flow frequency distributions for a given industrial category (SIC code). Revised by OPPT, the major purpose of SDFP is to (1) retrieve receiving stream flow data for facilities in a particular SIC code (direct dischargers), (2) calculate dilution factors for each facility (receiving stream flow divided by effluent flow), and (3) rank the flow data and dilution factors and report the results in terms of percentiles. See Appendix B for more details.) Harmonic mean, 30Q5, and 1Q10 flows are calculated from the 7Q10 flows and arithmetic mean flows. The units of flow are MLD.

The following are short descriptions of the percentiles and flows displayed in this tab:

- **50th Percentile Results** — exposure calculations based on the median (i.e., 50th percentile) surface water concentrations and represent central tendency exposure. These flows are used to represent mid-sized stream flows.

- **10th Percentile Results** — exposure calculations based on the high-end (i.e., upper 10th percentile) surface water concentrations and represent the bounding high-end exposures. These flows are used to represent small streams.

- **Harmonic Mean Flow ($SF_{harmonic}$)** — inverse mean of reciprocal daily arithmetic mean flow values. In other words, harmonic mean (H) is defined as $H = n/[(1/x_1) + (1/x_2) +...+ (1/x_n)]$ where x is a particular number in a group of measured values and n is the number of measurements in the series. These flows are used to generate estimates of chronic human exposures via drinking water and fish ingestion.

- **30Q5 Flow (SF_{30Q5})** — 30 consecutive days of lowest flow over a 5-year period. These flows are used to determine acute human exposures via drinking water.

- **7Q10 Flow (SF_{7Q10})** — 7 consecutive days of lowest flow over a 10-year period. These flows are used to calculate estimates of chronic surface water concentrations to compare with the concentrations of concern for aquatic life.

- **1Q10 Flow (SF_{1Q10})** — single day of lowest flow over a 10-year period. These flows are used to calculate estimates of acute surface water concentrations to compare with the concentrations of concern for aquatic life.

The calculations used to estimate the SIC Code-based surface water concentrations are presented in Section 3.1.4.1, Equations 3-1 to 3-4.

At the bottom of the page is a text box containing any comments entered by clicking on “SW comment” on the General Release Information page (See Section 3.1.1.1)

3.1.5.2 *SIC Code Results Page – Drinking Water Information*

The Drinking Water Information tab (Figure 3-15) presents the predicted exposure doses for individuals who ingest drinking water from streams and rivers that receive wastewater discharges containing the chemical of concern. The first column, "Exposure Type," lists three different measurements of exposure. To the right of each, under the "Results" heading, are the corresponding 50th and 10th percentile exposure values. The subsequent columns contain exposure factors that were entered in the Exposure Factors page (See Section 3.1.2). The exposure types and exposure factors are defined below.

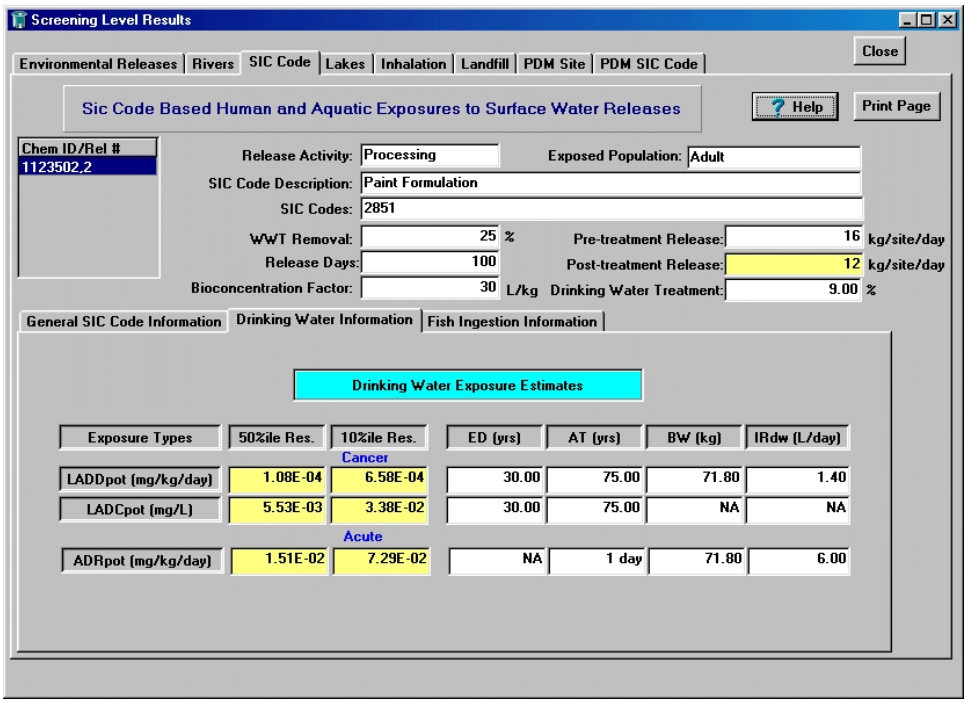

Figure 3-15. SIC Code Results Page – Drinking Water Exposure Estimates

<u>Exposure Types</u>

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from drinking water intake; calculated to represent chronic exposures to contaminated drinking water over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in drinking water; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from drinking water intake; normalized over a shorter time period (e.g., 1 day).

The calculations of these values are presented in Section 3.1.4.2, Equations 3-5 through 3-7.

- **Exposure Duration (ED)** — number of years a resident drinks contaminated water. E-FAST V2.0 uses a default value of 30 years; see Table 3-2.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Drinking Water Ingestion Rate (IR_{dw})** — used for calculating acute and chronic exposures.

3.1.5.3 *SIC Code Results Page – Fish Ingestion Information*

The Fish Ingestion Information tab (Figure 3-16) presents the acute and chronic exposure doses for individuals who ingest fish from streams and rivers that receive wastewater discharges containing the chemical of concern. The first column, "Exposure Types," lists three different measurements of exposure. To the right of each, under the "Results" heading, are the corresponding 50th and 10th percentile exposure values. The subsequent columns contain exposure factors that were entered in the Exposure Factors page (See Section 3.1.2). The exposure types and exposure factors are defined below.

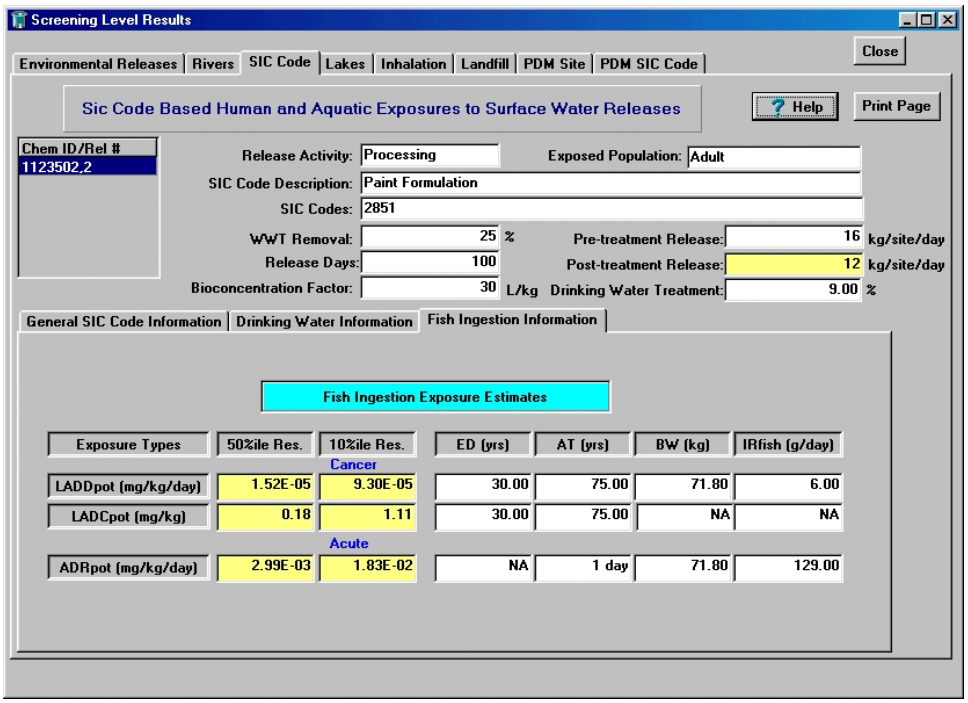

Figure 3-16. SIC Code Results Page – Fish Ingestion Exposure Estimates

<u>Exposure Types</u>

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from ingestion of fish tissue; calculated to represent chronic exposures to fish over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in ingested fish tissue; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from ingestion of fish tissue; normalized over a shorter time period (e.g., 1 day).

  The calculations of these values are presented in Section 3.1.4.3, Equations 3-8 through 3-10.

Exposure Factors

- **Exposure Duration (ED)** — number of years a resident consumes contaminated fish. E-FAST V2.0 uses a default value of 30 years; see Table 3-2.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Fish Ingestion Rate (IR_{fish})** — used for calculating acute and chronic exposures.

3.1.6 Lakes Results Page

Figure 3-17 shows an example Lakes Results page. The box in the upper left-hand corner shows all of the release activities that included discharges to lakes, bays estuaries, or oceans; you can click on any release activity to view the results for that activity. The following are short descriptions of the fields listed in the upper half of this page.

- **Release Activity** — can be manufacturing, processing, industrial use, or other. This was entered in a text field on the left-hand side of the General Release Information page (Figure 3-2).

- **Facility Name, Location, NPDES, Reach Number, Reach Name** — information on the discharging facility extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Facility on Reach?** — indicates whether the facility discharges to the identified reach, discharges to a tributary stream, or if the discharge point is unknown.

- **Exposed Population** — can be adults, youths 13 to 19 years, children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years, or infants less than one year old. This was entered on the Screening Level Main page (Figure 3-1).

- **Discharge Type —** indicates whether the facility is a direct discharger that discharges treated wastewater directly to a surface water body or an indirect discharger that discharges wastewater to a POTW for treatment.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release Days** — number of days per year that the chemical is discharged, as entered on the General Release Information page.

- **Pretreatment Release** — rate of release of the chemical by the facility to a wastewater treatment facility (kg/site/day), as entered on the General Release Information page.

- **Post-treatment Release** — rate of release of the chemical after treatment by a wastewater treatment facility. The post-treatment release amount is equal to the pretreatment release reduced by the wastewater treatment removal percentage.

- **Bioconcentration Factor —** indicates the tendency of the chemical to accumulate in living organisms. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

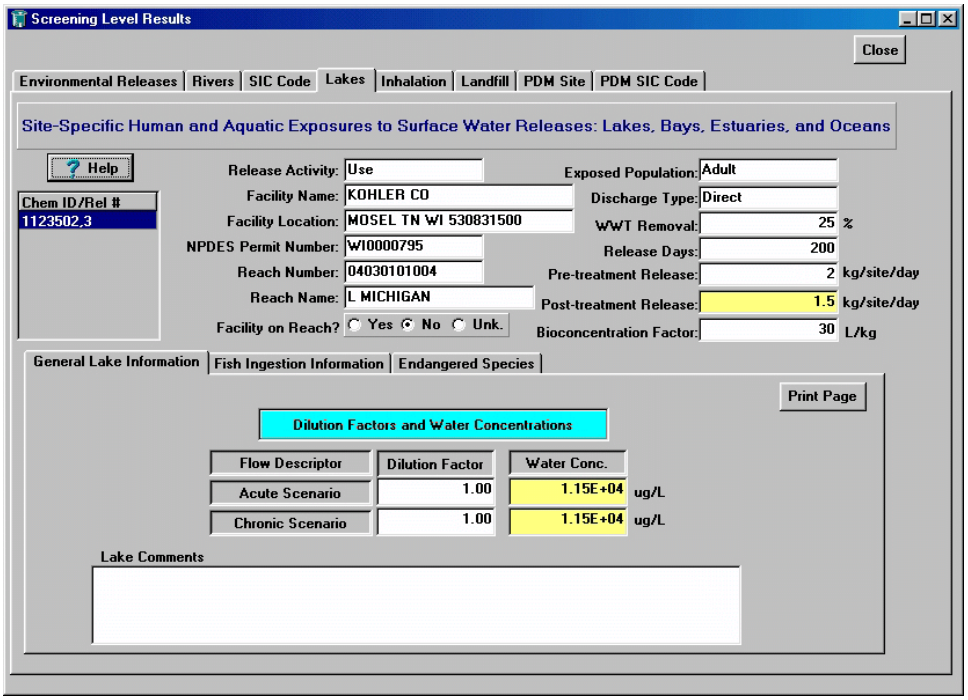

Figure 3-17. Lakes Results Page – Dilution Factors and Water Concentrations

Three tabs located in the lower half of the page allow you to view General Lake Information, Fish Ingestion Information, and Endangered Species. The "Print Page" button at the right-hand side of the tabs may be used to generate a hard copy of the data on the screen. The hard copy includes the data in all of the tabs in the lower portion of the screen (General Lake Information, Fish Ingestion Information, and Endangered Species), so there is no need to click the "Print Page" button for each of these tabs.

3.1.6.1 *Lakes Results Page – General Lake Information*

The General Lake Information tab contains dilution factors and resulting surface water concentrations for lakes, bays, estuaries, and oceans. No simple streamflow value represents dilution in these types of water bodies. To account for further dilution in the water body, dilution factors for the water body of interest are used. Measured dilution factors are typically between 1 (representing no dilution) and 200 and are based on NPDES permits or regulatory policy.

Dilution factors are used to calculate all fish tissue concentrations. Acute dilution factors are used to calculate potential ADR_{POT} and chronic dilution factors are used to calculate potential $LADD_{POT}$ and $LADC_{POT}$. If an acute dilution factor is available but a chronic dilution factor is not available, then

the chronic value is assumed to be equal to the acute value. If a chronic value is available, but no acute value is available, then the acute value is assumed to be one. E-FAST V2.0 does not calculate potential drinking water exposures resulting from releases to estuaries and bays because they are not potable waters. Potential drinking water exposures are also not calculated for releases to lakes because of high uncertainty about appropriate dilution factors.

Estimation of Surface Water Exposure Concentrations in Lakes, Bays, Estuaries, and Oceans

E-FAST V2.0 uses the following equation to calculate surface water concentrations in still bodies such as bays, lakes, and estuaries:

$$SWC \; 4 \; \frac{WWR \times \left(1 \;) \; \frac{WWT}{100} \right) \times CF1}{PF \times CF2 \times DF} \qquad \text{(Eq. 3-11)}$$

where:

SWC	=	Surface water concentration (ppb or µg/L)
WWR	=	Chemical release to wastewater (kg/day)
WWT	=	Removal from wastewater treatment (%)
PF	=	Effluent flow of the discharging facility (MLD)
DF	=	Acute or chronic dilution factor used for the water body (typically between 1 and 200)
CF1	=	Conversion factor (10^9 µg/kg)
CF2	=	Conversion factor (10^6 L/day/MLD)

Acute and chronic dilution factors, supplied by the States (or Federal Government), were used if they were available. If the dilution factors were not available, a value of 1 was assigned for the acute and chronic dilution factors.

Immediate mixing of effluent discharges to lakes, bays, and estuaries does not occur because these water bodies have slow-moving and/or tidal fluctuations that prevent complete mixing. Therefore, modeling techniques and tracer studies are used to develop mixing zone values for these types of water bodies. These mixing zone values are then used to develop dilution factors for estimating concentrations of chemicals in lakes, bays, and estuaries. A mixing zone is defined as an area within which water quality criteria can be exceeded. Mixing zones can be associated with either acute or chronic aquatic toxicity criteria. Acute mixing zones are sized to prevent lethality to passing organisms. Chronic mixing zones are sized to protect the ecology of the water body as a whole. The acute mixing zone is referred to as the "zone of initial dilution" and is smaller than the chronic mixing zone.

3.1.6.2 *Lakes Results Page – Fish Ingestion Information*

The Fish Ingestion Information tab (Figure 3-18) presents the estimated acute and chronic potential exposure doses for people who ingest fish from lakes, bays, estuaries, and oceans that receive wastewater discharges containing the chemical of concern. The first column, "Exposure Types," lists three different measurements of exposure. To the right of each, under the "Results" heading, is the corresponding exposure value. The subsequent columns contain exposure factors that were entered in the Exposure Factors page (Section 3.1.2). The exposure types and exposure factors are defined below.

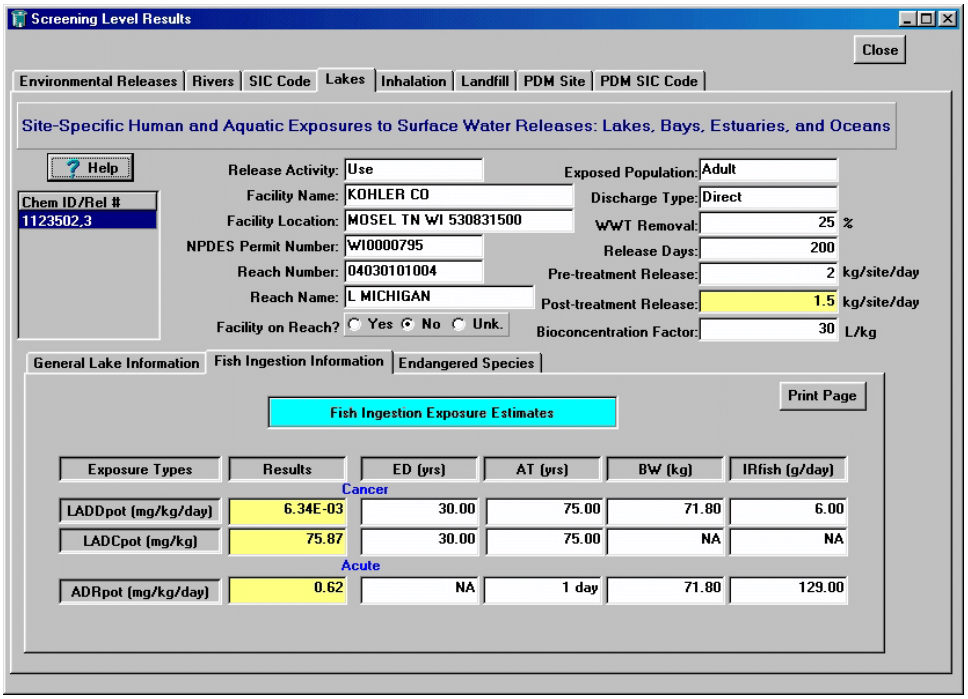

Figure 3-18. Lakes Results Page – Fish Ingestion Exposure Estimates

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from ingestion of fish tissue; calculated to represent chronic exposures to fish over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in ingested fish tissue; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from ingestion of fish tissue; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** — number of years a resident consumes contaminated fish. E-FAST V2.0 uses a default value of 30 years; see Table 3-2.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Fish Ingestion Rate (IR_{fish})** — used for calculating acute and chronic exposures.

Estimation of Potential Doses via Fish Ingestion

To estimate how much of a given chemical a person will ingest through eating fish, E-FAST V2.0 uses Equations 3-8 through 3-10 (See Section 3.1.4.3). These equations convert an estimated surface water concentration to a fish ingestion exposure estimate. The distinction between acute and chronic fish

ingestion is made on the basis of daily ingestion rate. The mean long-term fish ingestion rate is used to calculate chronic exposures and the mean serving size is used to calculate acute fish ingestion exposures for adults.

3.1.6.3 *Lakes Results Page – Endangered Species*

The Endangered Species tab presents the endangered species known (or possible) to exist in the vicinity of lakes, bays, estuaries, and oceans that receive wastewater discharges containing the chemical of concern. The Endangered Species tab in the Lakes Results page is identical to the Endangered Species tab in the Rivers Results page (Figure 3-13). The location of endangered species is correlated with the facility location via FIPS State and county codes. The endangered species information is presented in six columns and includes common name, county and State, taxonomic group (e.g., mammals, birds, fish, plants, reptiles, amphibians, clams, etc.), listing action (listing, proposed, delisting), and known occurrence. The data were obtained from EPA's Endangered Species Protection Program (ESPP) Databases (U.S. EPA, 2004). The ESPP is a cooperative effort between the U.S. Fish and Wildlife Service (FWS), EPA Regions, States, and pesticide users. ESPP is located in the Field and External Affairs Division (FEAD) of the Office of Pesticide Programs (OPP).

3.1.7 Landfill Results Page

Figure 3-19 shows an example Landfill Results page. The box in the upper left-hand corner shows all of the release activities that included discharges to landfills; you can click on any release activity to view the results for that activity. The "Print Page" button in the lower right-hand corner may be used to generate a hard copy of the data on the screen. The following are short descriptions of the fields listed in the upper half of this page.

E-FAST V2.0 uses a simple conservative method for estimating groundwater concentrations that may result from chemical releases to landfills. These releases may be in the form of waste material from manufacturing, processing, or commercial activities, or wastewater treatment plant sludge that contains the chemical and is placed in a landfill.

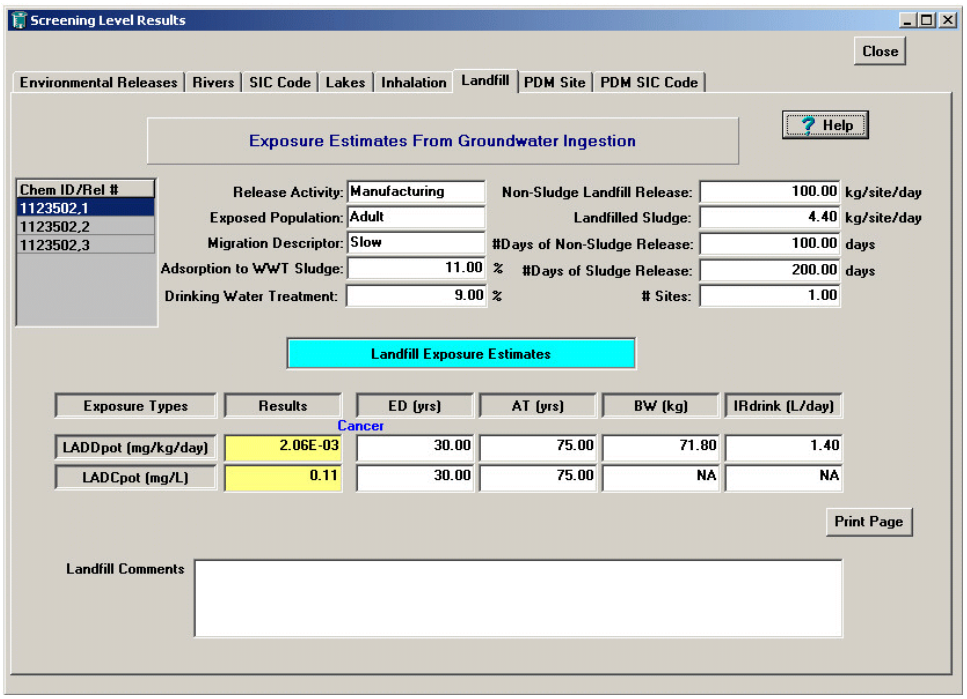

Figure 3-19. Landfill Results Page – Landfill Exposure Estimates

The following are short descriptions of the fields in this page:

- **Release Activity** — can be manufacturing, processing, industrial use, or other. This was entered in a text field on the left-hand side of the General Release Information page (Figure 3-2).

- **Exposed Population** — can be adults, youths 13 to 19 years, children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years, or infants less than one year old. This was entered on the Screening Level Main page (Figure 3-1).

- **Migration Descriptor** — an expression of the chemical's tendency to migrate from the waste being disposed of in the landfill to surrounding soil, and eventually to groundwater. The migration descriptors used by E-FAST V2.0 are negligible, negligible to slow, slow, moderate, and rapid; a rating of "negligible" indicates that the chemical does not reach groundwater. The migration descriptor should be selected on the basis of physical-chemical parameters such as the log of the organic carbon/water partition coefficient (log K_{OC}), the log of the n-octanol/water partition coefficient (log K_{OW}), the expected leachability of the chemical from the type of waste being disposed, and the reactivity of the chemical, which includes transformation processes such as biodegradation and hydrolysis (as applicable). A discussion of the E-FAST V2.0 default descriptor selection method is presented later in this section. This method may be useful when it is known that reactivity is not a factor controlling migration, and a measured log K_{OC} value is available or it is known that K_{OC} estimation methods yield reliable predictions. The migration descriptor was entered in the PChem/Fate Inputs screen (Figure 2-1).

- **Adsorption to Wastewater Treatment (WWT) Sludge** — percentage of chemical adsorbed to sludge during wastewater treatment. This value was entered in the PChem/Fate Inputs screen (Figure 2-1).

- **Drinking Water Treatment Removal** — removal percentage, which is based on the physical-chemical characteristics of the chemical and the expected efficiency of unit treatment processes at the drinking water treatment facility. This value was entered in the PChem/Fate Inputs Screen (Figure 2-1).

- **Number of Sites** — number of landfill release sites. This value was entered in a number field on the left-hand side of the General Release Information page (Figure 3-2).

- **Non-Sludge Landfill Release** — the per site daily release amount and release days of chemical wastes (excluding landfilled wastewater treatment sludge) to a landfill. These values were entered in the General Release Information Page (Figure 3-2b).

- **Landfilled Sludge** — the per site daily release amount and release days of chemical in contaminated wastewater treatment sludge that is landfilled. If you have specified a surface water release and a percent adsorption to wastewater releases in the PChem/Fate Inputs screen (Figure 2-1), E-FAST V2.0 will have calculated a sludge release for you. These values were entered in the General Release Information Page (Figure 3-2b).If you have specified non-sludge landfill and landfilled sludge as releases in the same release activity entry screen in Figure 3-2b, E-FAST V2.0 assumes the per site amounts are landfilled together at one location; non-sludge and sludge releases from one release site that are landfilled at different locations should be entered on separate release activity screens.

The lower half of the page presents the chronic exposure doses for individuals who ingest groundwater contaminated by landfill releases containing the chemical of concern. The first column, "Exposure Types," lists two different measurements of exposure. To the right of each, under the "Results" heading, is the corresponding exposure value. The subsequent columns contain exposure factors that were entered in the Exposure Factors page (See Section 3.1.2). The exposure types and exposure factors are defined below.

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from ingestion of groundwater contaminated by landfill releases; calculated to represent chronic exposure over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — in groundwater contaminated by landfill releases; calculated to represent chronic lifetime concentration. These concentrations are generally used for cancer calculations.

Potential Acute Dose Rate (ADR_{POT}) is not calculated because the algorithms used in the estimation method calculate long-term average groundwater concentrations rather than short-term acute concentrations (see below).

Exposure Factors

- **Exposure Duration (ED)** — number of years a resident drinks contaminated water. E-FAST V2.0 uses a default value of 30 years; see Table 3-2.

- **Exposure Frequency (EF)**— number of days per year a resident drinks contaminated water. E-FAST V2.0 uses a default value of 365 days/year.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.

Estimation of Groundwater Exposure Concentrations from Releases to Landfills

Site-specific estimation of groundwater (drinking water) exposure from landfills requires information on climate, soil, groundwater flow direction, and location of receptor drinking water wells. Because this level of information is commonly not available for screening-level estimates, E-FAST V2.0 uses a simple, conservative, generic method developed by EPA (U.S. EPA, 1987a). The only chemical-specific parameter required is the log K_{OC}, and it is assumed that a reliable value (measured or estimated) exists. It is also assumed that the substance does not degrade abiotically or biologically at a rate sufficient to significantly affect its potential to reach ground water.

This method is based on studies that modeled the groundwater concentrations that resulted from the landfill of hypothetical nonvolatile compounds (i.e., Henry's law constant $\leq$ 1E-05 atm-m^3/mol) of varying soil sorption characteristics (i.e., log K_{OC} values ranging from 0 to 4.5) in soil types with different organic carbon contents and groundwater hydraulic characteristics (GSC, 1987; U.S. EPA, 1987a). The transport of the chemicals through the soil and groundwater was modeled using the SESOIL and AT123D models, respectively. The loading of chemicals in a 1-hectare landfill was assumed to be 1,000 kg/year for 10 years. The distance to groundwater was assumed to be 8 meters, and the depth of a drinking water well 200 meters from the edge of the landfill was set at 20 meters.

EPA used the results of these studies to develop a conservative method for predicting groundwater exposures from landfill disposals by assigning migration descriptors based on log K_{oc} values and the maximum long-term ($\geq$70 year) average groundwater concentrations associated with those K_{oc} values, as follows:

Migration Descriptor	Log K_{oc}	Groundwater concentration (GWC) (mg/L per kg release)
Negligible - no migration		None
Negligible to slow	$\geq$ 4.5	3.21E-6
Slow	<4.5 to 3.5	2.67E-5
Moderate	<3.5 to 2.5	5.95E-5
Rapid	<2.5	7.55E-5

Estimation of Groundwater Potential Doses from Releases to Landfills

To estimate how much of a given chemical a person will ingest through groundwater (drinking water), E-FAST V2.0 uses the equations presented below. These equations convert an annual chemical release and its estimated groundwater concentration (from the preceding section) to a drinking water exposure estimate. The release amount is multiplied by the groundwater concentration (per kg release), the removal rate (if any) of the chemical during treatment of the drinking water, the estimated drinking water ingestion rate, the exposure frequency, and the exposure duration. This product is then divided by body weight and averaging time to yield the exposure dose.

$$LADD_{POT} = \frac{LFR \times GWC \times \left(1 - \frac{DWT}{100}\right) \times IR_{dw} \times EF \times ED}{BW \times AT \times CF1} \qquad \text{(Eq. 3-12)}$$

$$LADC_{POT} \; 4 \; \frac{LFR \times GWC \times \left(1 \;) \; \frac{DWT}{100}\right) \times EF \times ED}{AT \times CF1} \qquad \text{(Eq. 3-13)}$$

where:

$LADD_{POT}$	=	Potential Lifetime Average Daily Dose (mg/kg/day)
$LADC_{POT}$	=	Potential Lifetime Average Daily Concentration in drinking water (mg/L)
LFR	=	Chemical release rate to landfill per site (kg/yr)
GWC	=	Groundwater concentration (mg/L per kg release/yr)
IR_{dw}	=	Drinking water intake rate (L/day)
BW	=	Body weight (kg)
DWT	=	Removal during drinking water treatment (percent)
ED	=	Exposure duration (years)
AT	=	Averaging time (years)
EF	=	Exposure frequency (days/yr)
CF1	=	Conversion factor (365 days/yr)

3.1.8 Inhalation Results Page

As introduced in Section 3.1.1.3, E-FAST V2.0 uses EPA's SCREEN3 Model for estimating ambient air concentrations from stack and fugitive releases. Stack releases include but are not limited to incineration; an example of fugitive release is untreated local exhaust at ambient temperature. An example Inhalation Results page is shown in Figure 3-20. The box in the upper left-hand corner shows all of the fugitive air and stack release activities; you can click on any release activity to view the results for that activity. The following are short descriptions of the fields listed in the upper half of this page.

- **Release Activity** — can be manufacturing, processing, industrial use, or other. This was entered in a text field on the left-hand side of the General Release Information page (Figure 3-2).

- **Exposed Population** — can be adults, youths 13 to 19 years, children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years, or infants less than one year old. This was entered on the Screening Level Main page (Figure 3-1).

- **Number of Sites** — number of fugitive and/or stack release sites. This was entered in a number field on the left-hand side of the General Release Information page (Figure 3-2).

- **Per Site Fugitive Release** — total site release of fugitive emissions, presented in units of kg/site/day.

- **Release Days (fugitive) —** number of days per year that the chemical is released to the air via fugitive emissions. This was entered in a number field on the right-hand side of the General Release Information page (Figure 3-2c).

- **Per Site Stack Release** — total site release of stack emissions, presented in units of kg/site/day.

- **Release Days (stack) —** number of days per year that the chemical is released to the air via stack emissions. This was entered in a number field on the right-hand side of the General Release Information page (Figure 3-2c).

In addition to these fields, the top portion of the Inhalation results page displays a "Print Page" button that may be used to generate a hard copy of the data on the screen. The hard copy includes the data in all of the tabs in the lower portion of the screen (Inhalation Exposure Estimates, Release Information, Meteorological/Terrain and Downwash Information, and SCREEN3 Model Results), so there is no need to click the "Print Page" button for each of these tabs.

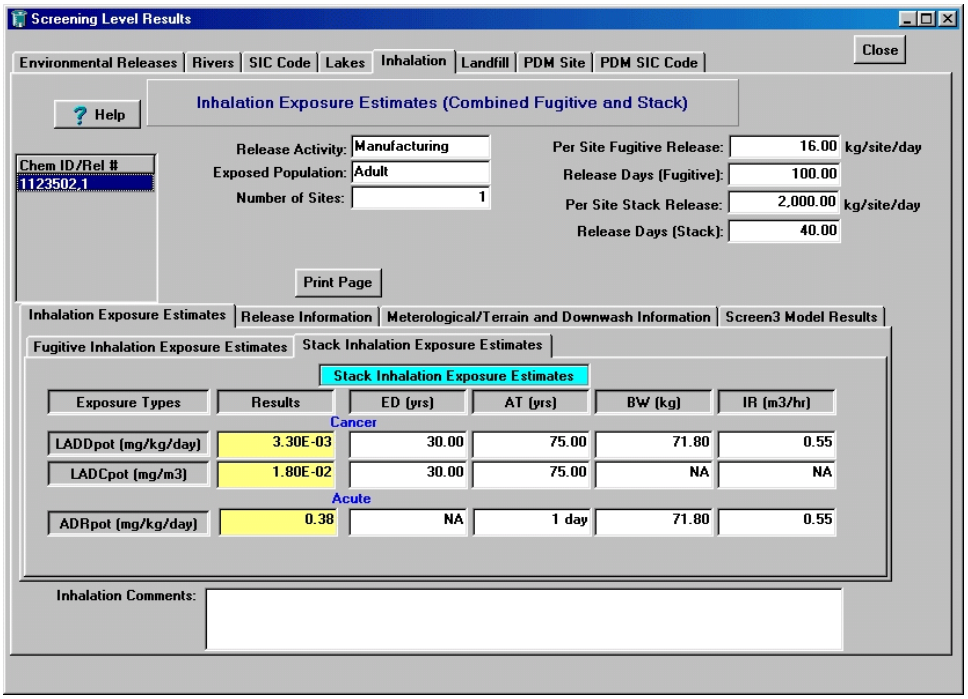

Figure 3-20. Inhalation Results Page – Inhalation Exposure Estimates

Three tabs located in the lower half of the page allow you to view Inhalation Exposure Estimates, Release Information, and Meteorological/Terrain and Downwash Information, and SCREEN3 Model Results.

3.1.8.1 *Inhalation Results Page – Inhalation Exposure Estimates*

The Inhalation Exposure Estimates tab (Figure 3-20) presents the acute and chronic exposure doses for individuals who breathe the air containing the chemical of concern. This tab contains two sub-tabs displaying exposure estimates for fugitive and stack releases. In each sub-tab, the first column, "Exposure Types," lists three different measurements of exposure. To the right of each, under the "Results" heading, is the corresponding exposure value. The subsequent columns contain exposure factors that were entered in the Exposure Factors page (See Section 3.1.2). The exposure types and exposure factors are defined below.

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from inhalation of stack and fugitive air emissions; calculated to represent chronic exposures over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — from inhalation of the chemical of concern in stack and fugitive air emissions; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from inhalation of stack and fugitive air emissions; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** — number of years the resident breathes contaminated air. E-FAST V2.0 uses a default value of 30 years; see Table 3-2.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Inhalation Rate (InhR)** — used for calculating acute and chronic exposures.

Estimation of Ambient Air Exposure Concentrations

E-FAST V2.0 uses EPA's SCREEN3 air dispersion model to estimate air concentrations. This section describes the approach used to develop the fate and transport modeling system for residential (outdoor) air exposures. It also includes an overview of the principles of ambient air dispersion modeling and a discussion of the input parameters, the default values used in E-FAST V2.0, and the assumptions needed to perform air dispersion modeling.

a) General Overview of Air Dispersion Models

Air quality models have become the primary analytical tool for assessing the effects of point sources on air quality. A point source is an emission that emanates from a specific point, such as a smokestack or vent. The modeling methods used are considered to be applicable for assessing impacts of a source from the facility fence line out to a 50-km radius of the source to be modeled (U.S. EPA, 1992a). These models use mathematical equations to simulate the rise of a plume from a source and the subsequent horizontal and vertical dispersion affected by wind, temperatures, terrain, and other environmental factors (Turner, 1994). Gaussian models are the most widely used techniques for estimating the impact of nonreactive pollutants (U.S. EPA, 1987b). These models use the Gaussian distribution to describe crosswind and vertical distributions that are the result of wind and other factors that produce mixing (Turner, 1994). According to Turner (1994), the basic Gaussian dispersion equation simulates the 3-dimensional behavior of pollutants in the atmosphere:

$$X = QVD/(2\pi\, u_s \sigma_y \sigma_z)\exp\left[-1/2((z_r - h_e)/\sigma_z)^2\right] + \sum_{N=1}^{k}\left[\exp -1/2((z_r - h_e - 2Nz_i)/\sigma_z)^2\right] \quad \text{(Eq. 3-14)}$$

where:

X	=	Concentration (g/m^3)
Q	=	Emission rate (g/s)
V	=	Vertical term
D	=	Dispersion term
u_s	=	Stack height wind speed (m/s)
σ_y	=	Lateral dispersion parameter (m)
σ_z	=	Vertical dispersion parameter (m)
z_r	=	Receptor height above ground (m)
h_e	=	Plume centerline height (m)
z_i	=	Mixing height (m)
k	=	Summation limit for multiple reflections of plume off of the ground and elevated inversion, usually ≤ 4

See Sections 1.1.6 and 1.1.7 of the User's Guide of the ISC3 Dispersion Model Vol. 2 for more information (U.S. EPA, 1995b).

The fate and transport modeling system depends on you to provide data which describe the local situation so the model can predict likely resulting concentrations at a residence some distance from the facility. It is necessary to have quantitative information about the sources to conduct air dispersion modeling. Screening models need less information than more sophisticated models. The main inputs include the following parameters for stack emissions:

- Source emission rate
- Stack height
- Inside stack diameter
- Exhaust gas exit velocity
- Exhaust gas exit temperature
- Dimensions of structures near each source
- Land use near the modeled facility
- Terrain features near the facility
- Distance to receptor
- Receptor height

and the following parameters for fugitive emissions:

- Source emission rate
- Release height
- Length of larger side
- Length of smaller side
- Wind Direction Search Option
- Land use near the modeled facility
- Terrain features near the facility
- Distance to receptor
- Receptor height

SCREEN3 is an EPA screening-level system that uses a Gaussian plume model, incorporating source-related factors and meteorological conditions to estimate the ambient pollutant concentration (U.S.

EPA, 1995a). The model requires relatively straightforward facility-specific input data on stack, meteorological conditions, and terrain. The main advantages of SCREEN3 are that it is simple to use and does not require much data (default values are provided for most parameters). SCREEN3 performs single-source calculations, estimating the maximum 1-hour average concentrations at prespecified distances. (Note: This value is not appropriate for assessing potential health impacts of long-term, i.e., chronic, exposure. According to EPA (1992b), risk assessment for chronic health effects should be based on the maximum annual concentration for a representative exposure concentration. The convention used in E-FAST V2.0 (based on general experience with elevated point sources) is to approximate the maximum annual average concentration by multiplying the 1-hour maximum average concentration by a generic conversion factor. (U.S. EPA, 1992b))

b) Input Parameters, Default Values, and Assumptions for SCREEN3 Dispersion Modeling

E-FAST V2.0 incorporates SCREEN3 by linking the output of one calculation (e.g., emission rate estimates) to the input of the subsequent model (e.g., air dispersion) and a post-processing program that incorporates SCREEN3's predicted concentrations into E-FAST V2.0's potential dose calculations. The user interface prompts you for the input parameters SCREEN3 needs to perform the dispersion calculations that result in estimated air concentrations at a residence at a given distance from the facility. E-FAST V2.0 provides default input values for all of these input parameters, except emission rate, which is generated by E-FAST V2.0 based on the release amount you entered in the ambient air section of the General Release Information Page (See Section 3.1.1.3). The main input parameters for stack emissions include:

- Emission Rate (g/s), which is generated by E-FAST V2.0, based on user inputs
- Stack Height (m)
- Inside Stack Diameter (m)
- Stack Gas Exit Velocity (m/s)
- Stack Gas Temperature (K)
- Ambient Temperature (K)

While E-FAST V2.0 uses the point source algorithms in SCREEN3 to generate emission concentrations for stack emissions, E-FAST V2.0 uses the area source algorithms in SCREEN3 to model downwind concentrations for fugitive emissions. Unlike stack emissions that exit a facility at a single stack or point, fugitive emissions exit a facility through cracks, vents, or openings; this type of emission is modeled as an area release. The main input parameters for fugitive emissions include:

- Emission Rate (g/m^2-s), which is generated by E-FAST V2.0, based on user inputs
- Release Height (m)
- Length of Release Opening (m)
- Width of Release Opening (m)

SCREEN3 also requires the distance to the residence, meteorological conditions, the height and usage of the surrounding terrain, downwash conditions (for stack releases only), and other related parameters. Prior to beginning any model calculations, you can review the default values for their appropriateness to your model run (See Table 3-1, Section 3.1.1.3). If you choose not to accept a default value for any parameter, you can enter a site-specific value. The user interface provides logical constraints on the range of possible values you can enter.

Below are several assumptions made for air dispersion modeling in E-FAST V2.0:

- **Ambient Transformation** — SCREEN3 and E-FAST V2.0 do not account for chemical reactions (transformation) in the atmosphere. This is a conservative assumption because the duration that emitted chemicals will be in the atmosphere before reaching the potential receptors (i.e., nearby residents) is relatively short.

- **Constant Emission Rate** — The air dispersion calculations performed by SCREEN3 rely on a source emission rate for each pollutant, in g/s or g/m^2-s. These emissions are assumed to be continuous and the rate not variable over time. Because of these assumptions, the emission rate inputs must be adjusted according to the desired outputs, which for E-FAST V2.0 are 24-hour and annual maximum average concentrations. For example, a 100 kg per day release that occurred two days per year would have a source emission rate based on 100 kg/d for the 24-hour concentration calculation, but the source emission rate for the annual maximum calculation would be calculated from the total amount emitted per year (200 kg). The source emission rate data are provided by E-FAST V2.0 from the earlier calculations in the ambient air section of the General Release Information page (Figure 3-2). These data are automatically input to the air dispersion modeling of E-FAST V2.0.

- **Single Point Emissions** — E-FAST V2.0 assumes that all stack emissions from a given facility are released from a single stack. E-FAST V2.0 treats fugitive emissions in a similar fashion, however the user can adjust the size of the release area so that it encompasses all of the fugitive releases. SCREEN3 cannot explicitly determine impacts from multiple sources; however, it can provide a conservative estimate for the downwind concentration if the emissions are merged into a single representative stack. (Note: SCREEN3 may provide an unacceptably high estimate for the downwind concentration using a "representative" stack, if the stacks are located more than 100m apart, or the stack parameters differ more than 20 percent.)

  To determine the parameter for the "representative" stack of multiple stacks, a merged stack parameter is calculated for each individual stack using the following equation:

$$M = \frac{h_s \times \left[\left(\pi/4\right) D_s^2 V_s\right] \times T_s}{Q} \qquad \text{(Eq. 3-15)}$$

where:

M	=	Merged stack parameter (m^{4}K/g)
h_s	=	Stack height (m)
D_s	=	Inside stack diameter (m)
V_s	=	Stack exit gas velocity (m/s)
T_s	=	Stack gas exit temperature (K)
Q	=	Pollutant emission rate (g/s)

Screen 3 inputs: use the stack with the lowest value of M as the representative stack and the sum of the emission rates from all of the stacks as the emission rate from the representative stack (U.S. EPA, 1992b).

Default Model Parameters

Table 3-1 in Section 3.1.1.3 shows the default values provided by E-FAST V2.0 for stack/incinerator releases and for fugitive/vent releases. Several other parameters and the considerations in selecting appropriate values for them require more extensive discussion and are provided below. These parameters influence the way the model simulates stability and turbulence in the atmosphere.

- **Meteorological Conditions** — With respect to information needed by SCREEN3, stability and wind speed are the two most important parameters of meteorological conditions that affect ambient pollutant concentrations emitted from an elevated stack. In a stable atmospheric environment, the plume is trapped at a certain height or even descends, resulting in a relatively high concentration. In an unstable atmospheric environment, the plume rises to a higher level by momentum and buoyancy forces. Horizontal winds transport pollutants away from the source and dilute ambient concentrations. The effect of horizontal wind speed is relatively straightforward: doubling the wind speed cuts concentrations in half. Modeling dispersion is easiest when winds are from one direction and of consistent speed, and when the terrain is flat and uninterrupted (as in a rural area).

  For simple elevated or flat-terrain screening, you have three choices of meteorological conditions: (1) full meteorological description, including all stability classes and wind speeds; (2) specification of a single stability class; and (3) specification of both stability class and wind speed. Full meteorology is recommended for a combination of stability and wind speed that will result in maximum ground-level concentrations. If you have particular meteorological conditions of concern, specify either stability only or both stability and wind speed for SCREEN3 modeling.

  Stability classes are indicators of atmospheric turbulence. The stability category depends on static stability (related to the change in temperature with height), thermal turbulence (caused by heating of the air at ground level), and mechanical turbulence (a function of wind speed and surface roughness). See *Screening Procedures for Estimating the Air Quality Impact of Stationary Sources, Revised* (U.S. EPA. 1992b) and *SCREEN3 User's Guide* (U.S. EPA 1995a) for more detailed information.

- **Surrounding Land Use** — This classification has a significant effect on estimates of downwind concentrations. The default value is rural, but you can modify this classification in the user interface. The selection of urban or rural dramatically affects the estimate of concentrations by giving a different wind speed profile at the same stability category. If more than 50 percent of an area 3 km around the source is of land use types heavy or medium industrial, commercial or multi-family residential, the site is deemed to be in an urban setting. Also, if the population density within a 3 km radius around the source is greater than 750 people per square km, the urban mode should be selected (U.S. EPA, 1995a, 1997b).

- **Terrain** — Air quality models are most accurate when simulating long-term averages in areas with relatively simple topography (U.S. EPA, 1987b). Terrain sometimes significantly affects ambient ground-level pollutant concentrations through its effects on plume behavior. The important topographic features to note are the location and height of the elevated terrain. SCREEN3 uses two types of terrain: simple or complex. Simple terrain is considered to be an area where terrain features are all lower in elevation than the top of the stack of the source(s) in question. Complex terrain is defined as terrain exceeding the height of the stack being modeled.

If terrain height is higher than stack height, the modeling techniques required to simulate such a situation become more demanding. Because of the potential for providing inappropriate information in such a circumstance, only the simple terrain option of SCREEN3 has been incorporated into E-FAST V2.0.

- **Conversion of 1-hour Maximum Concentration to 24-hour and Annual Maximum Average Concentrations** — The standard output from SCREEN3 is a 1-hour maximum average concentration. As stated in Section 3.1.1.3, E-FAST V2.0 does independent SCREEN3 model runs for use in calculating the desired 24-hour and annual maximum average concentrations. E-FAST V2.0 then converts these values to 24-hour and annual maximum concentrations by multiplying the SCREEN3 calculations by the following conservative conversion factors (U.S. EPA, 1992b):

	Stack (point source)	Fugitive (area source)
24-hour maximum average	0.4	1
Annual maximum average	0.08	0.08

These conversion factors were developed by the EPA Office of Air Quality Planning and Standards (U.S. EPA, 1992b). They are intended to be used for a general case with a degree of conservatism to ensure that the annual maximum concentration will not be underestimated.

Estimation of Ambient Air Potential Doses

As described in the previous section, SCREEN3 predicts the air concentration for the residential scenario based on emission rates, stack data, terrain, meteorological conditions, and other related information. Exposure via inhalation is estimated using the equations below:

$$ADR_{POT} = \frac{0.4 \times AAC_{24} \times InhR \times ED \times CF1}{BW \times AT} \quad \textit{for stack (point source) releases} \qquad \text{(Eq. 3-16)}$$

$$ADR_{POT} = \frac{AAC_{24} \times InhR \times ED \times CF1}{BW \times AT} \quad \textit{for fugitive (area source) releases} \qquad \text{(Eq. 3-17)}$$

$$LADD_{POT} = \frac{0.08 \times AAC_{yr} \times InhR \times EF \times ED \times CF1}{BW \times AT \times CF2} \qquad \text{(Eq. 3-18)}$$

$$LADC_{POT} = \frac{0.08 \times AAC_{yr} \times ED \times CF1}{AT} \qquad \text{(Eq. 3-19)}$$

where:

ADR_{POT} = Potential Acute Dose Rate (mg/kg/day)
$LADD_{POT}$ = Potential Lifetime Average Daily Dose (mg/kg/day)
$LADC_{POT}$ = Potential Lifetime Average Daily Concentration (mg/m^3)

AAC_{24}	=	24-Hour Maximum Average Ambient Air Concentration ($\mu g/m^3$)
AAC_{yr}	=	Annual Maximum Average Air Concentration ($\mu g/m^3$)
InhR	=	Inhalation rate (m^3/day, equal to m^3/hr × 24 hr/day)
EF	=	Exposure frequency (365 days/year; see explanation below.)
ED	=	Exposure duration (years for $LADC_{POT}$ and $LADD_{POT}$, day for ADR_{POT})
BW	=	Body weight (kg)
AT	=	Averaging time (years for $LADC_{POT}$ and $LADD_{POT}$, day for ADR_{POT})
CF1	=	Conversion factor (10^{-3} mg/µg)
CF2	=	Conversion factor (365 days/year)

The value of AAC_{24} in Equations 3-16 and 3-17 is calculated by running SCREEN3 using the emission rate occurring over the course of one day. For the AAC_{yr} used in Equations 3-18 and 3-19, the emission rate input for SCREEN3 is calculated by taking the amount released in one year, regardless of the number of release days, and dividing the annual release by 365 days. Therefore, in the above equation, the exposure frequency (EF) is 365 days per year. Because of this difference in emission rates for daily and annual dose calculations, SCREEN3 is run twice for each fugitive release and twice for each stack release. The results of the SCREEN3 model runs are presented with the inhalation results, as described in Section 3.1.8.4. The units of AAC_{24} and AAC_{yr} are presented as $\mu g/m^3$ to be consistent with the stand-alone SCREEN3 model that is familiar to many users of E-FAST V2.0.

3.1.8.2 *Inhalation Results Page – Release Information*.

The Release Information tab (Figure 3-21) presents the release information inputs that were entered into SCREEN3. These inputs include Stack Height (m), Inside Stack Diameter (m), Stack Gas Exit Velocity (m/s), Stack Gas Temperature (K), Release Height (m), Length of Release Opening (m), and Width of Release Opening (m). All of these parameters are described in detail in Section 3.1.8.1. In addition, the Pretreatment Release (kg/site/day) and Emissions Removal (%) as entered on the General Release Information page (Figure 3-2c) and the PChem/Fate Inputs screen (Figure 2-1) are shown.

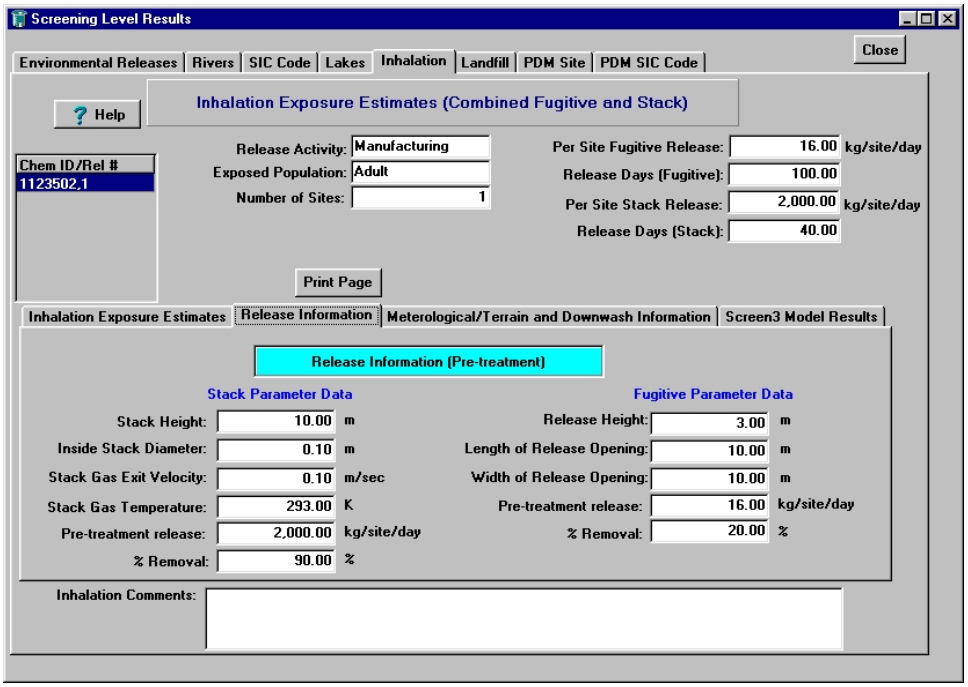

Figure 3-21. Inhalation Results Page – Release Information.

3.1.8.3 *Inhalation Results Page – Meteorological/Terrain and Downwash Information*

The Meteorological/Terrain and Downwash Information tab (Figure 3-22) presents the meteorological, terrain, and downwash information inputs that were entered into SCREEN3. These inputs include Surrounding Land Use, Terrain Height (m), Distance to Residence of Interest (m), and Meteorological Class (including Stability Class and Wind Speed, if applicable). In addition, the Facility Length (m), Facility Width (m), and Facility Height (m) will be presented, if applicable. All of these parameters are described in detail in Section 3.1.8.1.

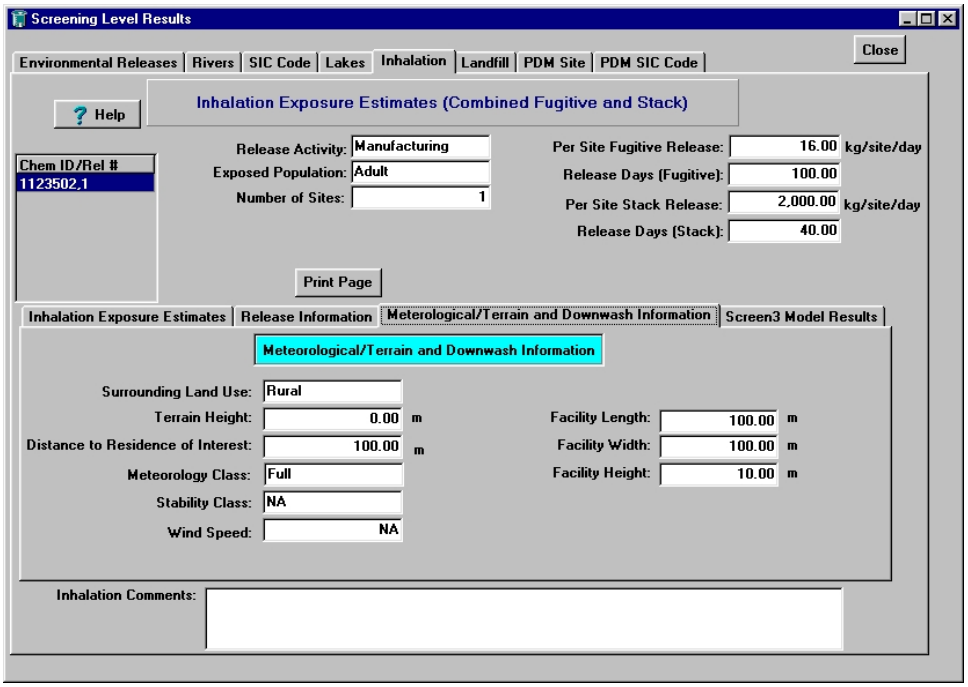

Figure 3-22. Inhalation Results Page – Meteorological/Terrain and Downwash Information

3.1.8.4 *Inhalation Results Page - SCREEN3 Model Results*

The SCREEN3 Model Results tab (Figure 3-23) presents the results of the SCREEN3 model runs. Results are presented for 24-hour average concentration and annual average concentration derived from stack and fugitive emissions. These are the AAC_{24} and AAC_{yr} values used in Equations 3-16, 3-17, 3-18, and 3-19. Note that the units are $\mu g/m^3$, which is consistent with the stand-alone SCREEN3 model.

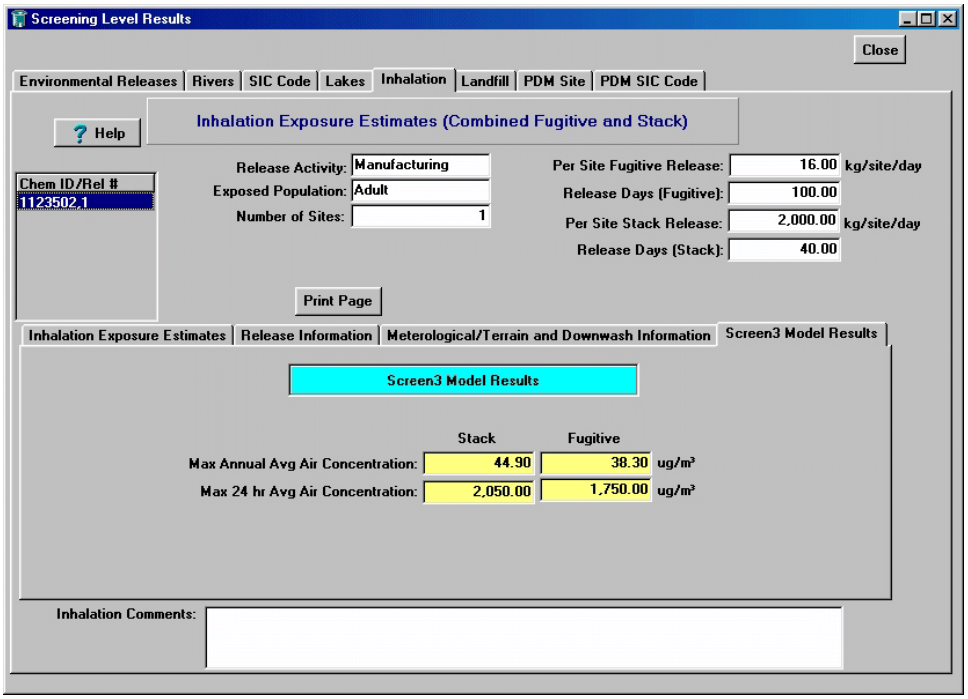

Figure 3-23. Inhalation Results Page – SCREEN3 Model Results

3.1.9 PDM Site-Specific Results Page

Running PDM is optional, as discussed in Section 3.1.1.1. In E-FAST V2.0, PDM predicts the number of days per year a chemical's COC in an ambient water body will be exceeded by the discharge from a facility. PDM analyses can be performed on reaches with measured flow data or reaches with only estimated flow values. An example of the PDM Site-Specific Results page is shown in Figure 3-24.

The model is based on the mathematical derivation presented by Di Toro (1984). A simple mass balance approach forms the basis of the model; however, the input variables are not single point estimates. In reality, these variables are not constant; streams follow a highly variable seasonal flow pattern and numerous variables in a manufacturing process can affect the chemical concentration and flow rate of the effluent. PDM uses probability distributions as inputs and calculates the resulting probability distribution of the concentration in the stream. See Appendix C for a description of the statistical framework of PDM.

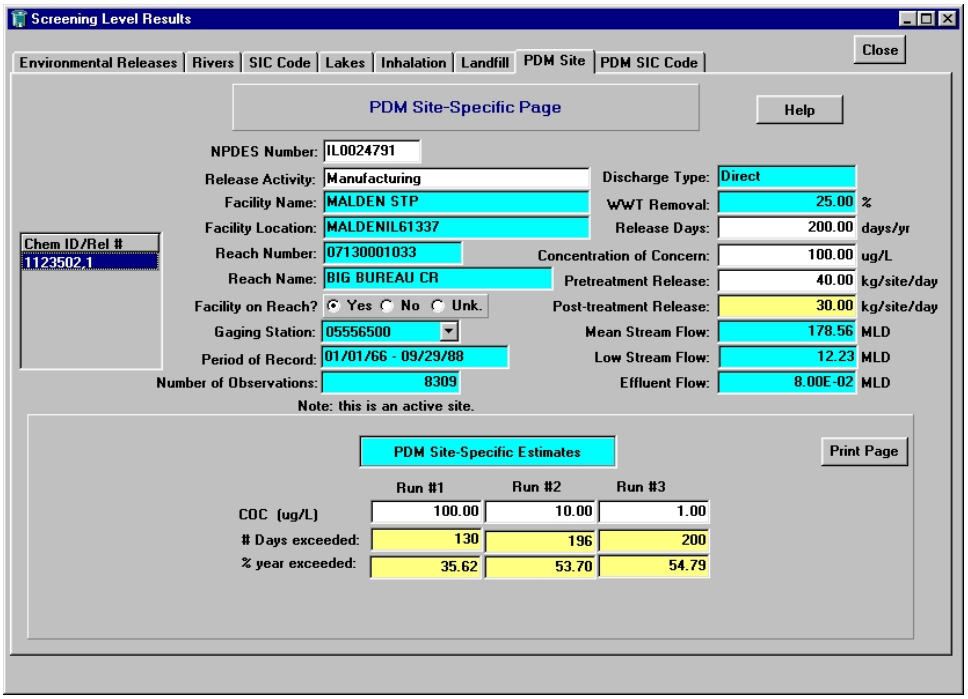

Figure 3-24. PDM Site-Specific Results Page

To run PDM, select "Include PDM run" on the General Release Information page (Figure 3-2a). (Selecting "Average PDM Analysis (SIC Code)" or "High-end PDM Analysis (SIC Code)" under "Select PDM Analysis" will yield the same results when performing a site-specific analysis.) On the Select a Facility screen (Figure 3-3), PDM uses the selected NPDES number to determine if the reach has a USGS gaging station (i.e., measured flow data are available). If the reach has a gaging station, the ranked measured daily flow values are used to determine the frequency of exceedence. If only estimated flow data are available, the program estimates the frequency of exceedence using a watershed-specific relationship between mean flow, 7Q10 flow, and the streamflow coefficients of variation for gaged streams in the watershed.

Using information entered in the PChem/Fate Inputs screen (Figure 2-1) and on the General Release Information page, PDM estimates the number of days per year and the percentage of the year the COC was exceeded. The Chemical ID/Release Number box on the left hand side of the page can be scrolled to show all the stored site-specific PDM results for all surface water releases analyzed using the site-specific surface water release scenario. The following are short descriptions of the fields that appear on the PDM Site-Specific Results page:

- **NPDES Number** — extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Release Activity** — can be manufacturing, processing, industrial use, or other. This was entered in a text field on the left-hand side of the General Release Information page (Figure 3-2a).

- **Facility Name, Location, Reach Number, Reach Name** — information on the discharging facility extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Facility on Reach?** — indicates whether the facility discharges to the identified reach, discharges to a tributary stream, or if the discharge point is unknown.

- **Discharge Type —** indicates whether the facility is a direct discharger that discharges treated wastewater directly to a surface water body or an indirect discharger that discharges wastewater to a POTW for treatment.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release Days** — number of days per year that the chemical is discharged, as entered on the General Release Information page.

- **Concentration of Concern (COC)** — threshold concentration, in micrograms per liter (µg/L), below which adverse effects on aquatic life are expected to be minimal. PDM in E-FAST V2.0 predicts how many days per year the concentration of the chemical in the receiving stream will exceed the COC. (Only the first COC value entered on the General Release Information page appears on the upper half of the page. Up to three of the COC values entered will appear on the lower half of the page.)

- **Pretreatment Release** — rate of release of the chemical by the facility to a wastewater treatment facility (kg/site/day), as entered on the General Release Information page.

- **Post-treatment Release** — rate of release of the chemical after treatment by a wastewater treatment facility (kg/site/day). The post-treatment release amount is equal to the pretreatment release reduced by the wastewater treatment removal percentage.

- **Mean Stream Flow** — arithmetic mean flow of the ambient water body receiving the facility's discharge (MLD), extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Low Stream Flow** — 7Q10 stream flow (i.e., 7 consecutive days of lowest flow over a 10-year period) (MLD), extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Effluent Flow** — Effluent flow of the discharging facility (MLD), extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

If the facility selected discharges to an ambient water body with a USGS gaging station, E-FAST 2.0 will not provide an effluent flow. However, the following additional information is provided:

- **Gaging Station** — identification number for the USGS streamflow monitoring site for the ambient water body receiving the facility's discharge. PDM accesses daily flow values collected between 1966 and 1991 to calculate the frequency of exceedence.

- **Period of Record** — period for which daily streamflow data are available for the selected gaging station.

- **Number of Observations** — number of times the daily stream flow was measured during the period of record.

The lower half of the page presents the PDM site-specific estimates. These results are: the estimated number of days that the COC will be exceeded in the ambient water body that receives discharge from the facility; as well as the percent of the year that the COC will be exceeded. These are described below:

- **Number of Days COC Exceeded** — estimate of the number of days/year that the COC is exceeded.

- **Percent of Year COC Exceeded** — the percentage of year that the COC is exceeded. This is calculated by dividing the exceedence days/year by 365 and multiplying the result by 100.

In addition to these fields, the PDM Site Results page displays a "Print Page" button that may be used to generate a hard copy of the data on the screen.

3.1.10 PDM SIC Code Results Page

To develop exposure estimates of surface water releases for which you entered an SIC code to characterize a facility on the General Release Information page (Figure 3-2a), E-FAST V2.0 performs an average or high-end analysis for the receiving streams of facilities in the particular industrial category to predict the exceedences of the COC. The Chemical ID/Release Number box on the left hand side of the page can be scrolled to show all the stored SIC Code PDM results for all surface water releases analyzed using the SIC Code surface water release scenario. An example of the PDM SIC Code Results page is shown in Figure 3-25.

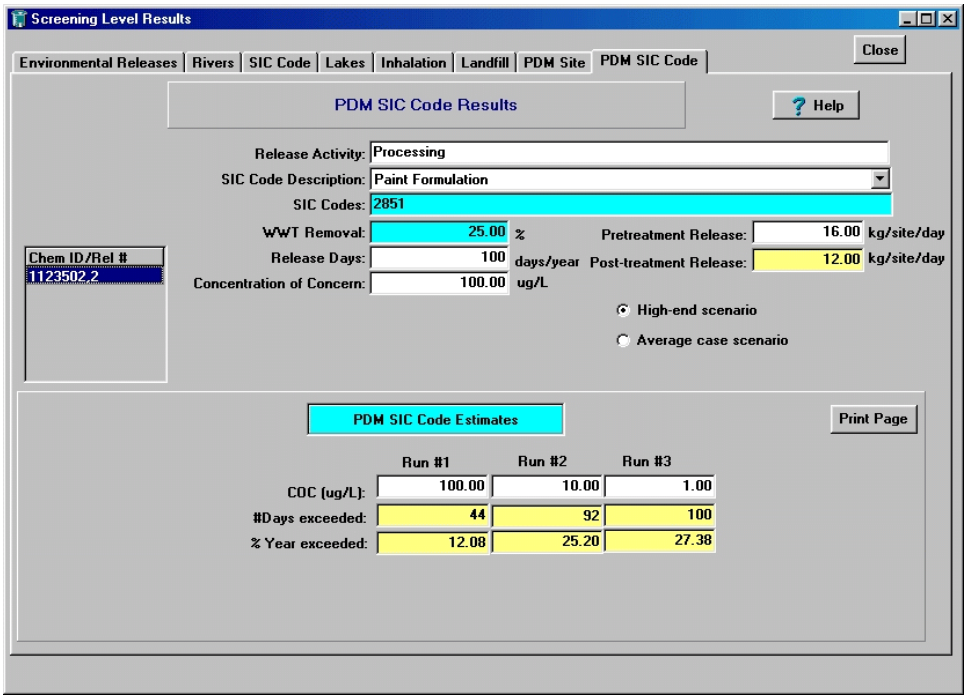

Figure 3-25. PDM SIC Code Results Page

The model is based on the mathematical derivation presented by Di Toro (1984). A simple mass balance approach forms the basis of the model; however, the input variables are not single point estimates. In reality, these variables are not constant; streams follow a highly variable seasonal flow pattern and numerous variables in a manufacturing process can affect the chemical concentration and flow rate of the effluent. PDM uses probability distributions as inputs and calculates the resulting probability distribution of the concentration in the stream. See Appendix C for a description of the statistical framework of PDM.

To run PDM, select "Include PDM run" on the General Release Information page (Figure 3-2a), and select "Average PDM Analysis (SIC Code)" or "High-end PDM Analysis (SIC Code)" under "Select PDM Analysis." Using information entered in the PChem/Fate Inputs screen (Figure 2-1) and on the General Release Information page, PDM estimates the number of days per year and the percentage of the year the COC was exceeded. The following are short descriptions of the fields that appear on the PDM SIC Code Results page:

- **Release Activity** — can be manufacturing, processing, industrial use, or other. This was entered in a text field on the left-hand side of the General Release Information page (Figure 3-2).

- **SIC Code Description** — text description of the industry selected in the Select an SIC code page.

- **SIC Codes** — the 4-digit code or codes assigned to the industry selected.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release Days** — number of days per year that the chemical is discharged, as entered on the General Release Information page.

- **Concentration of Concern (COC)** — threshold concentration, in micrograms per liter (µg/L), below which adverse effects on aquatic life are expected to be minimal. PDM in E-FAST V2.0 predicts how many days per year the concentration of the chemical in the receiving stream will exceed the COC. (Only the first COC value entered on the General Release Information page appears on the upper half of the page. Up to three of the COC values entered will appear on the lower half of the page.)

- **Pretreatment Release** — rate of release of the chemical by the facility to a wastewater treatment facility (kg/site/day), as entered on the General Release Information page.

- **Post-treatment Release** — rate of release of the chemical after treatment by a wastewater treatment facility (kg/site/day). The post-treatment release amount is equal to the pretreatment release reduced by the wastewater treatment removal percentage.

In addition, the results page identifies the type of scenario that was selected in the General Release Information page. The scenario will be identified as either a high-end or an average case scenario, as defined below.

- **High-end Scenario** — averaged probability of exceedence of the 10 percent of the facilities of the selected industrial category that have the highest probability of exceedence for the COC and the loading rate specified by you for worst-case scenarios.

- **Average Case Scenario** — mean exceedence probability for all facilities within an industrial category.

The lower half of the page presents the PDM SIC Code estimates. These results are: the estimated number of days that the COC will be exceeded in the ambient water body that receives discharge from the facility; as well as the percent of the year that the COC will be exceeded. These are described below:

- **Number of Days COC Exceeded** — estimate of the number of days/year that the COC is exceeded.

- **Percent of Year COC Exceeded** — percentage of year that the COC is exceeded. This is calculated by dividing the exceedence days/year by 365 and multiplying the result by 100.

In addition to these fields, the PDM Site Results page displays a “Print Page” button that may be used to generate a hard copy of the data on the screen.

3.2 Down-the-Drain

OPPT developed the Down-the-Drain module as a screening-level model for estimating concentrations of chemicals in surface waters that may result from the disposal of consumer products into household wastewater. The methodology assumes that household wastewater undergoes treatment at a local wastewater treatment facility and the treated effluent is subsequently discharged into surface waters. Down-the-Drain also provides estimates of aquatic exposure and human exposure from ingestion of drinking water and fish that may become contaminated by these household wastewater releases. In addition, you may select PDM (modified, See Section 3.2.2.2) which allows you to estimate the number of days per year that the concentration of a chemical in surface water exceeds the concentration of concern (COC) for aquatic life. Down-the-Drain currently uses data from various EPA water-related information systems.

Chemical constituents of some household products, such as detergents, are expected to end up in household wastewater, whereas others, such as fragrance in an air freshener, are not. Before proceeding with the methods presented below, you should evaluate the physical-chemical properties and the functional role of the chemical in a product, because these properties could preclude the presence of the chemical in household wastewater.

3.2.1 Consumer Disposal Inputs Page

In the Consumer Disposal Inputs page, enter a production volume (kg/year) and the exposure duration (years of use) as shown in Figure 3-26. Down-the-Drain inputs also include the Chemical ID for the chemical of interest, the bioconcentration factor (BCF), and wastewater treatment removal percentage previously entered in the Physical-Chemical Properties and Fate (PChem/Fate) Inputs screen (Figure 2-1). You have the option of running PDM when executing the Down-the-Drain module. If you select "Run PDM" under the PDM Option, you must enter at least one COC and whether you want it to run a high-end or average scenario. As was the case for water releases under the General Population and Ecological Exposure from Industrial Releases module, you may enter up to three COC values to be assessed.

PDM in E-FAST V2.0 predicts the number of days per year the concentration of the chemical in the receiving stream will exceed the COC. To execute the Down-the-Drain module and display the Disposal Results page, click on "Run the Disposal Model." The results also will be written to the output directory.

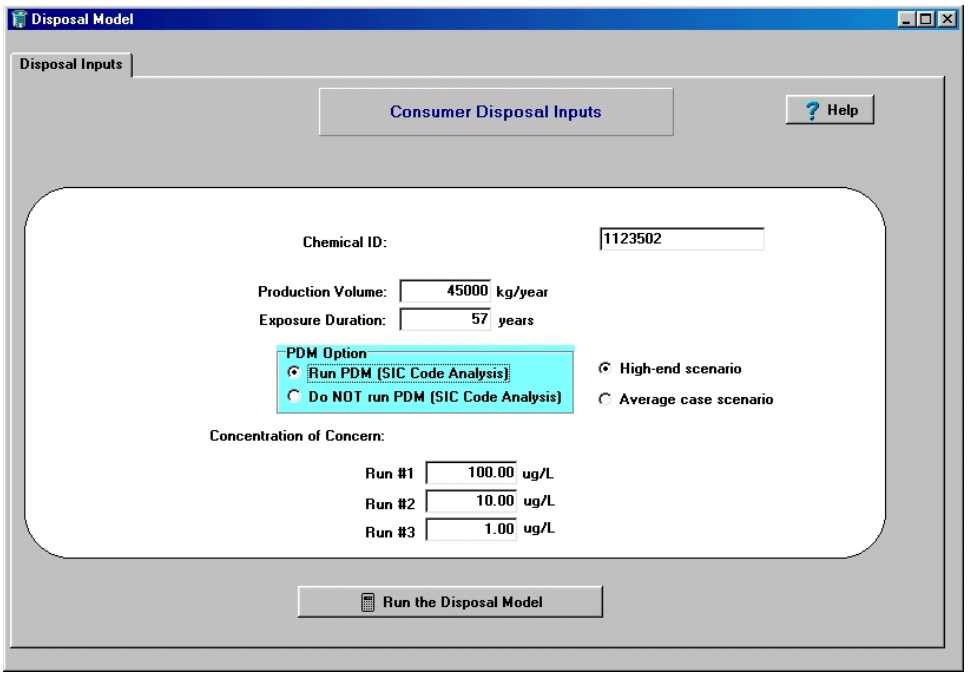

Figure 3-26. Consumer Disposal Inputs Page – Selecting PDM

The following are short descriptions of the fields in the Consumer Disposal Inputs page:

- **Production Volume** — mass of a chemical produced annually in the USA or an estimate of the mass that is discharged annually in the USA to wastewater by consumers.

- **Exposure Duration** — number of years that a product would be used by a person; E-FAST V2.0 uses a default value of 57 years (See Table 3-2).

- **Concentration of Concern (COC)** — threshold concentration, in micrograms per liter (**:**g/L), below which adverse effects on aquatic life are expected to be minimal.

3.2.2 Disposal Results Page

An example Disposal Results page (Figure 3-27) shows both the inputs to and the results of the Down-the-Drain module calculations. The following are short descriptions of the fields listed in the upper half of the page:

- **Production Volume** — mass of chemical produced annually in the USA or an estimate of the mass that is discharged annually in the USA to wastewater by consumers.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release days** — number of days per year that the chemical is discharged; assumed to be 365 days/year.

- **Bioconcentration Factor —** indicates the tendency of the chemical to accumulate in living organisms. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Exposed Population** — can be adults, youths 13 to 19 years, children 6 to 12 years, children 3 to 5 years, infants 1 to 2 years, or infants less than one year old. This was entered on the Screening Level Main page (Figure 3-1).

- **Pretreatment Release** — the daily per capita release of the chemical before effluent has been treated by a wastewater treatment facility.

- **Post-treatment Release** — the daily per capita release of the chemical after effluent has been treated by a wastewater treatment facility. The post-treatment release amount reflects the wastewater treatment removal percentage you supplied in Figure 2-1, the Physical-Chemical Properties and Fate component.

In addition to these fields, the top portion of the Disposal Results page displays a "Print Page" button that may be used to generate a hard copy of the data on the screen. The hard copy includes the data in all of the tabs in the lower portion of the screen (PDM Information, Drinking Water Information, Fish Ingestion Information, and Concentrations), so there is no need to click the "Print Page" button for each of these tabs.

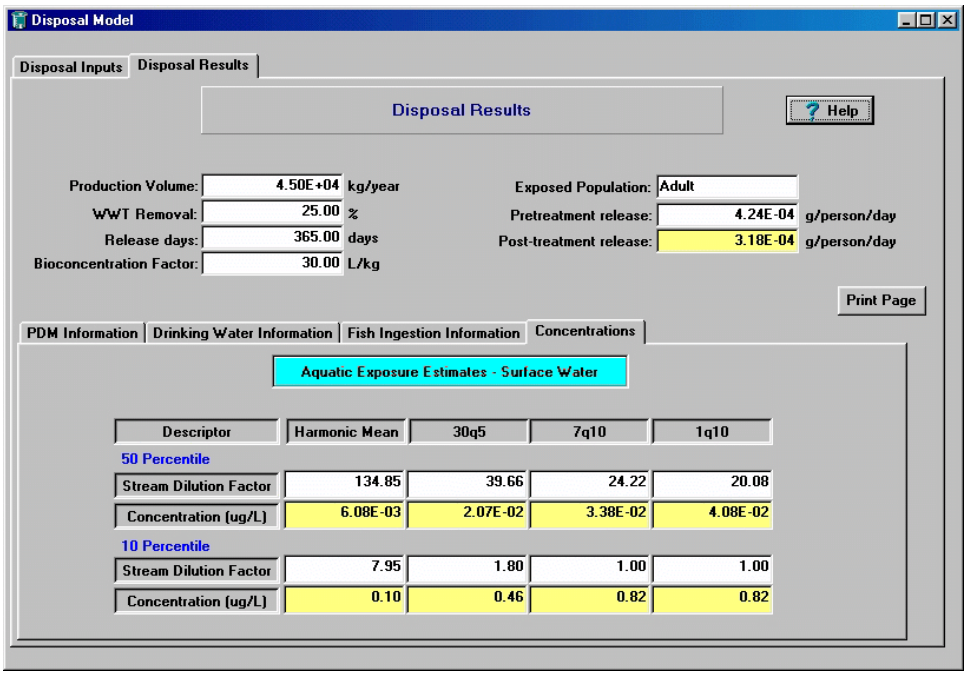

Figure 3-27. Disposal Results Page – Aquatic Exposure Estimates - Surface Water

The four tabs located in the lower half of the page allow you to view Concentrations, PDM Information, Drinking Water Information, and Fish Ingestion Information.

3.2.2.1 *Disposal Results Page – Concentrations*

Based on a specified annual production volume (mass of chemical produced annually or discharged annually to wastewater by consumers) and the U.S. population, Down-the-Drain estimates the total daily per capita release of a chemical in household wastewater. The household daily release and stream dilution factors, along with the specified wastewater treatment efficiency, are then used to calculate a screening-level estimate of the time-averaged surface water concentration (high-end and median) of a chemical substance released by a wastewater treatment facility receiving household wastewater (assuming all wastewater entering a treatment facility is from residential sources). Surface water concentrations are estimated under four receiving stream flow conditions (1Q10 low flow, 7Q10 low flow, 30Q5 low flow, and harmonic mean flow) as described in Section 3.1.4.1, using the stream dilution factors for all wastewater treatment facilities based on 10th and 50th percentile values.

Estimation of Household Wastewater Releases

E-FAST V2.0 uses the following equation to estimate the total daily per capita release of a chemical in household wastewater:

$$H_R \; 4 \; \frac{PV}{Pop} \times \frac{1000 \; grams}{1 \; kg} \times CF1 \qquad \text{(Eq. 3-20)}$$

where:

H_R	=	Daily per capita release of the chemical to a wastewater treatment facility (g/person/day)
PV	=	Production volume (kg/year)
Pop	=	2003 U.S. resident population (2.908×10^8 persons) (U.S. Bureau of the Census, 2004-2005)
CF1	=	Conversion factor (year/365 days)

Estimation of Surface Water Concentrations

The following equations are used to calculate a screening-level estimate of the time-averaged surface water concentration of a chemical released by a wastewater treatment facility receiving household wastewater:

$$SWC_{median} \; 4 \; \frac{H_R \times \frac{1}{Q_H} \times \left(1 \;) \; \frac{WWT}{100} \right) \times CF1}{SDF_{median}} \qquad \text{(Eq. 3-21)}$$

$$SWC_{high} \; 4 \; \frac{H_R \times \frac{1}{Q_H} \times \left(1 \;) \; \frac{WWT}{100} \right) \times CF1}{SDF_{low}} \qquad \text{(Eq. 3-22)}$$

where:

SWC_{median}	=	Median time-averaged surface water concentration (µg/L)
SWC_{high}	=	High-end time-averaged surface water concentration (µg/L)
H_R	=	Daily per capita release of chemical (i.e., pretreatment release) (g/person/day)

SDF_{median}	=	50th percentile stream dilution factor for streams to which wastewater treatment facilities discharge
SDF_{low}	=	10th percentile stream dilution factor for streams to which wastewater treatment facilities discharge
CF1	=	Conversion factor (10^6 **:** g/g)

The above factors, and the assumptions on which they are based, are discussed below. The underlying conservative assumption used in these equations is that all wastewater entering a wastewater treatment facility is from residential sources. With this assumption, readily available data can be used to estimate concentrations of the chemical in ambient receiving waters.

- **Daily Household Release of Chemical (H_R)** — pretreatment release; See Equation 3-20.

- **Household Wastewater Volume Released Daily (Q_H)** — based on the subset of POTWs that have an accessible domestic flow value and resident-population-served; derived from an EPA database of POTWs (See Appendix B). The household wastewater flow of 388 L/person/day was the 50th percentile value. This value is used as the daily per capita wastewater volume released in Down-the-Drain.

- **Wastewater Treatment (WWT) Removal** — estimate of chemical removal efficiency, dependent on the physical-chemical properties of the chemical of concern and the extent of wastewater treatment (e.g., primary, secondary). Most chemicals in household wastewater can be expected to be removed to some extent during wastewater treatment.

- **Stream Dilution Factor (SDF_{median}, SDF_{low})** — equal to the volume of the receiving stream flow under four flow conditions divided by the volume of the wastewater treatment facility effluent flow. These values were obtained from the Stream Dilution Factor Program (SDFP) for 36 industrial categories. (SDFP is a software program originally developed by the OW to obtain effluent and stream flow frequency distributions for a given industrial category (SIC code). Revised by OPPT, the major purpose of SDFP is to (1) retrieve receiving stream flow data for facilities in a particular SIC code (direct dischargers), (2) calculate dilution factors for each facility (receiving stream flow divided by effluent flow), and (3) rank the flow data and dilution factors and report the results in terms of percentiles. See Appendix B for more details. Harmonic mean, 30Q5, and 1Q10 flows are calculated from the 7Q10 flows and arithmetic mean flows.

3.2.2.2 *Disposal Results Page – PDM Information*

If the module is run with PDM, it predicts the number of days of exceedence of each of the user-specified surface water COC values (See Figure 3-28). The following is a short description of each field in the lower half of the page:

- **Concentration of Concern (COC)** - threshold concentration, in micrograms per liter (µg/L), below which adverse effects on aquatic life are expected to be minimal.

- **Number of Days COC Exceeded** — estimate of the number of days/year that the COC is exceeded.

- **Percent of Year COC Exceeded** — percentage of year that the COC is exceeded. This is calculated by dividing the exceedence days/year by 365 and multiplying the result by 100 (releases are assumed to occur 365 days per year).

- **High-end Scenario** — averaged probability of exceedence of the 10 percent of the facilities of the selected industrial category that have the highest probability of exceedence for the COC and the loading rate specified by you for the worst-case scenarios.

- **Average Case Scenario** — mean exceedence probability for all facilities within an industrial category.

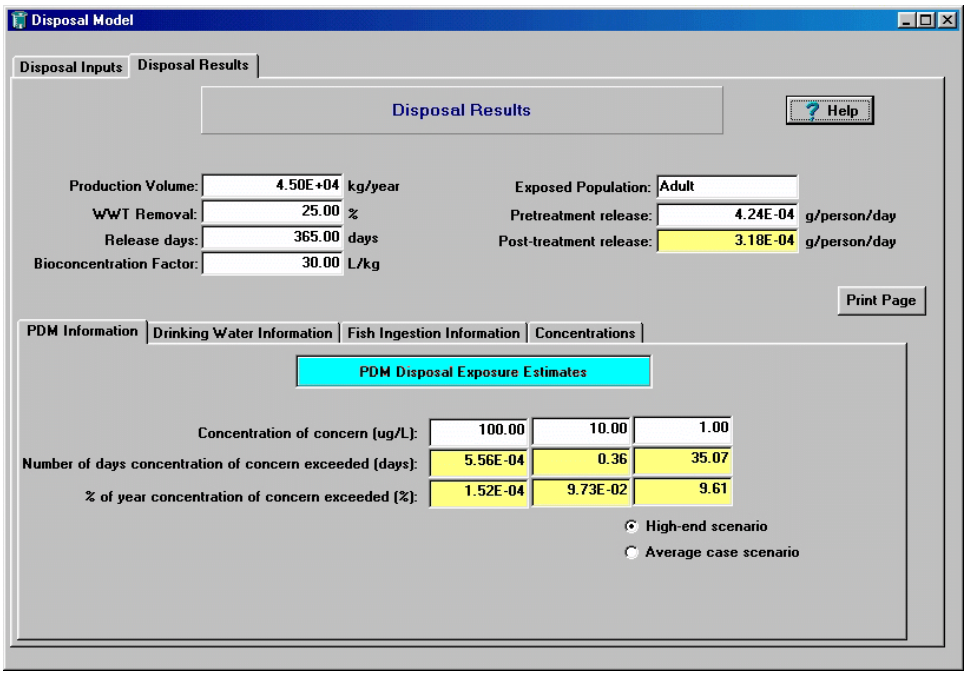

Figure 3-28. Disposal Results Page – PDM Disposal Exposure Estimates

<u>Estimating Probability of Exceeding Concentrations of Concern</u>

Down-the-Drain incorporates a modified version of PDM to calculate the number of days of exceedence of a surface water COC. This version is limited to the following:

- Addresses only POTWs;
- Uses data from an EPA survey of POTWs;
- Uses a typical per capita release (instead of discharge loading) to generate POTW loading

by multiplying estimates of population served by the estimates of per capita household releases.

The Probabilistic Dilution Model is based on the mathematical derivation presented by Di Toro (1984). A simple mass balance approach forms the basis of the model; however, the input variables are not single point estimates. In reality, these variables are not constant; streams follow a highly variable seasonal flow pattern and numerous variables in a manufacturing process can affect the chemical concentration and flow rate of the effluent. PDM uses probability distributions as inputs and calculates the resulting probability distribution of the concentration in the stream. See Appendix C for a description of the statistical framework of PDM.

3.2.2.3 *Disposal Results Page – Drinking Water Information*

The Drinking Water Information tab (Figure 3-29) presents the acute and chronic exposure doses for individuals who ingest drinking water from streams and rivers that receive wastewater discharges containing the chemical of concern. The first column, "Exposure Type," lists three different measurements of exposure. To the right of each, under the "Results" heading, are the corresponding 50th and 10th percentile exposure values. The subsequent columns contain the exposure factors for the age group selected (See Table 3.2 in Section 3.1.2). The following are short descriptions of the fields in the lower half of this page:

- **50th Percentile Results** — exposure calculations based on the median (i.e., 50th percentile) surface water concentrations and represent central tendency exposure. These flows are used to represent mid-sized stream flows.

- **10th Percentile Results** — exposure calculations based on the high-end (i.e., upper 10th percentile) surface water concentrations and represent the bounding high-end exposures. These flows are used to represent small streams.

The exposure types and exposure factors are defined below:

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from drinking water intake; calculated to represent chronic exposures to contaminated drinking water over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in drinking water; calculated to represent chronic lifetime concentration. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from drinking water intake; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** — number of years that a product would be used by a person; E-FAST V2.0 uses a default value of 57 years (See Table 3-2).
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Drinking Water Ingestion Rate (IR_{dw})** — used for calculating acute and chronic exposures.

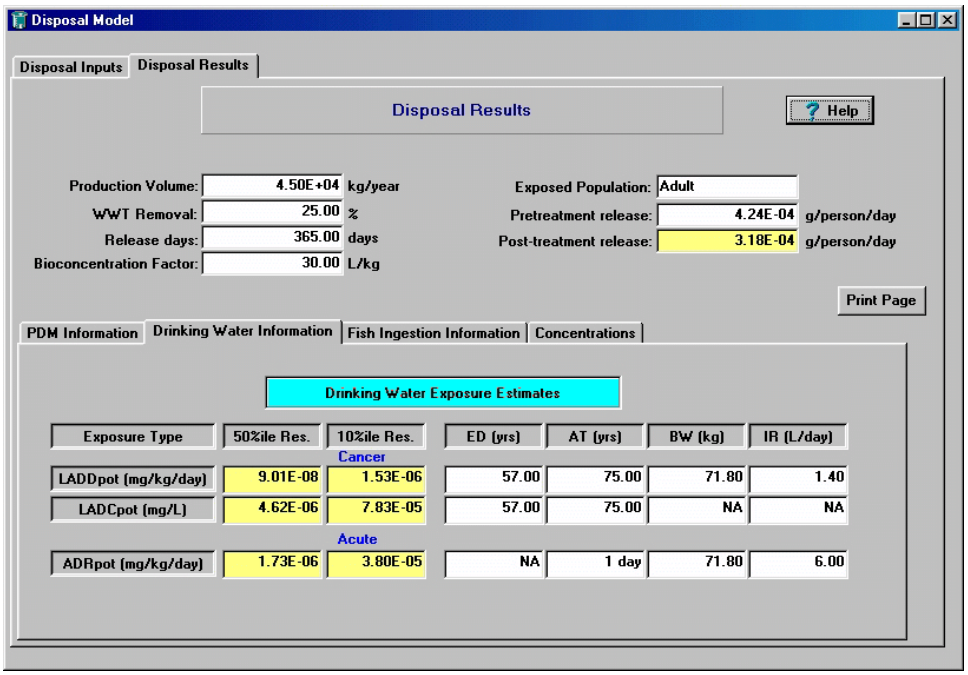

Figure 3-29. Disposal Results Page – Drinking Water Exposure Estimates

Estimation of Drinking Water Potential Doses

The following equations are used to calculate a screening-level estimate of the potential drinking water dose rate of a chemical release by a wastewater treatment facility receiving household wastewater.

10th percentile surface water concentrations:

$$ADR_{POT} \; 4 \; \frac{SWC_{high} \times IR_{dw} \times RD \times CF1}{BW \times AT} \qquad \text{(Eq. 3-23)}$$

$$LADD_{POT} \; 4 \; \frac{SWC_{high} \times IR_{dw} \times RD \times ED \times CF1}{BW \times AT \times CF2} \qquad \text{(Eq. 3-24)}$$

$$LADC_{POT} \; 4 \; \frac{SWC_{high} \times RD \times ED \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-25)}$$

50th percentile surface water concentrations:

$$ADR_{POT} \; 4 \; \frac{SWC_{median} \times IR_{dw} \times RD \times CF1}{BW \times AT} \qquad \text{(Eq. 3-26)}$$

$$LADD_{POT} \; 4 \; \frac{SWC_{median} \times IR_{dw} \times RD \times ED \times CF1}{BW \times AT \times CF2} \qquad \text{(Eq. 3-27)}$$

$$LADC_{POT} \; 4 \; \frac{SWC_{median} \times RD \times ED \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-28)}$$

where:

ADR_{POT}	=	Potential Acute Dose Rate from drinking water intake (mg/kg/day)
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose from drinking water intake (mg/kg/day)
$LADC_{POT}$	=	Potential Lifetime Average Daily Concentration (mg/L)
SWC_{high}	=	10th percentile time-averaged surface water concentration (µg/L)
SWC_{median}	=	50th percentile time-averaged surface water concentration (µg/L)
IR_{dw}	=	Drinking water intake rate (L/day)
RD	=	Days of release from wastewater treatment facility (1 day for ADR_{POT}; 365 days/year for $LADD_{POT}$ and $LADC_{POT}$)
ED	=	Exposure duration (years of product usage)
BW	=	Body weight (kg)
AT	=	Averaging time (day for ADR_{POT}; years for $LADD_{POT}$ and $LADC_{POT}$)
CF1	=	Conversion factor (10^{-3} mg/µg)
CF2	=	Conversion factor (365 days/year)

Descriptions of selected parameters are briefly discussed below:

- **Time-averaged Surface Water Concentration (SWC_{median}, SWC_{high})** — assumed to be the same as the drinking water concentration of the chemical as calculated using Equations 3-21 and 3-22 in Section 3.2.2.1. This conservative assumption implies either that water is ingested as raw stream water or, if treated before ingestion, that drinking water treatment removes none of the chemical.

- **Days of Release from a Wastewater Treatment Facility (RD)** — reflects the frequency of drinking contaminated water and is a constant. It is set at 1 day for acute scenarios and 365 days per year for chronic scenarios.

- **Exposure Duration (ED)** — reflects the number of years a product would be used by a person; E-FAST V2.0 uses a default value of 57 years (see Table 3-2). This parameter is not applicable for children's exposure because $LADD_{pot}$ and $LADC_{pot}$ are not calculated for children.

3.2.2.4 *Disposal Results Page – Fish Ingestion Information*

The Fish Ingestion Information tab of the Disposal Results page presents the predicted acute and chronic exposure doses for consumers who ingest fish from streams and rivers that receive wastewater discharges containing the chemical of concern. The exposure doses are calculated using the estimated median and high-end surface water concentrations in a water body receiving discharges from a POTW treating household wastewater (Figure 3-30).

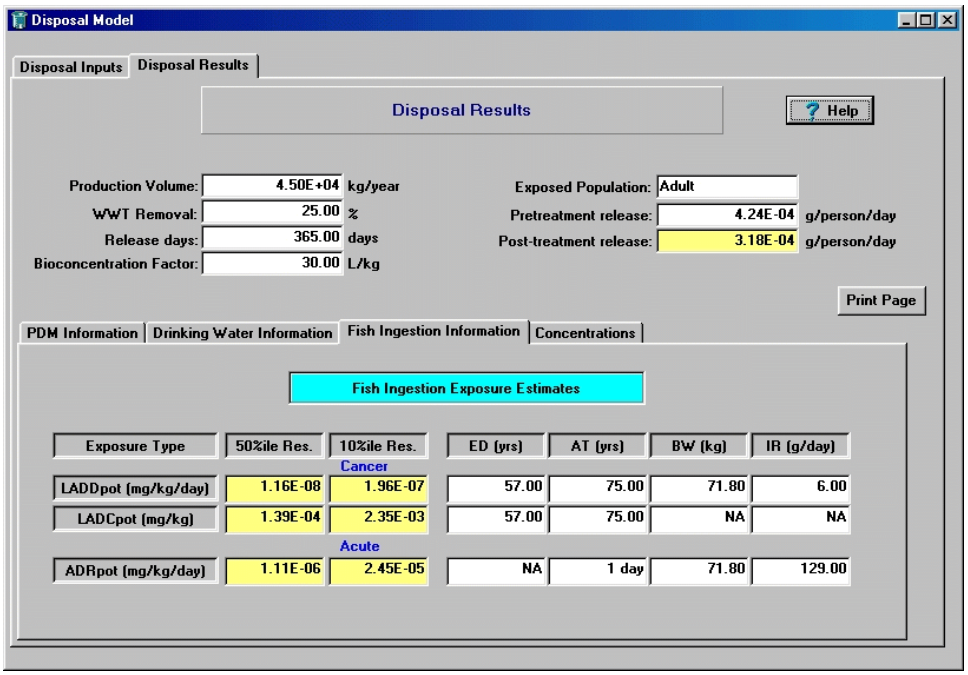

Figure 3-30. Disposal Results Page – Fish Ingestion Exposure Estimates

The following are short descriptions of the fields in the lower half of the page:

- **10th Percentile Results** — exposure calculations based on the high-end (i.e., upper 10th percentile) surface water concentrations (SWC_{high}) and represent the bounding high-end exposures. These flows are used to represent small streams.

- **50th Percentile Results** — exposure calculations based on the median (i.e., 50th percentile) surface water concentrations (SWC_{median}) and represent central tendency exposure. These flows are used to represent mid-sized stream flows.

<u>Exposure Types</u>

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from ingestion of fish tissue; calculated to represent chronic exposures to fish over a lifetime. These doses are generally used for cancer calculations.

- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in ingested fish tissue; calculated to represent chronic lifetime concentration. These concentrations are generally used for cancer calculations.

- **Potential Acute Dose Rate (ADR_{POT})** — from ingestion of fish tissue; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** —number of years that a product would be used by a person; E-FAST V2.0 uses a default value of 57 years (See Table 3-2).
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Fish Ingestion Rate (IR_{fish})** — used for calculating acute and chronic exposures.

Estimation of Potential Doses via Fish Ingestion

The following equations are used to calculate a screening-level estimate of the potential dose rate from ingestion of fish that may become contaminated with a chemical discharged by a wastewater treatment facility that receives household wastewater.

10th percentile surface water concentrations:

$$ADR_{POT} \; 4 \; \frac{SWC_{high} \times IR_{fish} \times RD \times BCF \times CF1 \times CF3}{BW \times AT} \qquad \text{(Eq. 3-29)}$$

$$LADD_{POT} \; 4 \; \frac{SWC_{high} \times IR_{fish} \times BCF \times RD \times ED \times CF1 \times CF3}{BW \times AT \times CF2} \qquad \text{(Eq. 3-30)}$$

$$LADC_{POT} \; 4 \; \frac{SWC_{high} \times RD \times ED \times BCF \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-31)}$$

50th percentile surface water concentrations:

$$ADR_{POT} \; 4 \; \frac{SWC_{median} \times IR_{fish} \times RD \times BCF \times CF1 \times CF3}{BW \times AT} \qquad \text{(Eq. 3-32)}$$

$$LADD_{POT} \; 4 \; \frac{SWC_{median} \times IR_{fish} \times BCF \times RD \times ED \times CF1 \times CF3}{BW \times AT \times CF2} \qquad \text{(Eq. 3-33)}$$

$$LADC_{POT} \; 4 \; \frac{SWC_{median} \times RD \times ED \times BCF \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-34)}$$

where:

ADR_{POT}	=	Potential Acute Dose Rate from fish ingestion (mg/kg/day)
$LADD_{POT}$	=	Potential Lifetime Average Daily Dose from fish ingestion (mg/kg/day)
$LADC_{POT}$	=	Potential Lifetime Average Daily Concentration in fish (mg/kg)
SWC_{high}	=	10th percentile time-averaged surface water concentration (µg/L)
SWC_{median}	=	50th percentile time-averaged surface water concentration (µg/L)
IR_{fish}	=	Fish ingestion rate (g/day)
BCF	=	Estimate of chemical's bioconcentration potential (L/kg)
RD	=	Days of release from a wastewater treatment facility (1 day for ADR_{POT}; 365 days/year for $LADD_{POT}$ and $LADC_{POT}$).
ED	=	number of years that a product would be used by a person; E-FAST V2.0 uses a default value of 57 years (see Table 3-2).
BW	=	Body weight (kg)
AT	=	Averaging time (day for ADR_{POT}; years for $LADD_{POT}$ and $LADC_{POT}$).
CF1	=	Conversion factor (10^{-3} mg/µg)
CF2	=	Conversion factor (365 days/year)
CF3	=	Conversion factor (10^{-3} kg/g)

3.3 Consumer Exposure Module (CEM)

The Consumer Exposure Module (CEM) is an interactive model within E-FAST V2.0 that calculates conservative estimates of potential inhalation exposure, and potential and absorbed dermal exposure to chemicals in certain types of consumer products. CEM allows for screening-level estimates of Potential Acute Dose Rates (ADR_{POT}), Potential Peak Concentrations ($C_{P\ POT}$), and Potential Lifetime Average Daily Concentrations ($LADC_{POT}$) and Dose Rates ($LADD_{POT}$). Because the model incorporates either a combination of upper percentile and mean input values or all upper percentile input values for various exposure factors in the calculation of potential exposures/doses, the exposure/dose estimates are considered "high-end" to "bounding" estimates.

CEM uses six data entry pages to collect the information necessary to calculate inhalation and dermal exposure. These pages are titled "Introduction," "Scenario," "Inhalation Input," "Day of Use," "Days After Use," and "Dermal Input." Additional data inputs necessary to run CEM (weight fraction of the chemical in the consumer product (central tendency and high-end (e.g., median and 90th percentile, respectively), molecular weight of the chemical (g/mol), and vapor pressure of the chemical) are previously entered in the Physical-Chemical Properties and Fate (PChem/Fate) Inputs screen (Figure 2-1).

3.3.1 Introduction Page

The opening page for CEM is shown in Figure 3-31. The introductory text describes the conservative nature of the CEM exposure results. *Exposure Factors Handbook* (U.S. EPA, 1997) was the main source from which many of the default values for the scenarios have been taken. The page prompts you for three pieces of information: an identification number (Chemical ID), a product name, and model run comments. These are optional and are not required for you to continue. The page also provides a "Quick Assist" button which provides help information. From the Introduction page you should then select the Scenario tab to go to the Scenario Data page which must be completed before you can continue to the other input screens.

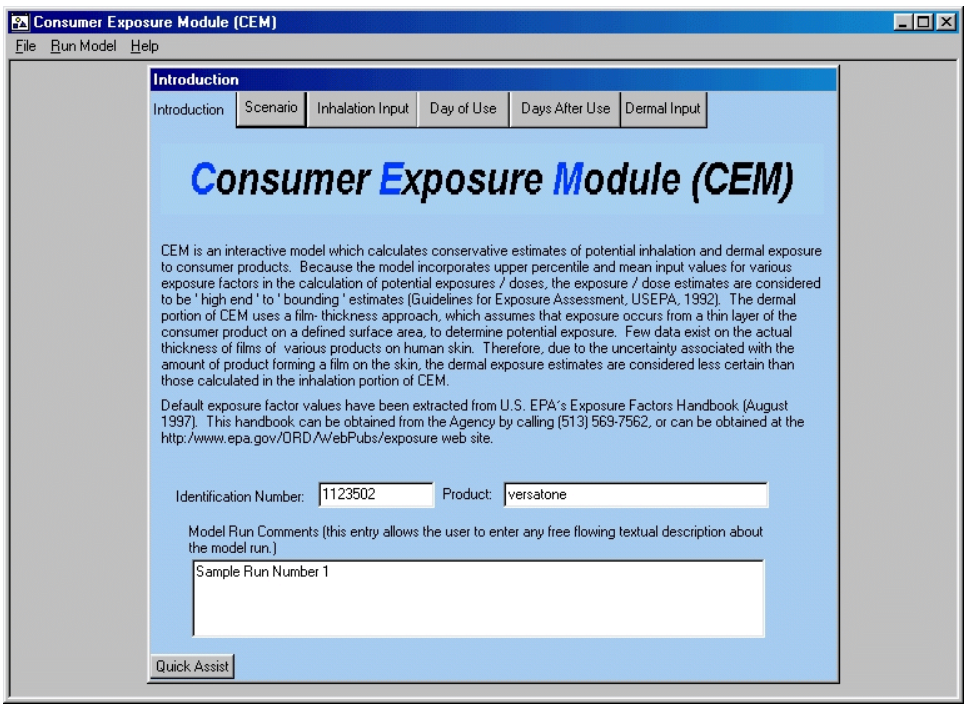

Figure 3-31. CEM Introduction Page

3.3.2 Scenario Page

The Scenario page (Figure 3-32) is divided into five general exposure categories, each with corresponding generic consumer product scenarios. The exposure categories with their corresponding consumer product scenarios are listed below. You also have the option to select the User-Defined scenario. To use this scenario, you must provide specific exposure factors (most defaults are not provided). More information on the User-Defined scenario is provided in Section 3.3.2.2.

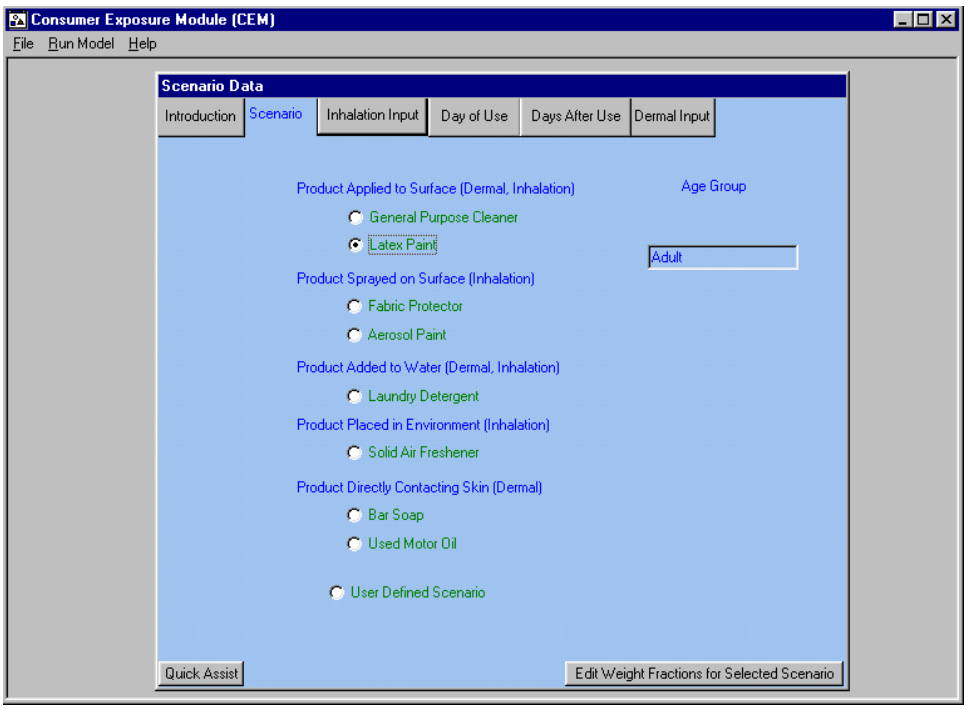

Figure 3-32. Scenario Page

The scenario selection portion of the screen allows you to choose the type of consumer product you are modeling. The model is based on the assumption that all exposure scenarios take place inside the home or car. The generic consumer product scenario (Section 3.3.2.1) assumes that the exposed population consists of individuals who stay at home, such as homemakers. The user-defined consumer product scenario (Section 3.3.2.2) requires the user to specify where the exposed individual spends each hour of his or her day.

The house used in CEM is considered to be a two-zone house. Zone 1 is the room where the consumer product is used and Zone 2 is the remainder of the house. The house contains a bedroom, a kitchen, a bathroom, a living room, and a utility room. The "Room of Use," where the product is used, depends on the scenario selected. For instance, the default room of use for the General Purpose Cleaner scenario is the kitchen and the default room of use for the Laundry Detergent scenario is the utility room. The magnitude of Zone 1 also changes with the room of use. For example, the volume of the kitchen is larger than the volume of the bathroom. The user may also specify a third zone of activity ("Out"), where no exposure to the consumer product occurs.

3.3.2.1 *Generic Consumer Product Scenarios*

General Purpose Cleaner - Dermal and Inhalation Scenario. Exposure occurs during cleaning of the outside of appliances and countertops. The model derived the number of events per lifetime and the years per use from the upper-end values of cleaning events from the Household Cleaning Products Survey (Westat, 1987a), then extrapolated this figure to a lifetime value using professional judgment. The model assumes six uses per week for 50 weeks per year (assumes one 2-week vacation per year) for 57 years (product users between the ages of 18 and 75). The duration of use and the mass of the product used were derived from the Source Ranking Database (Versar, 2003). The surface area to body weight ratio (SA/BW) of 15.6 cm^2/kg is based on both hands of an adult being exposed to the cleaning

solution (See Section 3.3.6). The film thickness of 2.10E-03 cm was derived from the initial film thickness of water uptake on the hands from handling a rag (U.S. EPA, 1987c). The dilution fraction of 0.016 and density of 1.04 g/cm^3 were estimated from the dilution of ¼ cup of cleaner per gallon of water (Versar, 1986).

Interior Latex Paint - Dermal and Inhalation Scenario. Exposure occurs during painting of the rooms of a house. The value of four events per year was taken from the Household Solvent Products Survey (Westat, 1987b). Professional judgment assumed that these painting events would occur 1 out of every 5 years, producing a years-of-use value of 11, occurring over the course of 57 years (product users between the ages of 18 and 75). Default values for mass of product used and duration of use also were derived from the Household Solvent Products Survey (Westat, 1987b). The adult SA/BW of 4.5 cm^2/kg was based on exposure of 10 percent of the face, hands, and forearms (See Section 3.3.6). The film thickness of 9.81E-03 cm was derived from the estimated film thickness of a bath oil and water mixture on the hands after immersion. The dilution fraction was assumed to be full strength (1.00); the density equals 1.16 g/cm^3. (U.S. EPA, 1987c; Versar, 1986).

Fabric Protector - Inhalation Scenario. Exposure occurs from using a fabric protector on clothes and furniture in a house. The frequency of use was assumed to be three times per year for 57 years (occurring between the ages of 18 and 75) and was derived from the Household Cleaning Products Survey (Westat, 1987a).

Aerosol Paint - Inhalation Scenario. Exposure occurs during spraying of aerosol paint indoors for small paint jobs. The value of six events per year was taken from the Household Solvent Products Survey (Westat, 1987b). Professional judgment assumed that these painting events occur 1 out of every 5 years, producing a years-of-use value of 11, occurring over a period of 57 years (product users between the ages of 18 and 75). Default values for mass of product used and duration of use also were derived from the Household Solvent Products Survey (Westat, 1987b).

Liquid Laundry Detergent - Inhalation Scenario. Exposure occurs when machine washing laundry at home. The number of events per lifetime and the years of use were derived from the Cleaning Products Survey (Westat, 1987a). The duration of use and the mass of the product used were derived from the Source Ranking Database (Versar, 2003). The frequency of use was assumed to be 312 events per year over a period of 57 years (product users between the ages of 18 and 75).

Liquid Laundry Detergent - Dermal Scenario. Exposure occurs when hand washing delicate clothing. The frequency of use was assumed to be once per week for 57 years (occurring between the ages of 18 and 75) and was derived from the Household Cleaning Products Survey (Westat, 1987a). The adult SA/BW of 15.6 cm^2/kg is based on exposure of both hands (See Section 3.3.6). The film thickness of 4.99E-03 cm was derived from the initial film thickness of water on the hands after initial immersion. The dilution fraction of 0.002 and density of 1.113 g/cm^3 were estimated from the dilution of ½ cup of detergent per medium load (U.S. EPA, 1987c; Versar, 1986). The frequency of use was assumed to be 312 events per year over a period of 57 years (product users between the ages of 18 and 75).

Solid Air Freshener - Inhalation Scenario. Exposure occurs from the use of a solid air freshener in the home. The number of events per year was based on the assumption that an air freshener is replaced every 60 days during the course of a year for 57 years (adult scenario). Product users are passively exposed to the air freshener. The mass of product used was derived from the Source Ranking Database (Versar, 2003). The duration of use assumed that an individual is exposed to a solid air freshener for a minimum of 24 hours a day for 30 days and a maximum of 24 hours a day for 90 days before replacing the air freshener.

Bar Soap - Dermal Scenario. Exposure occurs while washing the whole body and hands during showering, bathing, and washing the hands. The number of events assumed five showers or baths a week for individuals between the ages of 1 and 16 and 65 and 75 (6,500 times/lifetime), one shower per day between the ages of 16 and 65 (17,836 times/lifetime), and two hand washes per day between the ages of 1 and 75 (54,020 times/lifetime). These usage rates produce a frequency of use of 329 events per year for the body and a frequency of use of 730 events per year for the hands for 74 years (for the lifetime exposure estimate). The SA/BW ratios of 286 and 15.6 are based on exposure of the body and the hands, respectively. Table 3-3 presents the SW/BW ratios for all of the exposure age groups in E-FAST V2.0. The film thickness of 9.81E-03 cm was derived from the film thickness of bath oil and water mixture on the hands after immersion (U.S. EPA, 1987c). The dilution fraction of 0.001 and density of 0.94 g/cm^3 were estimated from the monthly consumption of soap and the amount of water needed to form lather (U.S. EPA, 1985a).

Used Motor Oil - Dermal Scenario. Exposure occurs while changing the oil in a car. The number of events was derived from the recommended length of time between oil changes (3 months), or four times a year for 57 years (performed between the ages of 18 and 75). The adult SA/BW of 7.8 cm^2/kg was derived from exposure of the insides (palms and fingers) of both hands (See Section 3.3.6). The film thickness of 1.19E-02 cm was derived from the uptake of mineral oil on the hands after immersion. (U.S. EPA, 1992c) The dilution fraction was assumed to be full strength (1.00); the density equals 0.88 g/cm^3. (Versar, 1986).

Table 3-3. Default Surface Area/Body Weight (SA/BW) Ratios Used in CEM Module for Bar Soap

Exposure Parameter	Population	Exposure Type	Default Value	Source	Comment
Total Body SA/BW ratio	Adult	All	286 cm^2/kg	U.S. EPA (1997)	Median adult SA/BW ratios (EFH Table 6-9). Based on an analysis of direct matched measurements of surface area and body weight for adults.
	Youth (age 13-19)	Acute	269 cm^2/kg	U.S. EPA (1997)	SA/BW ratio was calculated by treating surface area and body weight as independent variables. SA was calculated by averaging the median SAs for males and females in the 13 to <18 year age groups (EFH Tables 6-6 and 6-7) and body weight was calculated by averaging the mean body weights for 13 to 19 year olds (EFH Table 7-3). SA/BW was calculated as the ratio of the surface area to body weight.
	Child (age 6-12)	Acute	334 cm^2/kg	U.S. EPA (1997)	SA/BW ratio was calculated by treating surface area and body weight as independent variables. SA was calculated by averaging the median SAs for males and females in the 6 to <13 year age groups (EFH Tables 6-6 and 6-7) and body weight was calculated by averaging the mean body weights for 6 to 12 year olds (EFH Table 7-3). SA/BW was calculated as the ratio of the surface area to body weight.
	Small Child (age 3-5)	Acute	411cm^2/kg	U.S. EPA (1997)	SA/BW ratio was calculated by treating surface area and body weight as independent variables. SA was calculated by averaging the median SAs for males and females in the 3 to <6 year age groups (EFH Tables 6-6 and 6-7) and body weight was calculated by averaging the mean body weights for 3 to 5 year olds (EFH Table 7-3). SA/BW was calculated as the ratio of the surface area to body weight.
	Infants (age 1-2)	Acute	617 cm^2/kg	U.S. EPA (1997)	Median SA/BW ratio for children age 0-2 years (EFH Table 6-9).
	Infants (age <1)	Acute	617 cm^2/kg	U.S. EPA (1997)	Median SA/BW ratio for children age 0-2 years (EFH Table 6-9).

Table 3-3. Default Surface Area/Body Weight (SA/BW) Ratios Used in CEM Module for Bar Soap (Cont'd)

Exposure Parameter	Population	Exposure Type	Default Value	Source	Comment
Hand SA/BW ratio	Adult	All	15.6 cm^2/kg	Unpublished	Based on an analysis of direct matched measurements of surface area and body weight (Phillips et al., 1993).
	Youth (age 13-19)	Acute	14.3 cm^2/kg	U.S. EPA (1997)	SA/BW ratio for hands was calculated by multiplying the Total Body SA/BW shown above for this age group by the mean fraction of the total body represented by the hands for this age group (EFH Table 6-8).
	Child (age 6-12)	Acute	17.1 cm^2/kg	U.S. EPA (1997)	SA/BW ratio for hands was calculated by multiplying the Total Body SA/BW shown above for this age group by the mean fraction of the total body represented by the hands for this age group (EFH Table 6-8).
	Small Child (age 3-5)	Acute	24.0 cm^2/kg	U.S. EPA (1997)	SA/BW ratio for hands was calculated by multiplying the Total Body SA/BW shown above for this age group by the mean fraction of the total body represented by the hands for this age group (EFH Table 6-8).
	Infants (age 1-2)	Acute	34.0 cm^2/kg	U.S. EPA (1997)	SA/BW ratio for hands was calculated by multiplying the Total Body SA/BW shown above for this age group by the mean fraction of the total body represented by the hands for this age group (EFH Table 6-8).
	Infants (age < 1)	Acute	34.0 cm^2/kg	U.S. EPA (1997)	SA/BW ratio for hands was calculated by multiplying the Total Body SA/BW shown above for this age group by the mean fraction of the total body represented by the hands for this age group (EFH Table 6-8).

3.3.2.2 *User-Defined Scenario*

In the User-Defined scenario, you are responsible for providing all inputs, except those defined by the characteristics of the exposed individual, e.g., a child age 6-12 cannot be exposed for greater than 7 years, so the exposure duration entry should not exceed that value. Although you cannot specifically define the equations, you can select the way the emissions are determined by selecting how the product is used. Depending on the product's use or application, CEM will use one of the following to determine the inhalation emissions: an incremental source model, a double exponential model, or a constant emission rate model. For the generic scenarios already programmed in CEM, emissions are varied over time using equations that account for the manner in which the product is used or applied.

When you select the User-Defined scenario, a secondary pop-up screen (Figure 3-33) will query you for the general product type being considered, such as a "Product Applied to Surface." You may also select to calculate potential dermal dose rates or absorbed dermal dose rates for aqueous media.

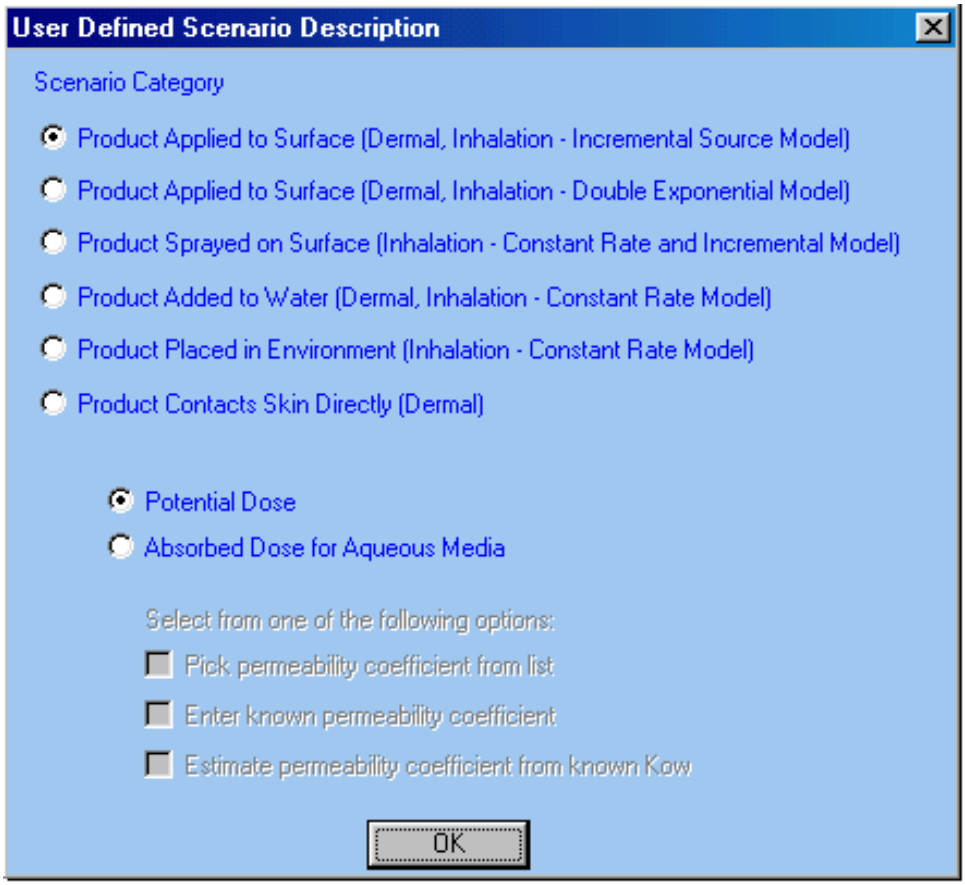

Figure 3-33. User-Defined Scenario Description Screen

Product Applied to Surface – Incremental Source Model. For a product applied to a surface, such as a general purpose cleaner, CEM uses an incremental source model. This model assumes a constant application rate over the user-specified duration of use; each instantaneously applied segment has an emission rate that declines exponentially over time, at a rate that depends on the chemical's molecular weight and vapor pressure.

Product Applied to Surface – Double Exponential Model. Latex paint is handled much like a general purpose cleaner, with two exceptions: (1) a double exponential model is used to account for an initial fast release that is governed primarily by evaporation, followed by a slow release dominated by diffusion; and (2) only 25 percent of the applied mass is released because a substantial fraction of the mass becomes trapped in the painted substrate when it dries. Empirical studies reported by Wilkes et al. (1996) support the assumption of 25 percent mass released and estimate a relationship between the fast rate of decline (k1) and vapor pressure (VP), and between the slow rate of decline and molecular weight (MW).

Product Sprayed on Surface – Constant Rate and Incremental Models. For a product sprayed on a surface, such as a fabric protector or an aerosol paint, a portion (default of 1 percent) is assumed to be aerosolized and therefore immediately available for uptake by inhalation. The remainder is assumed to contact the target surface, and to subsequently volatilize at a rate that depends upon the chemical's molecular weight and vapor pressure. The aerosolized portion is treated using a constant emission rate model. The remaining (non-aerosolized) mass is treated in the same manner as described for a general purpose cleaner, combining a constant application rate with an exponentially declining rate for each instantaneously applied segment.

Product Added to Water – Constant Rate Model. For a product added to water, such as a laundry detergent, the chemical is assumed to emit at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration is longer than the user-specified duration of use, then the chemical emissions are truncated at the end of the product-use cycle (i.e., in the case of a washing machine, the remaining chemical mass is assumed to go down the drain). The potential duration of emissions in this case is determined from the chemical's 90 percent evaporation time.

Product Placed in Environment – Constant Rate Model. For a product placed in the environment, such as a solid air freshener, the chemical is assumed to emit at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration exceeds the user-specified duration of use, then the chemical emissions are truncated at the end of the product-use period, because the product is assumed to be removed from the house after the use period.

Product Contacts Skin Directly – Potential and Absorbed Dose. For a product that comes in direct contact with the skin, the dermal portion of the User-Defined scenario allows you to model dermal exposure based on potential or absorbed doses. Potential dose is the amount of a chemical contained in bulk material that is applied to the skin. Absorbed dose is the amount of substance that penetrates the absorption barriers of an organism. CEM can calculate absorbed dose for aqueous media using a permeability coefficient. The permeability coefficient is a flux value, normalized for concentration that represents the rate at which the chemical penetrates the skin.

If you elect to calculate the absorbed dermal dose rate for an aqueous media, you will have to enter a permeability coefficient (K_p). The program gives you three options: "Pick Permeability Coefficient From List," "Enter Known Permeability Coefficient" and "Estimate Permeability Coefficient From Known K_{ow}." If you select "Pick Permeability Coefficient From List" another screen will prompt

you to select from a list of chemicals contained in the 1992 EPA document entitled *Dermal Exposure Assessment: Principles and Applications* (U.S. EPA, 1992d). If the you select "Enter Known Permeability Coefficient" or "Estimate Permeability Coefficient From Known K_{ow}", you must enter a selected value in units of cm/hr. More information on the permeability coefficient's relationship to K_{ow} can be found in Section 3.3.8.2.

3.3.2.3 *Exposed Population*

The age group that appears in the box on the right side of the Scenario page (Figure 3-32) is the exposed population selected on the Screening Level Main page (Figure 3-1). These age groups include: adults, youths 13 to 19 years, children 6 to 12 years, small children 3 to 5 years, infants 1 to 2 years, or infants less than one year old. However, the only scenarios for which you can calculate dermal exposure for a youth, infant or child are the Bar Soap and the User-Defined Scenarios. Dermal exposures for non-adults in the remaining scenarios are not calculated because the scenarios assume active and not passive exposure (e.g., adults are assumed to engage in cleaning and house painting activities; children are not), and individuals other than adults are assumed to have no direct contact with these products. Non-adults (youths, children, small children and infants) have significant changes in their physical qualities (e.g., body weight, surface area) over time. Therefore, for non-adults, CEM will calculate acute dermal exposures for the Bar Soap and User-Defined scenarios only. Although you can calculate chronic exposure for non-adults in the User-Defined scenario, these results may not reflect realistic exposures. In general, for inhalation scenarios, adults are assumed to be actively exposed (i.e., during product use); non-adults are assumed to be passively exposed.

When you select a scenario or an exposed population, only those inputs pages which are applicable can be selected, and that type of exposure assessment will be performed (e.g., if air freshener is selected, the dermal inputs page may not be selected because no dermal inputs are needed for this scenario).

3.3.3 Inhalation Input Page

To calculate inhalation exposure to a consumer product, enter the information requested on the Inhalation Inputs screen (Figure 3-34). Default exposure factor values, derived from EPA's *Exposure Factors Handbook* (1997) (See Table 3-2 in Section 3.1.2) appear in the appropriate fields, depending on the scenario you have selected. All values contained within the white boxes on the Inhalation Inputs page may be edited by the user.

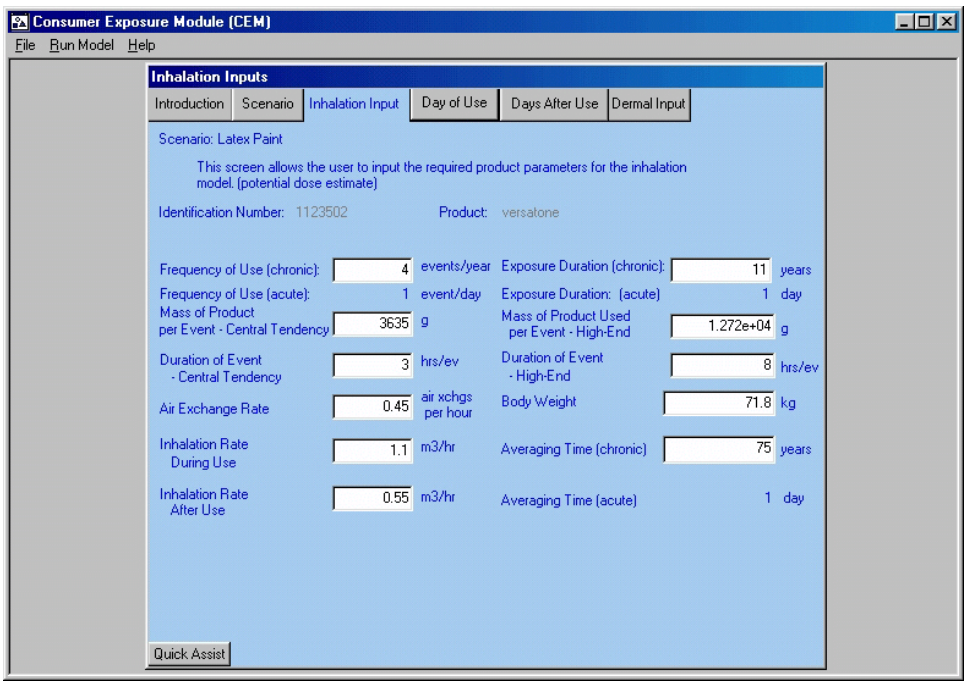

Figure 3-34. Inhalation Input Page

The following are short descriptions of the variables required for the Inhalation portion of CEM:

- **Frequency of Use (Chronic exposures)** — number of times per year the selected activity or scenario is performed (events per year).

- **Frequency of Use (Acute exposures)** — number of times per day the selected activity or scenario is performed (CEM assumes 1 event per day).

- **Exposure Duration (ED)** — Duration of product use (years for chronic, 1 day for acute)

- **Mass of Product Used per Event (Central Tendency)** — default value is 50th percentile amount of product used per activity or scenario (g).

- **Mass of Product Used per Event (High-End)** — default value is 90th percentile amount of product used per activity or scenario (g).

- **Duration of Event (Central Tendency)** — default value is 50th percentile amount of time it takes to complete the selected activity or scenario (hours per event).

- **Duration of Event (High-End)** — default value is 90th percentile amount of time it takes to complete the selected activity or scenario (hours per event).

- **Air Exchange Rate** — number of times over a specified period that the air leaves and enters the room where the activity or scenario occurs (air exchanges per hour).

- **Body Weight** — weight of the Exposed Population individual (kg).

- **Inhalation Rate During Use** — inhalation rate of the Exposed Population individual during the application of the product (m^3/hr).

- **Inhalation Rate After Use** — inhalation rate of the Exposed Population individual after the application of the product (m^3/hr).

- **Portion of Aerosol in the Air (Fabric Protector and Aerosol Paint scenarios only)** — fraction of the product that remains in the air as an aerosol during the product's use (unitless).

- **Averaging Time (Chronic)** — period of time over which exposures are averaged. For cancer, this number is generally assumed to be the lifetime of the product user (default is 75 years) and is used in calculating the Lifetime Average Daily Dose.

- **Averaging Time – (Acute), (Scenario dependent)** — period of time over which exposures are averaged. For acute toxicity in the exposed population, this value is assumed to be 1 day.

3.3.4 Day of Use Input Page

The Day of Use Input page (Figure 3-35) allows you to select various activities that the exposed individual would be performing during the day on which the consumer product is being used. The page consists of 26 drop-down lists, 24 that represent each hour of the day to record the location of the exposed individual throughout the course of the day, 1 that allows you to select the room where the product is used, and 1 that allows you to select the start time of the product use. This page also contains the volume of the room where the product is used (Zone 1 volume) and the volume of the house. The Day of Use Input page is used only for inhalation exposure assessments.

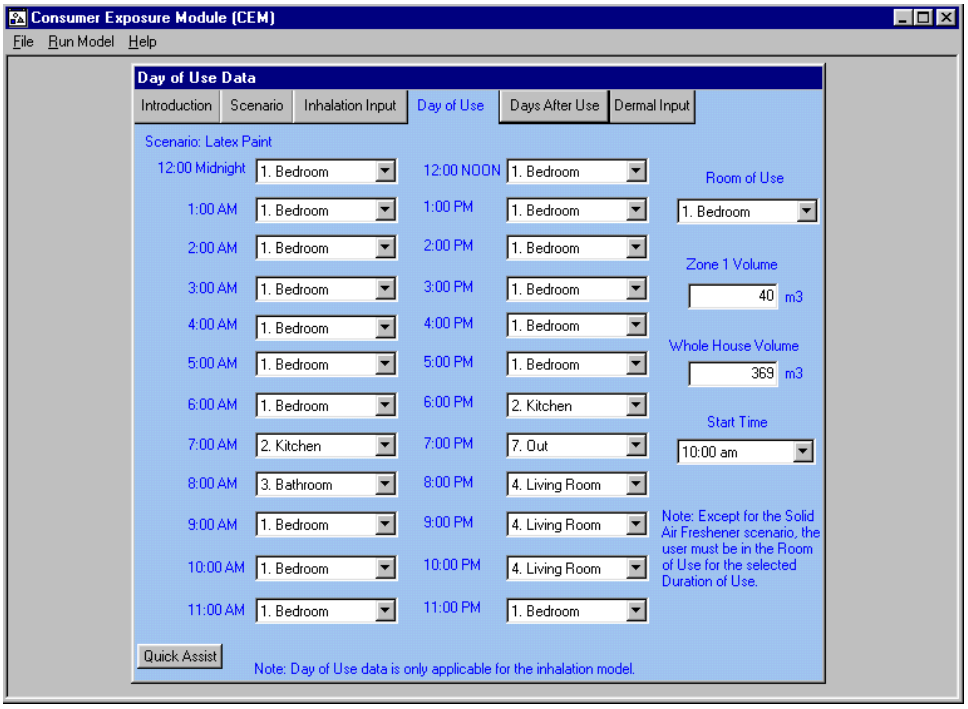

Figure 3-35. Day of Use Input Page

You can select from seven different activity locations: bedroom, kitchen, bathroom, living room, utility room, car, and out (outside the house). The table below lists the volumes of each activity location and its corresponding air exchange rate. There is no defined volume for "out" because exposure is assumed to be zero.

Activity Location	Estimated Volume, m^3	Reference	Air Exchange Rate (hr^{-1})	Reference
Bedroom	40	Versar, 1989	*	*
Kitchen	20	U.S. EPA, 1987c	*	*
Bathroom	9	U.S. EPA, 1987c	*	*
Living Room	40	U.S. EPA, 1987c	*	*
Utility Room	20	Assumed to be analogous to kitchen volume	*	*
Car	2.4	Versar, 1986	12.5	Versar, 1986 (assumes half of exchange rate for car at rest with engine running)
Whole House	369	U.S. EPA, 1997	0.45	U.S. EPA, 1997

*Whole house air exchange rate applies to all locations except "car."

The Room of Use input selections are the same as the activity locations, except for "out," which is not an option for the room of use. CEM sets the selection by default.

To begin, select the room of use and start time before entering the hourly locations (activity patterns). Make sure the room of use and start time correspond to the activity location of the exposed individual at that time; that is, you cannot select the bedroom as the room of use at a start time of 12:00 noon when the activity pattern for that time indicates the individual exposed is in the bathroom.

The model also will automatically change an activity location depending on the 90th percentile Duration of Use input on the Inhalation Input page; that is, if the scenario requires the individual to be exposed for 4 hours, CEM automatically changes the activity location so that 4 hours correspond to the room of use and the start time. If you attempt to change the location in this 4 hour block of time, the system will alert you that the room of use will be changed.

For scenarios modeling passive exposure of youths, infants or children, the default activity pattern of the day of use will be nearly identical to the day after use (non-use day) activity pattern for the user (adult). The infant or child will initially be placed (by default) outside the room of use during the time the product is being used. You can move the infant or child to any room at any time during the day of use.

Users should note that CEM requires that, except for the Solid Air Freshener scenario, the Duration of Use, both central tendency and high-end, must occur in its entirety during the Day of Use. CEM was not designed to model product-use durations that continue into the next day (e.g. indoor painting that starts at 10 PM and ends at 2:00 AM). If the user models this type of scenario, then CEM will not function properly. In these situations, it is suggested that the user select an earlier start time, such that the entire use period occurs on the day of use.

3.3.5 Days After Use (Non-Use Days) Input Page

The Days After Use (Non-Use Days) Input Page (Figure 3-36) allows you to select from the same locations as the Day of Use Input Page. The screen consists of 24 drop-down list boxes to allow you to fill in the location of the exposed individual during the course of the day or days after use. The Days After Use (Non-Use Days) Input Page is used only for inhalation exposure assessments.

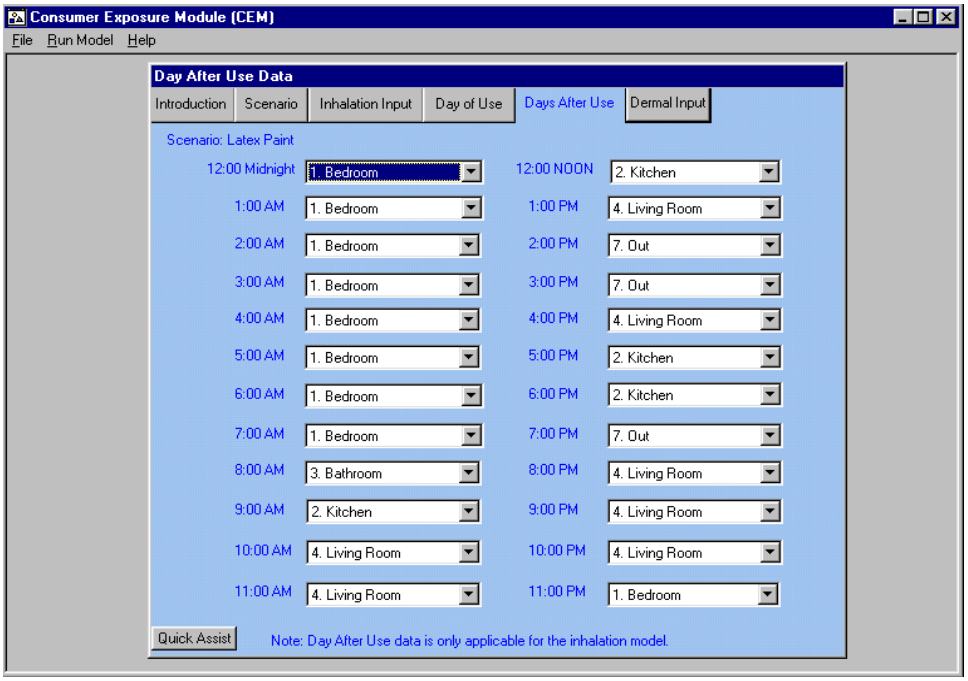

Figure 3-36. Days After Use (Non-Use Days) Input Page

3.3.6 Dermal Input Page

The Dermal Input page (Figure 3-37) allows you to enter the parameters necessary to calculate dermal exposure from the consumer product or use default exposure factor values. Default exposure factor values, derived from EPA's *Exposure Factors Handbook* (1997) (See Table 3-2 in Section 3.1.2) appear in the appropriate fields, depending on the scenario you have selected. You can edit all of the entries on the Dermal Input page except for the identification number, product name, and scenario fields.

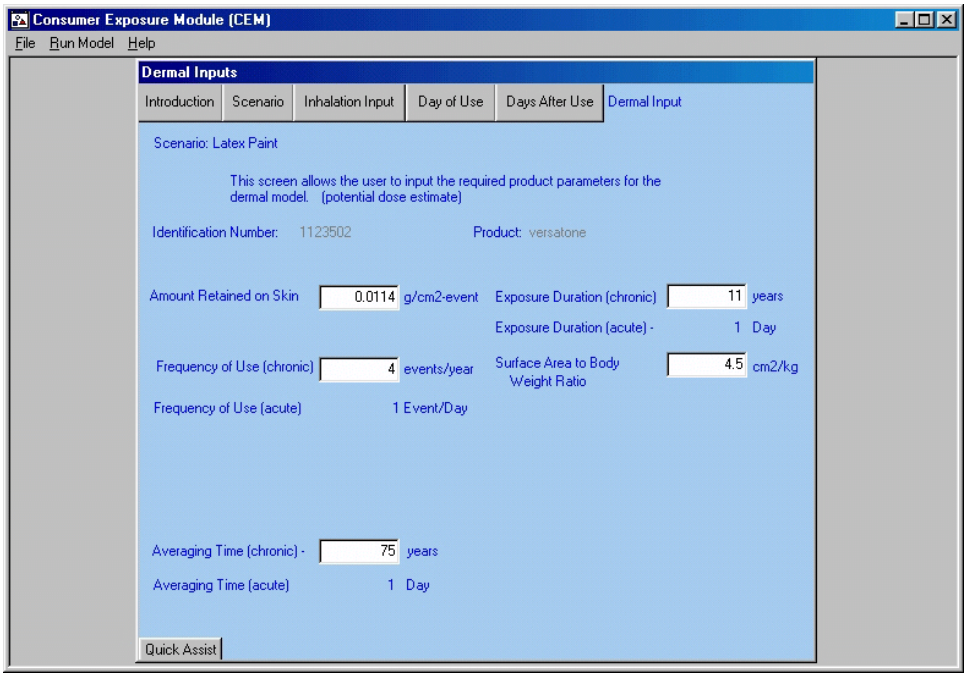

Figure 3-37. Dermal Input Page

Dermal doses can be categorized as potential doses or absorbed doses. A potential dose is the amount of a substance ingested, inhaled, or applied to the skin. An absorbed dose is the amount of a substance penetrating a specific absorption border (e.g., the exchange boundaries of skin, lung, and digestive tract) of an organism through either physical or biological processes. You can calculate the absorbed dose for an aqueous media exposure scenario by choosing the User-Defined Scenario on the Scenario page (Figure 3-32) to determine the permeability coefficient for the chemical of concern. The permeability coefficient is a flux value, normalized for concentration, that represents the rate at which the chemical penetrates the skin. The units for the permeability coefficient are centimeters per hour You can choose a permeability coefficient from a compiled list on the User-Defined Scenario Description screen (Figure 3-33), enter a known permeability coefficient, or calculate a permeability coefficient from a known K_{ow} value.

The following are short descriptions of the fields in the Dermal Input page:

- **Amount Retained on the Skin** — amount of product that is retained on the skin (grams of product per square centimeter of skin surface per event or g/cm^2-event). This variable is the product of the film thickness of the liquid on the skin's surface, the density of the formulation, and the dilution fraction (grams of product per square centimeter of skin surface per event or g/cm^2-event).

- **Exposure Duration (ED)** — Duration of product use (years for chronic, 1 day for acute)

- **Frequency of Use (Chronic exposures)** — number of times per year the selected activity or scenario is performed (events per year).

- **Frequency of Use (Acute exposures)** — number of times per day the selected activity or scenario is performed (CEM assumes 2 events per day for bar soap hand washing scenario and 1 event per day for all other scenarios).

- **Surface Area to Body Weight (SA/BW) Ratio** — ratio of the surface area of the exposed population's exposed skin during the scenario to the exposed population's body weight (cm^2/kg). For more information, see the discussion at the end of this section.

- **Frequency of Use – Hands (Bar Soap Scenario only)** — number of times the product is used and comes in contact with the product user's hands (events per year). This input variable is only used if you selected the Bar Soap scenario. People use bar soap several times during the course of a day to wash their hands and generally once a day during bathing. The Frequency of Use variable becomes the Frequency of Use – Body variable and is used in conjunction with the Frequency of Use – Hands variable in the Bar Soap scenario.

- **SA/BW Ratio – Hands (Bar Soap Scenario only)** — ratio of the surface area of the exposed skin of the product user's hands during the scenario to the user's body weight (cm^2/kg). This input variable is only used during the Bar Soap scenario (see Frequency of Use – Hands for explanation). For more information, see the discussion at the end of this section.

- **Averaging Time – (Chronic)** — period of time over which exposures are averaged. For cancer, this number is generally assumed to be the lifetime of the product user (default is 75 years) and is used in calculating the Lifetime Average Daily Dose.

- **Averaging Time – (Acute), (Scenario Dependent)** — period of time over which exposures are averaged. For acute toxicity in the exposed population, this value is assumed to be 1 day.

- **Duration of Event (User-Defined Scenario, Absorbed Dose only)** — length of time it takes to complete selected activity or scenario (hours/event). This variable is only used during user-defined dermal scenarios calculating absorbed dose.

- **Dilution (User-Defined Scenario, Absorbed Dose only)** — ratio of the amount of chemical of concern to the amount of product (unitless). This variable is only used during user-defined dermal scenarios calculating absorbed dose.

- **Density (User-Defined Scenario, Absorbed Dose only)** — ratio of the mass of the product to its volume (g/cm^3). This variable is only used during user-defined dermal scenarios calculating absorbed dose.

To determine potential exposure, the dermal portion of CEM uses a film-thickness approach, which assumes that exposure occurs from a thin layer of the consumer product on a defined skin surface area. Data on the actual thickness of films of various products on human skin are limited. The aqueous-based film-thickness data used in CEM were derived from the 1987 EPA report, *Methods for Assessing Exposure to Chemical Substances: Volume 7, Methods for Assessing Consumer Exposure to Chemical Substances* (1987c); The oil-based film-thickness data used in CEM were derived from the 1992 EPA report (*A Laboratory Method to Determine the Retention of Liquids on the Surface of Hands* (1992c). The 1992 report stated that retention measurements for the aqueous-based liquids presented in the 1987c report were not uniform and were difficult to reproduce. For these reasons, the 1992 report dropped such data from further consideration. However, the data under question are still the best known to EPA for

aqueous dermal exposures, so EPA has decided to retain the data in this model until better data are available. Because of the uncertainty associated with the amount of product forming a film on the skin, the dermal exposure estimates are considered less certain than those calculated in the inhalation portion of CEM. Absorbed dermal dose rates can be calculated using a permeability coefficient or a log octanol/water coefficient, log K_{ow}, but these values and their use in calculating exposure also involve uncertainty. Absorbed exposure can only be calculated for the User-Defined scenario in CEM.

Where possible, CEM uses the ratio SA/BW rather than the dermally exposed surface area and body weight because there is a direct relationship between the surface area of an individual and his or her body weight. Combining surface area distributions with unrelated body weight data may lead to biases in estimating exposures (Phillips et al., 1993). For example, combining an upper-percentile surface area value with a median or lower-percentile body weight could result in an unrealistic body type (i.e., an unrealistically tall individual). SA/BW ratios for adults and children (ages <1 years and 1-2 years) in CEM are derived from subsets of direct measurements of surface area and body weight data from 401 individuals (U.S. EPA, 1985b); for example, matched hand surface areas and body weights from 32 men and 12 women were used to develop the SA/BW ratios for adult hand dermal exposures. The measured body weight data from these individuals are different from those used to calculate the default body weights presented in Table 3-2 and used in E-FAST/CEM potential ingestion and inhalation dose calculations, so attempts to back-calculate surface areas in dermal dose calculations with the default body weight data are not valid. SA/BW ratios calculated in this way (i.e., from matched direct measurements) were not available for children ages 3-5 years, 6-12 years, and 13-19 years. Thus, the SA/BW ratios for these age groups were developed using median surface area data for each age group from EPA's *Exposure Factors Handbook* (U.S. EPA, 1997) divided by the mean body weight for these age groups. Note that in most cases dermal exposures in CEM applies only to adults actively engaged in product use. (e.g., children are not assumed to engage in house cleaning or painting activities). The SA/BWs used differ depending on scenarios. For example, some scenarios assume that only the palms of the hands are exposed while others assume whole hand exposure or that some other portion of the body is dermally exposed (See Section 3.3.2.1 for details.) The exception is in the Bar Soap scenario which also applies to all ages of children.

3.3.7 Estimation of Indoor Air Concentrations

CEM predicts indoor air concentrations by implementing a deterministic, mass-balance calculation. The model uses a two-zone representation of a house, with zone 1 representing the area where the consumer product is used (e.g., a kitchen) and zone 2 being the remainder of the house. The modeled concentrations in the two zones are a function of the time-varying emission rate in zone 1, the volumes of zones 1 and 2, the air flows between each zone and outdoors, and the air flows between the two zones. For a conservative estimate of exposure, indoor sinks are assumed not to exist.

The model requires the conservation of pollutant mass as well as the conservation of air mass. CEM uses a set of differential equations whereby the time-varying concentration of the chemical in each zone is a function of the rate of pollutant loss and gain for that zone. These relationships can be expressed as follows (Sandberg, 1984):

3.3.7.1 *Pollutant Mass Balance*

$$\frac{Change\ in\ Pollutant\ Mass}{Change\ in\ Time} \ 4\ Production \pm Transport\ )\ Removal \pm Reactions \qquad \text{(Eq. 3-35)}$$

Neglecting reactions:

$$\frac{dMass}{dt} = \sum Sources + \sum Mass\ in - \sum Mass\ out \pm \sum Sinks \qquad \text{(Eq. 3-36)}$$

Or:

$$V_i \frac{dC_i}{dt} = \sum Sources + \sum C_j Q_{ji} - \sum C_i Q_{ij} \pm \sum Sinks \qquad \text{(Eq. 3-37)}$$

where:

C_{air}	=	Air concentration
Q	=	Flow rate
V	=	Volume of the zone
i and j	=	Two indoor zones plus outdoors

The "±" for sinks accounts for the possibility that they may be reversible. As noted above, sinks are ignored in CEM, but are shown here for completeness.

3.3.7.2 *Air Mass Balance*

$$\Sigma\ Flows\ into\ a\ zone \ \ 4 \ \ \Sigma\ Flows\ out\ of\ a\ zone \qquad \text{(Eq. 3-38)}$$

Or:

$$\Sigma\ Qij \ \ 4 \ \ \Sigma\ Qji \qquad \text{(Eq. 3-39)}$$

where Q, i, and j are defined as in Equations 3-35 through 3-37.

The flow rates are input as constants. The pollutant mass balance (Equation 3-37) is used in conjunction with the flow rates to predict the time-varying pollutant concentrations in each of the two indoor zones.

The differential equations can be solved by a variety of numerical methods. The fourth-order Runge-Kutta method (also referred to as the Kutta-Simpson equation) is used for temporal integration (Mathews, 1992). Although this method is not as computationally efficient as some others, it is very stable, self-starting, and accurate. The equation takes the following form:

$$C(t+\Delta t) = C(t) + 1/6\left[K1 + 2K2 + 2K3 + K4\right] \qquad \text{(Eq. 3-40)}$$

where:

K1 = $\frac{dC}{dt}$ (Δt), evaluated at time = t, C = C (t)

K2 = $\frac{dC}{dt}$ (Δt), evaluated at time = t + (Δt)/2, C = C (t) + K1/2

K3 = $\frac{dC}{dt}$ (Δt), evaluated at time = t + (Δt)/2, C = C (t) + K2/2

K4 = $\frac{dC}{dt}$ (Δt), evaluated at time = t + (Δt), C = C (t) + K3.

The Runge-Kutta technique has been evaluated for stability over a wide range of values for time step, zone volumes, and flow rates.

How a product's chemical emissions are represented in CEM depends on how the product is used and its chemical makeup. Emissions are estimated over a period of 60 days using the following equations and methods that account for how a product is used or applied, the total applied mass of the product, the weight fraction of the chemical in the product, and the molecular weight and vapor pressure of the chemical.

For a **product that is applied to surface**, such as a general purpose cleaner or a latex paint, an incremental source model is used. This model assumes a constant application rate over the specified duration of use; each instantaneously applied segment has an emission rate that declines exponentially over time, at a rate that depends on the chemical's molecular weight (MW) and vapor pressure (VP).

In the case of a general purpose cleaner, the equation for exponentially declining emissions for each instantaneously applied segment is as follows:

$$E(t) = E(0) \times \exp(-kt) \qquad \text{(Eq. 3-41)}$$

where E (t) is the emission rate (mass/time) at time t (in hours), E (0) is the initial emission rate at time 0, k is a first-order rate constant for the emissions decline (inverse hours), and t is elapsed time (hours). The value of k is determined from an empirical relationship, developed by Chinn (1981), between the time (in hours) required for 90 percent of a pure chemical film to evaporate (EvapTime) and the chemical's molecular weight and vapor pressure:

$$EvapTime = \frac{145}{(MW \times VP)^{0.9546}} \qquad \text{(Eq. 3-42)}$$

The value of k is determined from the 90 percent evaporation time as follows:

$$k = \frac{\ln(10)}{EvapTime} \qquad \text{(Eq. 3-43)}$$

E (0) can be determined from the fact that the integral of Equation 3-41, which accounts for all chemical mass released (i.e., applied mass times chemical weight fraction), is equal to E (0)/k. However, the equation for the time-varying emission rate resulting from the combination of constant application and exponentially declining emissions (Evans, 1994) requires knowledge of only the total mass released and k.

$$ER(t) = \frac{M}{ta}\left[(1 - e^{-kt}) - (1 - e^{-k(t-ta)}) \times H_{(t-ta)}\right] \qquad \text{(Eq. 3-44)}$$

where:

ER(t)	=	Emission rate at time t (mg/hr)
M	=	Chemical mass to be emitted (mg)
ta	=	Application time (hr)
k	=	First-order rate constant for emissions decline (1/hr); see Eq. 3-43
t	=	Time (hr)
$H_{(t-ta)}$	=	0 if t-ta < 0
	=	1 if t-ta > 0

Latex paint is handled much like a general purpose cleaner, with two exceptions: (1) a double exponential model is used to account for an initial fast release that is governed primarily by evaporation, followed by a slow release dominated by diffusion; and (2) only 25 percent of the applied chemical mass is released, because a substantial fraction of the mass becomes trapped in the painted substrate when it dries. Empirical studies reported by Wilkes et al. (1996) support the assumption of 25 percent mass released and have estimated a relationship between the fast rate of decline (k1) and vapor pressure (VP), and between the slow rate of decline (k2) and molecular weight, leading to the following equation for the time-varying emission rate (Evans, 1994):

$$ER(t) = \frac{M}{ta} \times \left(\left[f \times \left(1 - e^{-k1t}\right) + \left(1 - f\right) \times (1 - e^{-k2t})\right] - \left[f \times (1 - e^{-k1(t-ta)}) + (1 - f) \times (1 - e^{-k2(t-ta)}) - 1\right] \times H_{(t-ta)}\right) \qquad \text{(Eq. 3-45)}$$

where:

ER(t)	=	Emission rate at time t (mg/hr)
M	=	Chemical mass to be emitted (0.25 × mass of product) (mg)
ta	=	Application time (hr)
f	=	Fraction of mass emitted from first exponential (0.1) (unitless)
t	=	Time (hr)
$H_{(t-ta)}$	=	0 if t-ta < 0
	=	1 if t-ta > 0
k1	=	233.25 × VP/24 (1/hr)
k2	=	0.0000584 × MW/24 (1/hr)
VP	=	Vapor pressure (torr)
MW	=	Molecular weight (g/mol)

The equation for the resultant emission profile requires estimates of the total mass released, k1 and k2, and the fraction of released mass associated with the first exponential (Evans, 1994). Based on the empirical studies reported by Wilkes et al. (1996), CEM associates 10 percent of the released mass with the first exponential.

For a **product sprayed on a surface**, such as a fabric protector or an aerosol paint, a portion of the applied chemical mass (default of 1 percent) is assumed to be aerosolized and is therefore immediately available for uptake by inhalation. The remainder is assumed to contact the target surface and to subsequently volatilize at a rate that depends upon the chemical's molecular weight and vapor pressure.

The constant emission rate (ER, in mass/time) for the aerosolized portion is as follows:

$$ER = \frac{\textit{Applied Chemical Mass} \times \textit{Fraction Aerosolized}}{\textit{Duration of Product Use}} \qquad \text{(Eq. 3-46)}$$

The remaining (non-aerosolized) chemical mass is treated in the same manner as described above for a general purpose cleaner, combining a constant application rate with an exponentially declining rate for each instantaneously applied segment.

For a **product added to water**, such as a laundry detergent, the chemical is assumed to emit at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration is longer than the user-specified duration of use, then the chemical emissions are truncated at the end of the product use cycle (i.e., in the case of a washing machine, the remaining chemical mass is assumed to go down the drain).

The potential duration of emissions in this case is determined from the chemical's 90 percent evaporation time, as in Equation 3-42. The constant emission rate (ER) is

$$ER = \frac{Chemical\ Mass}{EvapTime} \qquad \text{(Eq. 3-47)}$$

It is possible, however, for evaporation time to be longer than the duration of product use. In that case, the emission rate in Equation 3-47 is applied only through the end of the use cycle, resulting in loss of some mass down the drain before evaporation time is reached.

For a **product placed in the environment**, such as a solid air freshener, the chemical is assumed to emit at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration exceeds the user-specified duration of use, then the chemical emissions are truncated at the end of the product-use period, because the product is assumed to be removed from the house after the use period. Equation 3-47 applies equally here, with the loss of some mass when evaporation time is longer than the use cycle.

In certain cases the above source models could lead to predicted concentrations that exceed the chemical's saturation concentration in air. However, the model adjusts the time-varying emission rate so that the saturation concentration is never exceeded. In such cases, the chemical mass will be released at a slower rate than implied by the above source models, once the saturation concentration is reached. The same chemical mass ultimately will be released, except in cases where emissions are truncated at the end of the product use period.

The following equation is used to estimate the value for the saturation concentration:

$$C_{sat} = \frac{VP \times CF1 \times MW \times CF2 \times CF3}{R \times T} \qquad \text{(Eq. 3-48)}$$

where:

C_{sat} = Saturation concentration (mg/m^3)
VP = Vapor pressure (mm Hg)
MW = Molecular weight (g/mol)
R = Gas constant = 0.0821 L-atm/mol-K
T = Temperature of the air (296 K)
CF1 = Conversion factor (atm/760 mmHg)

CF2 = Conversion factor (10^3 mg/g)
CF3 = Conversion factor (10^3 L/m^3)

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds C_{sat}. If so, then the emission rate is reduced to a value that results in the indoor concentration equaling C_{sat}. In such a case, CEM keeps track of the cumulative mass that has been subtracted to meet the C_{sat} constraint. Release of this accumulated excess mass is initiated at a later point in time, when the modeled concentration otherwise would be below the C_{sat} value. This procedure is continued until all excess mass has been release, unless the model run period of 60 days ends first (or the product is removed or goes down the drain).

3.3.8 Estimation of Consumer Exposures

After you have entered the applicable information in the various input pages (as described above), click on "Run Model" on the pull-down bar at the top of the screen and then click on "Submit Data." to calculate the consumer exposures for the scenario of interest. CEM prompts you with a pop-up box when it is finished with the calculations; Click "OK" to display the results screen. The first page (Figure 3-38) displays the values you entered as inputs in the various scenario input pages. The remaining page(s) display the exposure estimates for the inhalation and dermal results, as applicable. Figure 3-39 is an example of the CEM Inhalation Exposure Estimates page, and Figure 3-40 is an example of the CEM Dermal Exposure Estimates page. The following sections (3.3.8.1 and 3.3.8.2) discuss the calculation of these exposure estimates. For further discussion regarding inhalation concentration and dose estimation, please refer to Appendix D.

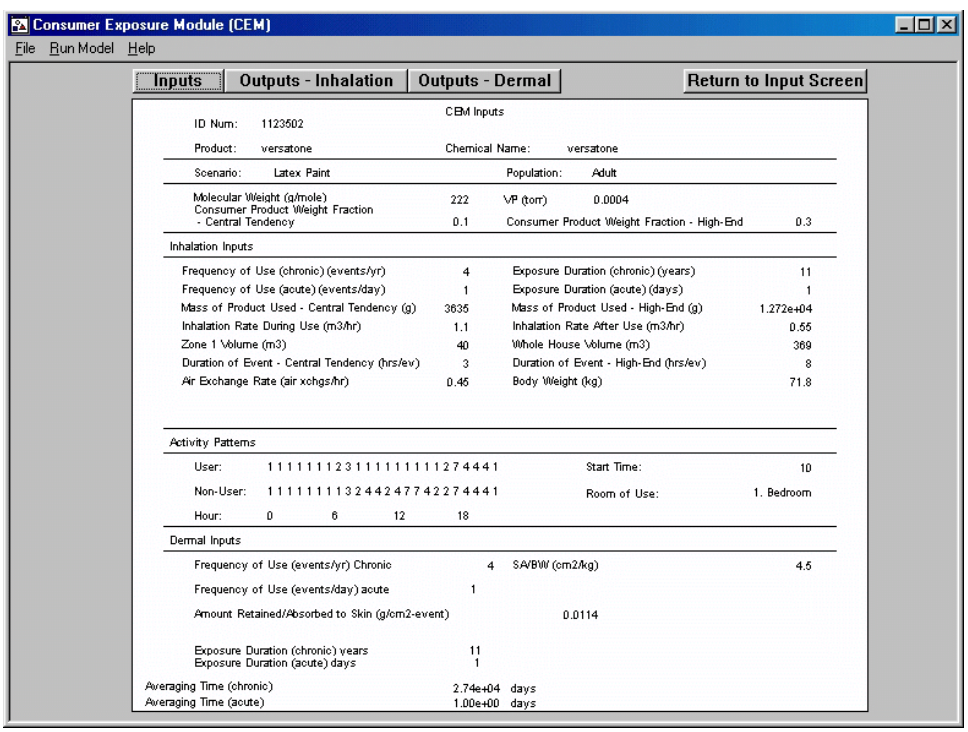

Figure 3-38. CEM Inputs

Consumer Exposure Module (CEM)

File Run Model Help

Inputs | Outputs - Inhalation | Outputs - Dermal | Return to Input Screen

CEM Inhalation Exposure Estimates

ID Num: 1123502 Product: versatone

Scenario: Latex Paint Population: Adult

Inhalation Rate(m3/hr) 1.1
BodyWeight (kg) 71.8

Exposure Duration (years) Chronic 11
Exposure Duration (days) Acute 1
Frequency of Use (events/year) Chronic 4
Frequency of Use (events/day) Acute 1

Exposure Units	Result	AT (days)
Chronic, Cancer		
$LADD_{pot}$ (mg/kg-day)	1.72e-03	2.74e+04
$LADC_{pot}$ (mg/m3)	9.36e-03	2.74e+04
Acute		
ADR_{pot} (mg/kg-day)	3.62e-01	1.00e+00

Cp_{pot} (mg/m3)	2.436	

LADDpot - Lifetime Average Daily Dose (mg/kg-day)

LADCpot - Lifetime Average Daily Concentration (mg/m3)

ADRpot - Acute Dose Rate (mg/kg-day)

Cppot - Peak Concentration (mg/m3)

Note: 75 years = 2.738e+04 days

pot - potential dose

Note: The general Agency guidance for assessing short-term, infrequent events (for most chemicals, an exposure of less than 24 hours that occurs no more frequently than monthly) is to treat such events as independent, acute exposures rather than as a chronic exposure. (Methods for Exposure-Response Analysis for Acute Inhalation Exposure to Chemicals (External Review Draft). EPA/600/R-98/051. April 1998)

Figure 3-39. CEM Inhalation Exposure Estimates

Consumer Exposure Module (CEM)

File Run Model Help

Inputs | Outputs - Inhalation | Outputs - Dermal | Return to Input Screen

CEM Dermal Exposure Estimates

ID Num: 1123502 Product: versatone

Scenario: Latex Paint Population: Adult

Exposure Duration (years) chronic 11
Exposure Duration (days) acute 1
SA/BW (cm2/kg) 4.5
Frequency of Use (events/year) chronic 4
Frequency of Use (events/day) acute 1

Exposure Units	Result	AT (days)
Chronic, Cancer		
$LADD_{pot}$ (mg/kg-day)	8.25e-03	2.74e+04
Acute		
ADR_{pot} (mg/kg-day)	1.54e+01	1.00e+00

LADDpot - Lifetime Average Daily Dose (mg/kg-day)

ADRpot - Acute Dose Rate (mg/kg-day)

pot - Potential Dose

Note: 75 years = 2.738e+04 days

Note: The general Agency guidance for assessing short-term, infrequent events (for most chemicals, an exposure of less than 24 hours that occurs no more frequently than monthly) is to treat such events as independent, acute exposures rather than as a chronic exposure. (Methods for Exposure-Response Analysis for Acute Inhalation Exposure to Chemicals (External Review Draft). EPA/600/R-98/051. April 1998)

Figure 3-40. CEM Dermal Exposure Estimates

3.3.8.1 *Estimation of Inhalation Exposures*

Two different inhalation dose calculations are performed in CEM: the Potential Lifetime Average Daily Dose ($LADD_{POT}$) and the Potential Acute Dose Rate (ADR_{POT}). The general expression for the Potential Lifetime Average Daily Dose ($LADD_{POT}$) is as follows:

$$LADD_{POT} = \frac{C_{air} \times InhR \times FQ \times DEv \times ED}{BW \times AT \times CF1} \qquad \text{(Eq. 3-49)}$$

where:

$LADD_{POT}$	=	Potential Lifetime Average Daily Dose (mg/kg-day)
C_{air}	=	Exposure concentration (mg/m^3)
InhR	=	Inhalation rate (m^3/hr)
FQ	=	Frequency of product use (events/year)
DEv	=	Duration of an event (hr/event)
ED	=	Exposure duration (years of product usage; see Table 3-2)
BW	=	Body weight (kg)
AT	=	Averaging time (years)
CF1	=	Conversion factor (365 days/year)

Within CEM, the inhalation dose is calculated iteratively, in time steps of 10 seconds, taking into account the chemical emission rate over time, the volume of the house and each zone, the air exchange rate and interzonal airflow rate, and the exposed individual's locations and inhalation rates during and after product use. Because of this iterative process, Equation 3-49 may not be directly used to calculate the $LADD_{POT}$ from the $LADC_{POT}$ presented in the model results. Therefore, the $LADD_{POT}$ is calculated using the following expression:

$$LADD_{POT} = \frac{Dose_{ati} \times FQ \times ED}{BW \times AT \times CF1} \qquad \text{(Eq. 3-50)}$$

where the variables are defined as they are for Equation 3-49, and $Dose_{ati}$ is the time-integrated, air dose for an event given by Equation 3-51. For $LADD_{POT}$ calculations, the averaging time is the lifetime of the individual.

$$Dose_{ati} = \sum_{ST}^{ET} (C_{i,t} \times \Delta t \times InhR_{i,t} \times CF2) \qquad \text{(Eq. 3-51)}$$

where

$Dose_{ati}$	=	Time-integrated air dose for an event (mg/event) from start time (ST) to end time (ET), where ET = ST + 60 days.
$C_{i,t}$	=	Concentration in Zone i at time t (mg/m^3)
Δt	=	time interval (1.16 x 10^{-4} days/event)
$InhR_{i,t}$	=	Inhalation Rate for Zone i at time t (m^3/hr)
CF2	=	Conversion factor (24 hours/day)

For cases where the evaporation time estimated in Equation 3-42 exceeds 60 days, the model will truncate the emissions at 60 days. Conversely, for cases where the evaporation time is less than 60 days, emissions will be set to zero between the end of the evaporation time and 60 days.

The general expression for the Potential Acute Dose Rate (ADR_{POT}) is as follows:

$$ADR_{POT} = \frac{C_{air} \times InhR \times FQ \times DEv \times ED}{BW \times AT} \qquad \text{(Eq. 3-52)}$$

where:

ADR_{POT}	=	Potential Acute Dose Rate (mg/kg-day)
C_{air}	=	Exposure concentration (mg/m^3)
InhR	=	Inhalation rate (m^3/hr)
FQ	=	Frequency of product use (events/year)
DEv	=	Duration of an event (hr/event)
ED	=	Exposure duration (years of product usage; see Table 3-2)
BW	=	Body weight (kg)
AT	=	Averaging time (days)

For the ADR_{POT} calculations, an averaging time of one day is used; the ADR_{POT} therefore represents the maximum time-integrated dose over a 24-hour period during the exposure event.

As was the case with the $LADD_{POT}$ in Equation 3-49, Equation 3-52 cannot be directly used to calculate an ADR_{POT} from a time-integrated air concentration. Instead, the following expression is used:

$$ADR_{POT} = \frac{Dose_{ati} \times FQ \times ED}{BW \times AT} \qquad \text{(Eq. 3-53)}$$

where

ADR_{POT}	=	Potential Acute Dose Rate (mg/kg-day)
$Dose_{ati}$	=	Time-integrated, air dose (mg/event)
FQ	=	Frequency of product use (1 event/day)
ED	=	Exposure duration (1 day)
BW	=	Body weight (kg)
AT	=	Averaging time (1 day)

The time-integrated air dose is defined by the following equation

$$Dose_{ati} = Max\left[\sum_{0}^{24}(C_{i,t} \times \Delta t \times InhR_{i,t} \times CF2)\right]\Bigg|_{ST}^{ET} \qquad \text{(Eq. 3-54)}$$

where

$Dose_{ati}$	=	Time-integrated air dose for an event (mg/event) evaluated from start time (ST) to end time (ET), where ET = ST + 60 days.
$C_{i,t}$	=	Concentration in Zone i at time t (mg/m^3)
) t	=	time interval (1.16 x 10^{-4} days/event)
$InhR_{i,t}$	=	Inhalation Rate for Zone i at time t (m^3/hr)
CF2	=	Conversion factor (24 hours/day)

For cases where the evaporation time estimated in Equation 3-42 exceeds 60 days, the model will truncate the emissions at 60 days. Conversely, for cases where the evaporation time is less than 60 days, emissions will be set to zero between the end of the evaporation time and 60 days.

The exposure concentration in the above equation is calculated differently for ADR_{POT} than for $LADD_{POT}$. For the $LADD_{POT}$ calculations, CEM uses the central tendency consumer product weight fraction, duration of use, and mass of product used. In the ADR_{POT} calculation, it uses the high-end consumer product weight fraction, duration of use, and mass of product used. CEM calculates all possible ADRs, over the 60-day modeling period, as running 24-hour integrations (i.e., hours 1-24, 2-25, etc.), and then reports the highest of these computed values as the ADR.

Two different inhalation concentration calculations are performed in CEM: Potential Lifetime Average Daily Concentration ($LADC_{POT}$), and Potential Peak Concentration (Cp_{POT}). They are defined as follows:

$$LADC_{POT} = \frac{C_{ati} \times FQ \times ED}{AT \times CF1} \quad \text{where:} \qquad \text{(Eq. 3-55)}$$

$LADC_{POT}$	=	Potential Lifetime Average Daily Concentration (mg/m^3)
C_{ati}	=	Time-integrated air concentration per product-use event (mg/m^3-days/event)
FQ	=	Frequency of use (events/year)
ED	=	Exposure Duration – duration of product use (years) (see Table 3-2)
AT	=	Averaging time (years)
CF1	=	Conversion factor (365 days/year)

The time-integrated air concentration is estimated using the following equation

$$C_{ati} = \sum_{ST}^{ET} (C_{i,t} \times \Delta t) \qquad \text{(Eq. 3-56)}$$

where

C_{ati}	=	Time-integrated air concentration for an event (mg/m^3-days/event) from start time (ST) to end time (ET), where ET = ST + 60 days.
$C_{i,t}$	=	Concentration in Zone i at time t (mg/m^3)
Δt	=	time interval (1.16×10^{-4} days/event)

For cases where the evaporation time estimated in Equation 3-42 exceeds 60 days, the model will truncate the emissions at 60 days. Conversely, for cases where the evaporation time is less than 60 days, emissions will be set to zero between the end of the evaporation time and 60 days.

The potential peak concentration (Cp_{POT}) provided in the model output is defined as the highest *instantaneous* air concentration that is calculated by the model during any 10-second time step, and should not be interpreted as a *daily* maximum concentration. Cp_{POT} is estimated using the following equation:

$$Cp_{POT} = Max(C_{i,t})\Big|_{t=0}^{t=ET} \qquad \text{(Eq. 3-57)}$$

where

Cp_{POT}	=	Potential Peak Concentration (mg/m^3), evaluated as the maximum $C_{i,t}$ from t=0 to t=ET
$C_{i,t}$	=	Concentration in Zone i at time t (mg/m^3)

3.3.8.2 *Estimation of Dermal Exposures*

Two different dermal exposure calculations are performed in CEM: the Potential Lifetime Average Daily Dose ($LADD_{POT}$) and the Potential Acute Dose Rate (ADR_{POT}). The following equations are used to calculate these results:

$$LADD_{POT} = \frac{AR \times SA/BW \times FQ \times ED \times WF \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-58)}$$

$$ADR_{POT} = \frac{AR \times SA/BW \times FQ \times ED \times WF \times CF1}{AT} \qquad \text{(Eq. 3-59)}$$

where:

AR	=	Amount retained on the skin (g/cm^2-event)
SA/BW	=	Surface area to body weight ratio (cm^2/kg)
FQ	=	Frequency of use (events/year for $LADD_{POT}$, 1 event/day for ADR_{POT} (*exception*: 2 events/day for Bar Soap (hand) scenario))
ED	=	Exposure Duration–duration of product use (years for $LADD_{POT}$, 1 day for ADR_{POT}) (see Table 3-2)
WF	=	Weight fraction of chemical in product (unitless) - central tendency for $LADD_{POT}$, high-end for ADR_{POT}
AT	=	Averaging time (years for $LADD_{POT}$, 1 day for ADR_{POT})
CF1	=	Conversion factor (10^3 mg/g)
CF2	=	Conversion factor (365 days/year)

In the dermal calculations for Bar Soap, the SA/BW term and the FQ term is split into two terms, a SA/BW and FQ for the body and a SA/BW and FQ for the hands. The dose for the body and hands is calculated and then summed to provide an overall dose for Bar Soap.

The consumer product weight fraction (WF) term in the above calculations varies. For the LADD calculations, the central tendency consumer product weight fraction is used. In the ADR_{POT} calculation, the high-end consumer product weight fraction is used.

The above calculations are performed for scenarios to calculate the potential dose. Potential dose is the amount of a chemical contained in bulk material applied to the skin. In the User-Defined scenario you can select to calculate absorbed dermal exposure using the permeability coefficient method. Absorbed dose is the amount of substance penetrating across the absorption barriers of an organism. You can choose a permeability coefficient by one of three methods:

- Entering a permeability coefficient
- Selecting a permeability coefficient value from a list of common chemicals
- Entering a K_{ow} value and having the model calculate the permeability coefficient using the following equation (U.S. EPA, 1992d):

$$\log(K_p) = -2.72 + 0.71 \times \log(K_{ow}) - 0.0061 \times MW \qquad \text{(Eq. 3-60)}$$

where:

K_p	=	Permeability coefficient (cm/hr)
K_{ow}	=	Octanol/water partition coefficient (unitless)
MW	=	Molecular weight (g/mol)

The permeability coefficient is then entered into the following equations to calculate dermal exposure:

$$LADD_{ABS} = \frac{Kp \times DEv \times Dil \times Den \times SA/BW \times FQ \times ED \times WF \times CF1}{AT \times CF2} \qquad \text{(Eq. 3-61)}$$

$$ADR_{ABS} = \frac{Kp \times DEv \times Dil \times Den \times SA/BW \times FQ \times ED \times WF \times CF1}{AT} \qquad \text{(Eq. 3-62)}$$

where:

K_p	=	Permeability coefficient (cm/hr)
DEv	=	Duration of an event (hr/event)
Dil	=	Dilution (unitless)
Den	=	Density (g/cm^3)
SA/BW	=	Surface area to body weight ratio (cm^2/kg)
FQ	=	Frequency of use (events/year for $LADD_{ABS}$, 1 event/day for ADR_{ABS})
ED	=	Exposure Duration–duration of product use (years for $LADD_{ABS}$, 1 day for ADR_{ABS}) (see Table 3-2)
WF	=	Weight fraction of chemical in product (unitless) - central tendency for $LADD_{ABS}$, high-end for ADR_{ABS}
AT	=	Averaging time (years for $LADD_{ABS}$; 1 day for ADR_{ABS})
CF1	=	Conversion factor (10^3 mg/g)
CF2	=	Conversion factor (365 days/year)

This approach assumes a constant supply of product on the skin throughout the exposure duration.

3.4 Probabilistic Dilution Model (Stand-alone PDM)

PDM is a software program developed by OPPT to predict downstream chemical concentrations from an industrial discharge. PDM calculates the probability that a given target stream concentration will be exceeded, and the number of days per year the exceedence condition will likely occur. PDM analyses can be performed on reaches with measured flow data (i.e., from U.S. Geological Survey gaging stations) or reaches with only estimated flow values. PDM does not estimate exceedences for chemicals discharged to still waters, such as bays, lakes, or estuaries. PDM may be executed within the General Population Exposure and Down-the-Drain modules or may be run as a stand-alone model from the PDM module. An example of the Stand-alone PDM Site-Specific Results page is shown in Figure 3-41.

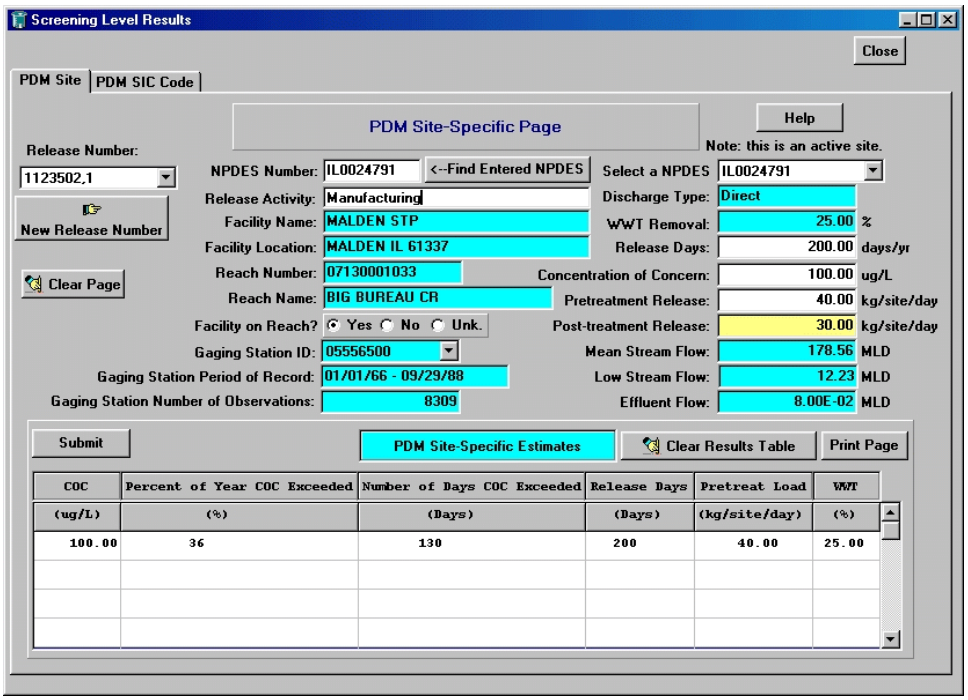

Figure 3-41. PDM Site-Specific Results Page (Stand-alone)

PDM employs a simple mass balance approach to calculate stream concentrations. However, input variables are not constant; streams follow a highly variable seasonal flow pattern and numerous variables in a manufacturing process can affect the chemical concentration and flow rate of the effluent. PDM uses probability distributions as inputs and calculates the resulting probability distribution of the concentration in the stream. PDM currently uses data from various EPA water-related information systems (See Appendix B). See Appendix C for a description of the statistical framework of PDM.

PDM has two options available for performing analyses, depending on the extent of data available. The first option addresses site-specific cases. The second option allows for a high-end or average-case analysis of potential exceedences for an unspecified facility in an industrial category This option serves as a screening-level analysis to assess the impacts on potentially hundreds of facilities in an industrial category. The following two sections describe the two options.

3.4.1 PDM Site-Specific Page

Upon selecting the PDM module, on the Screening-Level Main page (Figure 3-1), the PDM Site-Specific page will appear (Figure 3-41). Enter a complete or partial National Pollutant Discharge Elimination System (NPDES) permit number in the NPDES Number field, click on the "Find Entered NPDES" button, then select a NPDES number from the pull-down list in the "Select a NPDES" field. (Under the Clean Water Act, discharges of chemicals to surface waters are required to obtain a permit. A NPDES permit number is a unique nine-character code, beginning with the two-letter state abbreviation. E-FAST V2.0 only contains NPDES numbers for permitted facilities in the format IL*xxxxxxx*, where *x* is numeric. NPDES numbers for general permits and non-permitted facilities are not included.) Once you select the NPDES permit number for the facility of interest in the "Select a NPDES" field, the program will immediately determine if the reach has a USGS gaging station (i.e., measured flow data are available) or not (i.e., only estimated flow data are available). If the reach has gaging station data available, the ranked measured daily flow values are used to determine the frequency of exceedence. If only estimated flow data are available, the program estimates the frequency of exceedence using an integration procedure presented by Di Toro (1984).

PDM inputs include information entered in the PChem/Fate Inputs screen (Figure 2-1), information on the discharging facility extracted from the E-FAST V2.0 database, and the Release Days, Concentration of Concern (COC), and Pretreatment Release information you enter on the PDM Site-Specific page. Click on the "Submit" button and the results will be added to the table in the lower portion of the page. PDM estimates the number of days per year and the percentage of the year the COC will be exceeded. Click on the "Save" button to save the results from this PDM run in your chosen format (MS Word or WordPerfect); you will be prompted for a name and location for the file. After two or more releases have been run, the Release Number box on the left hand side of the page can be scrolled to show all the stored site-specific PDM results.

The following are short descriptions of the fields that appear on the PDM Site-Specific Results page:

- **NPDES Number** — Under the Clean Water Act, discharges of chemicals to surface waters are required to obtain a permit. A NPDES permit number is a unique nine-character code, beginning with the two-letter state abbreviation.

- **Release Activity** — your description of the release activity (entered on PDM Site-Specific page). You may leave this field blank.

- **Facility Name, Location, Reach Number, Reach Name** — information on the discharging facility extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Facility on Reach?** — indicates whether the facility discharges to the identified reach, discharges to a tributary stream, or if the discharge point is unknown.

- **Select a NPDES —** NPDES permit number you entered for the facility of interest.

- **Discharge Type —** indicates whether the facility is a direct discharger that discharges treated wastewater directly to a surface water body or an indirect discharger that discharges wastewater to a POTW for treatment.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release Days** — number of days per year that the chemical is discharged, as entered on the General Release Information page.

- **Concentration of Concern (COC)** — threshold concentration, in micrograms per liter (µg/L), below which adverse effects on aquatic life are expected to be minimal. PDM in E-FAST V2.0 predicts how many days per year the concentration of the chemical in the receiving stream will exceed the COC.

- **Pretreatment Release** — rate of release of the chemical by the facility to a wastewater treatment facility (kg/day), as entered on this page.

- **Post-treatment Release** — rate of release of the chemical after treatment by a wastewater treatment facility (kg/day). The post-treatment release amount is equal to the pretreatment release reduced by the wastewater treatment removal percentage.

- **Mean Stream Flow** — arithmetic mean flow of the ambient water body receiving the facility's discharge (MLD), extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Low Stream Flow** — 7Q10 stream flow (i.e., 7 consecutive days of lowest flow over a 10-year period) (MLD), extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

- **Effluent Flow** — Effluent flow of the discharging facility (MLD), extracted from the E-FAST V2.0 database when searching for a facility during the data entry procedure (See Section 3.1.1.1).

If the facility selected discharges to an ambient water body with a USGS gaging station, the following additional information is provided:

- **Gaging Station** — identification number for the USGS streamflow monitoring site for the ambient water body receiving the facility's discharge. PDM accesses daily flow values collected between 1966 and 1991 to calculate the frequency of exceedence.

- **Period of Record** — period for which daily streamflow data are available for the selected gaging station.

- **Number of Observations** — number of times the daily stream flow was measured during the period of record.

The lower half of the page presents the following PDM site-specific estimates in a table: the estimated number of days that the COC will be exceeded in the ambient water body that receives discharge from the facility; as well as the percent of the year that the COC will be exceeded. These are described below. In addition to the results, the table includes the following input fields: COC, release days, pretreatment release load, and the WWT removal rate. These are described above.

- **Number of Days COC Exceeded** — estimate of the number of days/year that the COC is exceeded.

- **Percent of Year COC Exceeded** — the percentage of year that the COC is exceeded. This is calculated by dividing the exceedence days/year by 365 and multiplying the result by 100.

In addition to these fields, the PDM Site Results page displays a "Print Page" button that may be used to generate a hard copy of the data on the screen.

3.4.2 PDM SIC Code Results Page

Upon selecting the PDM module on the Screening-Level Main page, the PDM Site-Specific page will appear. If you are modeling releases by an industrial category, select the PDM SIC Code tab, and the PDM SIC Code page will appear (Figure 3-42). The SIC codes within E-FAST V2.0 are used to classify facilities that discharge wastewater to ambient water bodies. The 36 SIC Code categories available for use with PDM can be viewed and selected from the pull down box labeled "SIC Code Description." To predict the exceedences of the COC, E-FAST V2.0 performs a high-end or average-case analysis for the receiving streams of facilities in the selected industrial category.

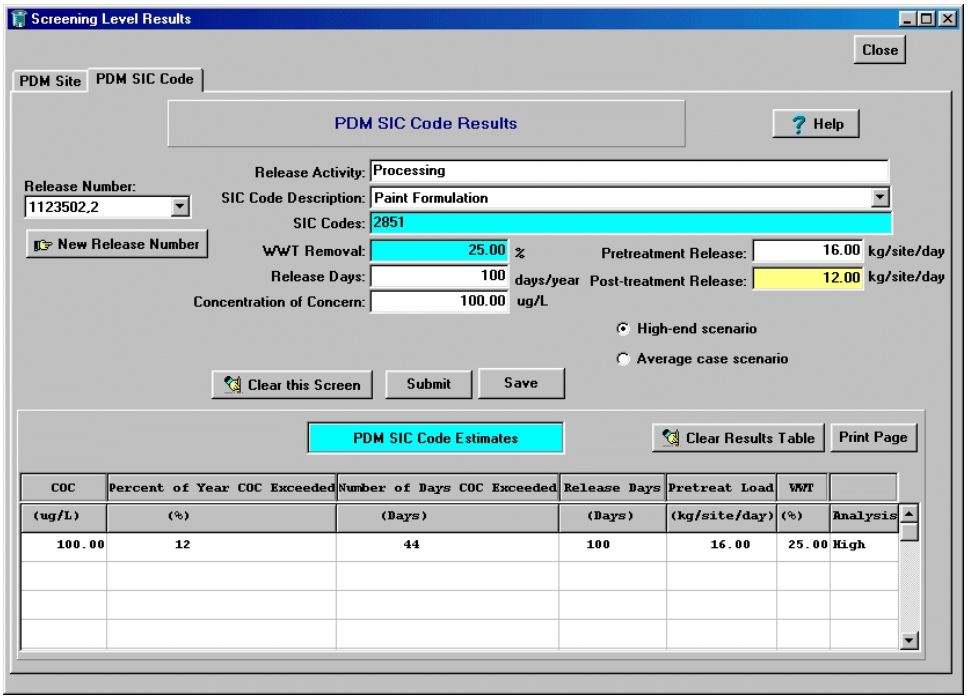

Figure 3-42. PDM SIC Code Results Page (Stand-alone)

PDM inputs include information entered in the PChem/Fate Inputs screen (Figure 2-1); stream flow information for the SIC Code category extracted from the E-FAST V2.0 database; Release Days, COC and Pretreatment Release information you enter; and the type of analysis (i.e., high-end or average) you select on this page. Click on the "Submit" button and the results will be added to the table in the lower portion of the page. PDM estimates the number of days per year and the percentage of the year the COC was exceeded. Click on the "Save" button if you want to save the results from this PDM run in your chosen format (MS Word or WordPerfect); you will be prompted for a name and location for the

file. After two or more releases have been run, the Release Number box on the left hand side of the page can be scrolled to show all the stored site-specific PDM results.

The following are short descriptions of the fields that appear on the PDM SIC Code Results page:

- **Release Activity** — your description of the release activity (entered on the PDM SIC Code page). You may leave this field blank.

- **SIC Code Description** — text description of the selected industry. The Standard Industrial Classification (SIC) system was developed by the U.S. Government to provide agencies with a uniform framework for organizing economic, engineering, and scientific data for a wide range of economic activities. These activities include agriculture, mining, manufacturing, construction, utilities, retail trade, and finance. Under the SIC system, every establishment, defined as a single economic production unit such as a factory, a mill, or a mine, is assigned a four-digit numerical code.

- **SIC Codes** — 4-digit code or codes assigned to the selected industry.

- **Wastewater Treatment (WWT) Removal** — percentage of the chemical removed from wastewater during treatment before discharge to a body of water. This is a chemical-specific property entered on the PChem/Fate Inputs screen (See Section 2.0).

- **Release Days** — number of days per year that the chemical is discharged, as entered on this page.

- **Concentration of Concern (COC)** — threshold concentration (in µg/L), below which adverse effects on aquatic life are expected to be minimal. PDM in E-FAST V2.0 predicts how many days per year the concentration of the chemical in the receiving stream will exceed the COC.

- **Pretreatment Release** — rate of release of the chemical by the facility to a wastewater treatment facility (kg/day), as entered on this page.

- **Post-treatment Release** — rate of release of the chemical after treatment by a wastewater treatment facility (kg/day). The post-treatment release amount is equal to the pretreatment release reduced by the wastewater treatment removal percentage.

- **High-end Scenario** — averaged probability of exceedence of the 10 percent of the facilities of the selected industrial category that have the highest probability of exceedence for the COC and the loading rate specified by you for worst-case scenarios.

- **Average Case Scenario** — mean exceedence probability for all facilities within an industrial category.

The lower half of the page presents the following PDM SIC Code estimates in a table: the estimated number of days that the COC will be exceeded in the ambient water body that receives discharge from the facility; as well as the percent of the year that the COC will be exceeded. These are described below. In addition to the results, the table includes the following input fields: COC, release days, pretreatment release load, WWT removal rate and the type of scenario (i.e., high-end or average case) selected. These are described above.

- **Number of Days COC Exceeded** — estimate of the number of days/year that the COC is exceeded.

- **Percent of Year COC Exceeded** — the percentage of year that the COC is exceeded. This is calculated by dividing the exceedence days/year by 365 and multiplying the result by 100.

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Appendix A

Definitions for Physical-Chemical/Fate Properties

DEFINITIONS FOR PHYSICAL-CHEMICAL/FATE PROPERTIES

The following are definitions for physical-chemical constants used in E-FAST V2.0. The particular physical constants used depend on which model is selected. The physical constants are defined below:

Adsorption to wastewater treatment sludge — expressed as a percentage, the amount of the chemical of concern that accumulates in wastewater treatment sludge divided by the total amount of the chemical in the untreated wastewater. The percentage adsorbed depends on the physical-chemical properties of the chemical, the biodegradability of the chemical, and the unit-treatment processes at the treatment plant. You should assume that industrial discharges to surface water are treated in a wastewater treatment facility before release to a body of water. The percent adsorbed cannot be greater than the wastewater treatment removal.

Bioconcentration factor (BCF) — the ratio (mg/kg in fish, divided by mg/L in water, = L/kg) of a chemical's concentration in the tissue of an aquatic organism to its concentration in the ambient water. The BCF is used to estimate the potential equilibrium concentration of a chemical in fish tissue resulting from the predicted concentration in surface water; the BCF factor times the chemical's surface water concentration equals the chemical concentration in fish tissue. Potential human exposure via fish ingestion is based on this estimated fish tissue concentration.

BCF factors can be for whole fish, fish muscle, specific fish organs, etc.. The appropriate BCF factor to use depends on the endpoint to be determined, e.g., since people generally eat fish fillets rather than whole fish, fish muscle BCF is more appropriate for potential human dose estimates of fish than the whole fish BCF. However, if only whole fish BCF values are available, those values can still be used to calculate the human potential dose rate to the chemical from ingestion of fish, as long as it is understood that the BCF for the fish fillet may be different—it is usually expected to be lower than the whole fish BCF, since the latter includes organs where greater bioconcentration usually occurs. This means the estimated dose would be higher than the actual dose; however, this is an acceptable approach for a screening-level analysis that estimates high-end to bounding exposure values. How different may the whole fish BCF be from the fish fillet BCF? In EPA's *EPI Suite BCFWIN* model, BCFs for whole fish and fish fillet are very close, probably not significantly different (Personal communication from Dr. Vince Nabholz, U.S. EPA to Conrad Flessner, U.S. EPA, March 2004).

Another consideration in the use of the BCF factor is whether it reflects the potential for metabolism. Measured BCF values do, of course, but estimation methods for BCF may or may not. For example, the Structure Activity Relationships the *EPI Suite BCFWIN* model uses to estimate BCFs are based on measured fish BCFs for chemicals with nil to average metabolism; chemicals with rapid metabolism, e.g., benzo(a)pyrene, were not included in this BCF model, so it cannot be used to estimate BCFs for chemicals that are analogs to those with rapid metabolism.

Chemical Abstracts Service (CAS) number — the unique number assigned to a substance when it enters the CAS Registry database. Numbers are assigned in sequential order to unique, new substances identified by CAS scientists for inclusion in the database. Each CAS Registry number is a unique numeric identifier, represents only one substance, has no chemical significance, and is a link to a wealth of information about a specific chemical substance.

Chemical name — the name of the chemical being modeled. This parameter can be different from the product name.

Consumer product weight fraction (central tendency) — for example, the median or the ratio of the 50th percentile weight of the chemical being analyzed found in the product to the weight of the product. This parameter is unitless.

Consumer product weight fraction (high-end) — for example the ratio of the 90th percentile weight of the chemical being analyzed found in the product to the weight of the product. This parameter is unitless.

Drinking water treatment removal — the removal percentage that is based on the physical-chemical characteristics of the chemical and the expected efficiency of unit treatment processes at the drinking water treatment facility.

Fugitive air emissions removal — the removal percentage that is based on the physical-chemical characteristics of the chemical and the expected efficiency of processes used to reduce fugitive emissions from the facility.

Henry's law constant — the ratio of a chemical's vapor pressure to its solubility. Henry's law constant gives a relative measure of a compound from water by measuring the extent to which a compound will partition between water and the air.

Log organic carbon/water partition coefficient (log K_{OC}) — chemical-specific adsorption parameter for organic substances that is largely independent of the properties of soil or sediment and can be used as a relative indicator of adsorption to such media. The larger the K_{oc}, the more likely that the chemical will adsorb to solid material. K_{oc} is highly inversely correlated with solubility, well correlated with octanol-water partition coefficient, and fairly well correlated with BCF.

Log octanol/water partition coefficient (log K_{ow}) — the ratio of the chemical concentration in octanol divided by the concentration in water. K_{ow} indicates whether a chemical will be found predominantly in water or in the fatty tissue of an animal.

Migration Descriptor — an expression of the chemical's tendency to migrate from the waste being disposed of in the landfill to surrounding soil, and eventually to groundwater. The migration descriptors as used by E-FAST V2.0 are negligible, negligible to slow, slow, moderate, and rapid; a rating of "negligible" indicates that the chemical does not reach groundwater. The migration descriptor should be chosen selected on the basis of physical-chemical parameters such as the log of the organic carbon/water partition coefficient (log K_{OC}), the log of the n-octanol/water partition coefficient (log K_{OW}), the expected leachability of the chemical from the type of waste being disposed, and the reactivity of the chemical, which includes transformation processes such as biodegradation and hydrolysis (as applicable).

Molecular weight — the sum of the atomic weights of the atoms that constitute the chemical being analyzed. The units for this parameter are grams per mole (g/mol).

Permeability coefficient (K_p) — flux value, normalized for concentration, that represents the rate at which the chemical penetrates the skin (cm/hr). The permeability coefficient for a chemical of concern can be calculated from the chemical's octanol/water partition coefficient K_{ow} (unitless) and the molecular weight (g/mol).

Stack air emissions removal — the removal percentage that is based on the physical-chemical characteristics of the chemical and the expected efficiency of treatment unit processes that are used to reduce point source emissions from the facility.

Vapor pressure (scenario-dependent) — the pressure exerted by a vapor in equilibrium with its solid or liquid phase. This parameter is only required for inhalation scenarios. There are various units for this parameter. Vapor pressure can be entered in E-FAST V2.0 in units of Atmospheres, Torr (millimeters of Mercury), Millibars, or Pascals.

Wastewater treatment removal — the removal percentages at a wastewater treatment plant. The percentage removed depends on the physical-chemical properties of the chemical, the biodegradability of the chemical, and the unit-treatment processes at the treatment plant. Removal of some or possibly all of the chemical substance usually occurs during wastewater treatment. You should assume that industrial discharges to surface water are treated in a wastewater treatment facility before release to a body of water.

Appendix B

Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2)

Surface Water Discharge Information Organization and Sources

TABLE OF CONTENTS

Page No.

PREAMBLE iii

GLOSSARY v

1.0 INTRODUCTION 1-2

2.0 GENERAL POPULATION AND ECOLOGICAL EXPOSURE (GPE) INDUSTRIAL RELEASES PATHWAY 2-2
- 2.1 Background 2-2
  - 2.1.1 Site-Specific Option 2-4
  - 2.1.2 SIC Code Option 2-4
  - 2.1.3 Probabilistic Dilution Model (PDM) 2-5
  - 2.1.4 Revisions to GPE Model 2-5
- 2.2 Data Sources in GPE 2-7
  - 2.2.1 Facility Discharge Information 2-7
  - 2.2.2 Receiving Stream Information 2-12
  - 2.2.3 Stream Dilution Factor Program (SDFP) 2-14
  - 2.2.4 Endangered Species Database 2-14
- 2.3 Hierarchy Used in Selection of Data Elements 2-15

3.0 DOWN-THE-DRAIN PATHWAY 3-2
- 3.1 Background 3-2
  - 3.1.1 Revisions to Down-the-Drain 3-3
- 3.2 Data Sources in Down-The-Drain 3-4
  - 3.2.1 E-FAST2 Main Facility File 3-4
  - 3.2.2 Stream Dilution Factor Program 3-5
  - 3.2.3 Basin Coefficient File 3-6

4.0 PROBABILISTIC DILUTION MODEL (PDM) PATHWAY 4-2
- 4.1 Background 4-2
  - 4.1.1 Site-Specific Option 4-2
  - 4.1.2 SIC Code Option 4-3
  - 4.1.3 Revisions to PDM 4-4

TABLE OF CONTENTS (cont'd)

Page No.

4.2 Data Sources in PDM 4-5
4.2.1 E-FAST2 Main Facility File 4-5
4.2.2 STORET Daily Flow Statistical File 4-6
4.2.3 Basin Coefficient File 4-7

5.0 REFERENCES 5-1

Tables

Table 2-1 Data Elements in E-FAST2 Main Facility File of Direct Dischargers 2-16

Figures

Figure 1-1 Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2) Pathways 1-1

Figure 2-1 Module 1 of Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2) - General Population and Ecological Exposure (GPE) from Industrial Releases Pathway 2-1

Figure 3-1 Module 2 of Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2) - Down-the-Drain Pathway 3-1

Figure 4-1 Module 3 of Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2) - Probabilistic Dilution Model (PDM) Pathway 4-1

PREAMBLE

The Exposure and Fate Assessment Screening Tool (E-FAST) was developed by the Office of Pollution Prevention and Toxics' (OPPT) Exposure Assessment Branch for use as a screening tool to assess potential exposure from chemical discharges to air (stack and fugitive releases), surface water, and landfills, as well as to assess inhalation and dermal exposures to chemicals in consumer products. E-FAST is composed of four separate exposure assessment modules: (1) the General Population and Ecological Exposure (GPE) from Industrial Releases Pathway; (2) the Down-the-Drain Pathway; (3) the Consumer Exposure Pathway; and (4) the Probabilistic Dilution Model (PDM) Pathway. Three of these four pathways (GPE, Down-the-Drain, and PDM) address discharges to surface water as discussed in more detail in the following sections of this report.

The surface water discharge information for the three pathways has been revised in the March 2007 E-FAST Version 2.0 (E-FAST2) to utilize the most current readily available and accurate facility and receiving stream information that would be consistent with data throughout the three pathways. These data are contained within the E-FAST2 Main Facility File. Separate files, as in the original E-FAST, will no longer be used for each module, and when the Main Facility File is updated, all of the surface water modules will be automatically updated. The Main Facility File was created by extracting various information from six water-related information systems, as well as supplemental information. While information for indirect dischargers was included in the original E-FAST model, it is not included in the E-FAST2 Main Facility File due to limitations. The original source of data for indirect dischargers has become outdated and limitations in obtaining and using data from alternate sources precludes their use at this time. More information on the data sources used to create the E-FAST2 Main Facility File is available in Section 2.2 of this report.

Additional data files are used in the various pathways of E-FAST2 in conjunction with the Main Facility File. These include the files of statistical stream data used in the Down-the-Drain and PDM Pathways (also included in the original E-FAST). As a new feature, an additional data file of endangered species is now included in the E-FAST2 GPE Pathway. The user may now search for a list of endangered species in the vicinity of a facility's discharge to surface waters.

Analyses performed using the Stream Dilution Factor Program (SDFP) in the GPE and Down-the-Drain Pathways have also been revised in E-FAST2. SDFP now only includes data for direct dischargers (including POTWs) as contained within the Main Facility File. While the same methodology employed in the original SDFP is used, the retrieval of receiving stream data, calculation of dilution factors, and ranking of the flow data and dilutions are now all conducted within the GPE and Down-the-Drain Pathways in E-FAST2. This ensures that future updates will be made efficiently and cost-effectively. Additional changes to SDFP include the loss of four of the original 40 industries due to the use of data for only direct dischargers that are included in the Main Facility File and a change in the "POTWs-Industrialized" category. This category was originally based on POTWs that received discharges from indirect facilities in select industrial categories. In E-FAST2, these POTWs are selected based on their pretreatment designation in the Permit Compliance System (PCS).

Revisions to the PDM Pathway (including the probability calculations in the GPE and Down-the-Drain Pathways) in E-FAST2 have been extensive. PDM now utilizes an approach that is more transparent and flexible for the average model user. The approach uses the most current readily available data from the E-FAST2 Main Facility File; the same data used in the other pathways (GPE and Down-the-Drain) of E-FAST2. The probability of exceedence calculations are now performed within PDM rather than using a matrix probability/ratio/interpolation method. The original E-FAST PDM required statistical "matrix files" that were created by performing thousands of stochastic calculations and storing the results. The files became out-of-date following any update of data and required interpolation before they were used. The current approach in the E-FAST2 PDM makes the use of "look-up" matrix files obsolete and ensures that future updates of PDM can be made efficiently and cost-effectively.

All of the revisions that have been incorporated into E-FAST2, along with recommended future revisions, are discussed in more detail in the following sections of this report (Sections 2.1.4 - GPE, Sections 3.1.1 - Down-the-Drain, and Sections 4.1.3 - PDM).

GLOSSARY

305(b) Assessments - Water quality assessment reports prepared by States, and submitted to EPA every two years. EPA summarizes these reports, as required under Section 305(b) of the Clean Water Act of 1972, into the National Water Quality Inventory Report to Congress, or the 305(b) report.

303(d) Lists - Lists of stream segments that do not meet water quality standards. Section 303(d) of the federal Clean Water Act requires each State to maintain these lists.

10th Percentile Receiving Stream Flows – The stream flow value that is greater than one-tenth and less than nine-tenths of the stream flow distribution under consideration.

50th Percentile Receiving Stream Flows – The stream flow value that is the median for the stream flow distribution under consideration.

CEM - Consumer Exposure Model

COC - concentration of concern - The concentration of a chemical in a water body (e.g., receiving stream, lake, etc.), above which there is a high risk to the aquatic life in the stream.

CSO - Combined Sewer Overflow

CWNS - Clean Water Needs Survey

Dilution Factor - The number calculated by dividing the receiving stream flow by the facility effluent flow.

Direct Discharger (Direct) - A municipal or industrial facility which introduces pollution through a defined conveyance or system; a point source. Direct dischargers include industrial facilities that discharge wastewater directly into a surface body of water (e.g., lake, river, stream).

EDSS - Effluent Data Statistics System

E-FAST2 - Exposure and Fate Assessment Screening Tool, Version 2.0

ESPP - Endangered Species Protection Program

GIS - Geographic Information System

GPE - General Population and Ecological Exposure

GLOSSARY (Cont'd)

Hydrologic Unit Maps - Maps developed by USGS that provide a classification of the United States based on watersheds. The United States is divided and sub-divided into successively smaller hydrologic units which are four levels: regions, sub-regions, accounting units, and cataloging units.

IFD - Industrial Facilities Discharge File

Indirect Discharger (Indirect) - A municipal or industrial facility which introduces pollutants from a non-domestic source into a publicly-owned waste treatment system. Indirect dischargers can be commercial or industrial facilities that discharge wastes into the local sewers.

Mixing Zone - An area where an effluent discharge undergoes initial dilution and is extended to cover the secondary mixing in the ambient waterbody.

NHD - National Hydrography Dataset

NOAA - National Oceanic and Atmospheric Administration

NPDES - National Pollutant Discharge Elimination System (NPDES) is an EPA permit program that regulates discharges from point sources into waters of the U.S. Facilities are issued NPDES permits regulating their discharge as required by the Clean Water Act.

OW - U.S. EPA, Office of Water

PCS - Permit Compliance System

PDM - Probabilistic Dilution Model

PMN - Premanufacture Notification; refers to a stage in the assessment process applied to new chemical products under the Toxic Substances Control Act (TSCA).

POTW - Publicly-Owned Treatment Works; a wastewater treatment facility.

Pretreatment - Processes used to reduce, eliminate, or alter pollutants from nonresidential sources before they are discharged into POTWs.

REACH - Stream segment that is part of the U.S. surface water drainage system.

GLOSSARY (Cont'd)

Receiving Stream Flows:

7Q10 - lowest consecutive 7-day average flow during any 10-year period
1Q10 - lowest 1-day flow during any 10-year period
30Q5 - lowest consecutive 30-day flow during any 5-year period
Harmonic Mean Flow - inverse mean of reciprocal daily arithmetic mean flow values

SDFP - Stream Dilution Factor Program

SDWIS - Safe Drinking Water Information System

SIC Code - Standard Industrial Classification (SIC) System; 4-digit numerical code established by the Office of Management and Budget used to classify the economic activities of most of the industries and kinds of business establishments in the United States

SSO - Sanitary Sewer Overflow

STORET (short for STOrage and RETrieval) - EPA's largest computerized environmental data system that serves as a repository for water quality, chemical, biological, and physical data used by state environmental agencies, EPA and other federal agencies, universities, private citizens, tribes, and volunteer groups.

USGS - United States Geological Survey

WEG - File of estimated streamflows prepared for EPA's Office of Water, Monitoring Branch by W. E. Gates and Associates, Inc. in 1982.

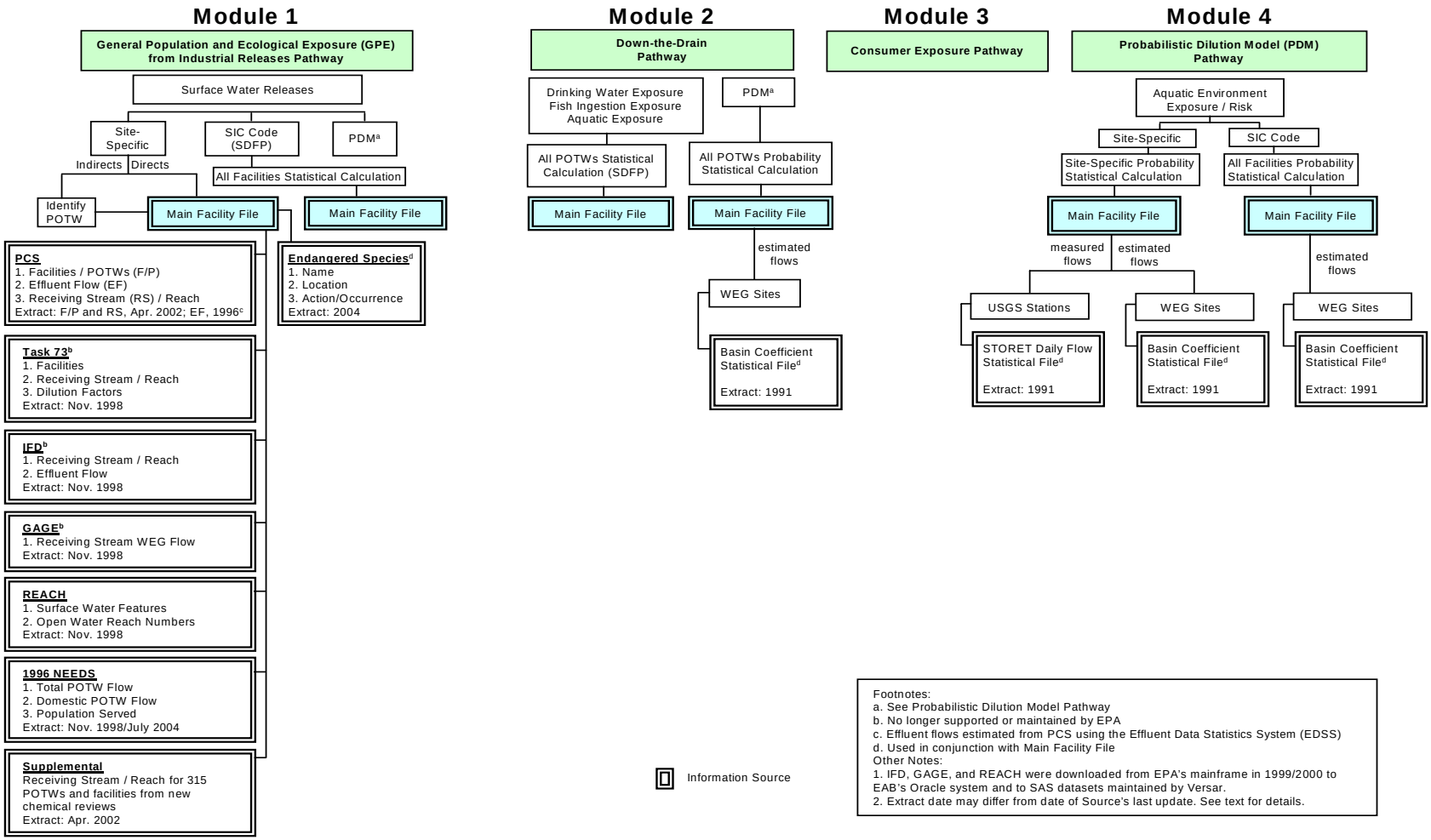

Figure 1-1
Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2) Pathways
(Surface Water Discharge Information Organization and Sources)

1.0 INTRODUCTION

The Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2) March 2007, is a screening-level computer model that allows users to estimate chemical concentrations in water to which aquatic life may be exposed, as well as generate human inhalation, drinking water ingestion, and fish ingestion exposures resulting from chemical releases to air, water, and land. E-FAST2 also may be used to assess inhalation and dermal exposures to chemicals that may result from the use of certain types of consumer products. The exposed populations assessed by the model are either some segment of the general population or consumers. Worker exposures are not assessed in this model.

E-FAST2 is composed of four separate exposure assessment modules:

- **General Population and Ecological Exposure (GPE) from Industrial Releases Pathway** - addresses human and aquatic ecological exposures resulting from facility releases to air, water, and land.

- **Down-the-Drain Pathway** - addresses human and aquatic ecological exposures to chemical releases in household wastewater.

- **Consumer Exposure Pathway** - addresses various consumer exposure pathways (i.e., dermal and inhalation) using the Consumer Exposure Model (CEM). The model calculates exposure resulting from consumer use. In addition to eight generic scenarios, CEM also allows for user-defined scenario inputs.

- **Probabilistic Dilution Model (PDM) Pathway** - addresses aquatic ecological exposures. PDM is used by the GPE and Down-the-Drain modules to calculate concentrations and to predict the number of days per year a chemical's concentration of concern (COC) in an ambient water body will be exceeded by the discharge from a facility. This module allows the user to run the model independently of the release scenarios that are used in the GPE and the Down-the-Drain modules.

Three of the four pathways (GPE, Down-the-Drain, and PDM) address discharges to surface waters. Figure 1-1 presents an overview of the surface water discharge information organization and sources for the three pathways. The primary source of facility and basic receiving stream information in all pathways of E-FAST2, the Main Facility File, has been

highlighted. The pathways are discussed in more detail in the following sections (Section 2.0 - GPE, Section 3.0 - Down-the-Drain, and Section 4.0 - PDM). Included in each section is information on the development and use of the pathway (background), including changes from the original E-FAST, data elements and sources used in the pathway. Only water releases are discussed.

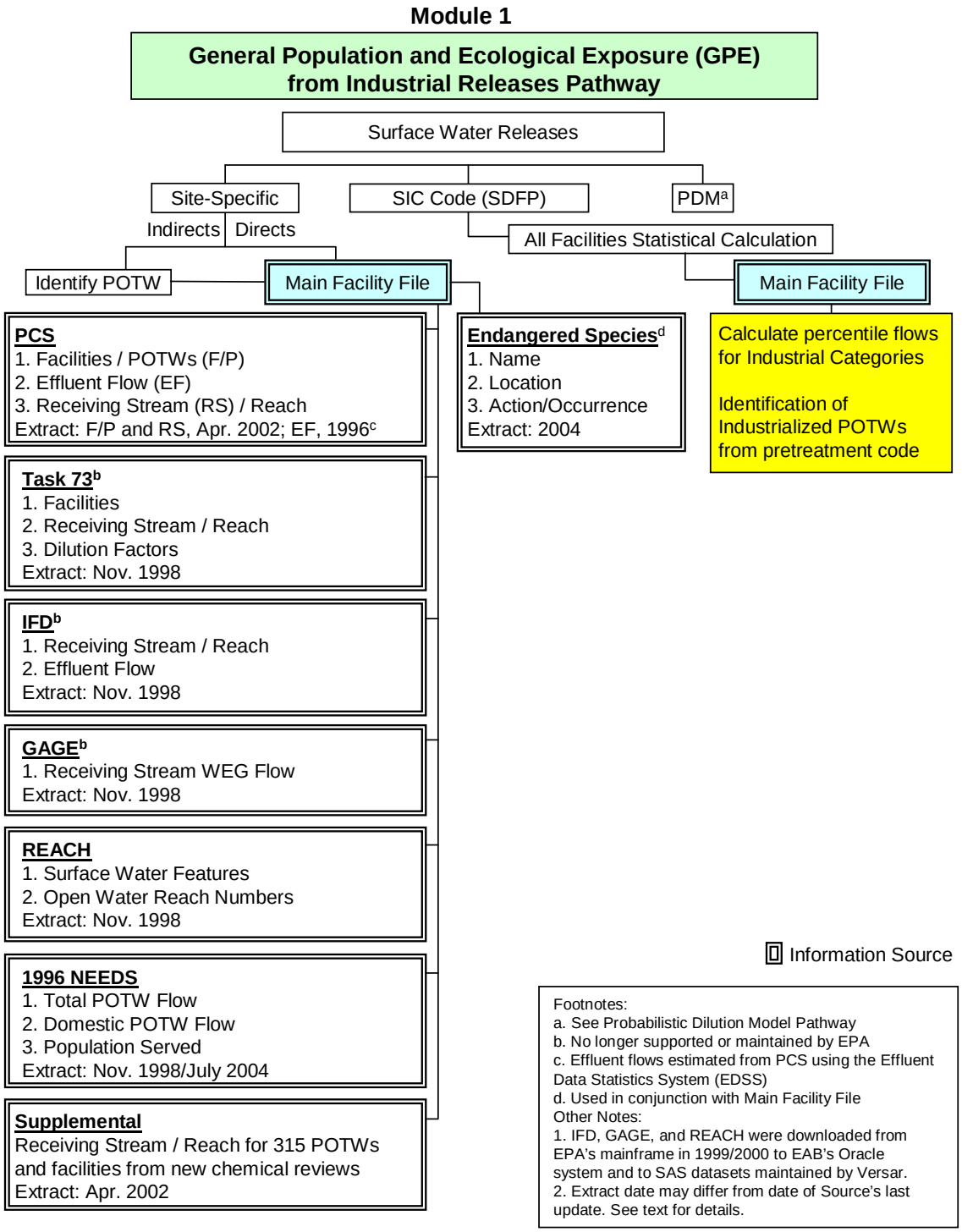

Figure 2-1
Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2)
General Population and Ecological Exposure (GPE) from Industrial Releases Pathway
(Surface Water Discharge Information Organization and Sources)

2.0 GENERAL POPULATION AND ECOLOGICAL EXPOSURE (GPE) INDUSTRIAL RELEASES PATHWAY

2.1 Background

The GPE Pathway is a screening level model. Based on information contained in an internal database and user inputs, GPE generates estimates of chemical concentrations in surface waters to which aquatic life may be exposed and estimates of human inhalation and drinking water exposures (potential dose rates) resulting from chemical releases to water, air and land. Developed as part of the original E-FAST in 1999, the GPE Model is used to support the U.S. Environmental Protection Agency (EPA) assessments of the potential exposures to new chemicals which are submitted to EPA under Section 5 of the Toxic Substances Control Act (TSCA).

Wastewaters generated by manufacturing, processing, and industrial and commercial use are typically sent to on-site treatment or are sent to publicly-owned treatment works (POTWs) prior to release to surface waters. The receiving water will dilute the discharge from the facility or the POTW, and an instream concentration of the chemical can be estimated using stream flow information in a simplified dilution analysis that does not account for fate processes other than complete and immediate mixing.

The GPE Model estimates surface water concentrations in rivers and streams under four receiving stream flow conditions (1Q10 low flow, 7Q10 low flow, 30Q5 low flow, and harmonic mean flow) as recommended in the *Technical Support Document for Water Quality-based Toxics Control* (U.S. EPA, 1991). Harmonic mean flows are used to generate estimates of chronic human exposure via drinking water and fish ingestion. EPA defines the harmonic mean flow as the inverse mean of reciprocal daily arithmetic mean flow values. EPA recommends using the long-term harmonic mean to assess potential human health impacts because it provides a more conservative estimate than the arithmetic mean flow. The 30Q5 flows (lowest consecutive 30-day flow during any five-year period) are used to generate estimates of acute human exposure via drinking water. To estimate potential acute and chronic aquatic life impacts, the model uses 1Q10 and 7Q10 flows, which are the lowest 1-day and the lowest consecutive 7-day average

flows during any 10-year period, respectively. The stream data used are estimated flows at the downstream end of specific stream segments (reaches), and are presumed to include the discharge flow from any facility on that reach.

In some cases, the mean effluent flow from a facility is larger than the estimated 7Q10 flow of the receiving reach. This may be a case where the facility effluent flow is intermittent, and the reach 7Q10 flow represents the stream flow at the time of zero or low effluent flow. For E-FAST2, OPPT has used the assumption that the value to be used to represent the stream flow in the vicinity of the facility should be the greater of the following two flow values: (1) the effluent flow for the facility of interest or (2) the stream flow.

If the effluent flow is greater than the stream flow, the effluent flow is used to represent the stream flow because the effluent flow represents the least amount of flow available.

For cases where the stream flow is greater than the effluent flow, there is a possibility that the effluent is included in the stream flow. If the stream flow includes the effluent, dividing by the stream flow yields the most accurate estimate of the in-stream chemical concentration. If the stream flow does not include the effluent, then the stream flow represents the least amount of water available for dilution, and therefore, the most conservative chemical concentration value. (Note: As stated in the E-FAST2 Introduction, the model is intended to be conservative.)

Because stream flows are not available for hydrologically complex waters such as bays, estuaries, and oceans, the model uses site-specific critical dilution factors (DFs) to estimate chemical concentrations for facilities discharging to these types of waterbodies. A survey of States and Regions, conducted by Versar for OPPT, *Mixing Zone Dilution Factors for New Chemical Exposure Assessments (Versar, 1992a) and Development of Mixing Zone Dilution Factors (Versar, 1997),* provide the site-specific critical DFs.

As seen in Figure 2-1, the GPE Model has two options available for performing analyses, depending on the extent of data available. The first option addresses site-specific cases. The second option addresses generic releases from unspecified facilities in an industrial category or specific SIC code(s). Within each option, a user may select the PDM to predict the number of days per year a chemical's COC(s) would be exceeded in a receiving body of water (stream, river, lake, etc.) due to the discharge from a facility. The following sections briefly describe the

two options and PDM, as well as recent revisions to the GPE Model. PDM is discussed in greater detail in Section 4.0.

2.1.1 Site-Specific Option

The Site-Specific Option is selected when the identity of the discharging facility is known. The GPE Model searches for a facility in the E-FAST2 Main Facility File based on the National Pollutant Discharge Elimination System (NPDES) number, facility name, SIC Code, or reach number. After finding the facility of interest and entering the number of release days and the loading (i.e. mass of chemical discharged per day), the model determines the surface water concentrations under the four flow conditions. Harmonic mean, 30Q5, and 1Q10 flows are calculated from estimated 7Q10 and arithmetic mean flows (Versar, 1992b). The E-FAST2 Main Facility File contains records for over 27,000 direct discharging facilities.

To perform an analysis for an indirect facility, the NPDES number (or some other identifying information such as the name and/or location) of the POTW that receives the discharge needs to be known. The POTW information is then used by the GPE model, as if the facility is discharging to the receiving stream of the POTW. If the removal rate for the chemical at the POTW is known, this can also be taken into account. Otherwise a worst-case scenario of zero percent removal can be assumed.

2.1.2 SIC Code Option

The SIC Code Option is selected when the exact location of a chemical loading is unknown, but, the representative industry or SIC code(s) is known. The option uses the same facility information and calculations as the site-specific option, except the calculations are performed using the 10th and 50th percentile receiving stream flows for representative dischargers in the selected SIC code(s) using the Stream Dilution Factor Program (SDFP). SDFP is currently used to (1) retrieve receiving stream flow data from the E-FAST2 Main Facility File for facilities in a particular industry or SIC code(s); (2) calculate dilution factors for each facility (receiving stream flow divided by effluent flow); and (3) rank the flow data and dilution factors, and report the results in terms of percentiles.

The majority of facilities in the E-FAST2 Main Facility File are POTWs. The facilities that comprise the category of “POTWs - Industrialized” are those POTWs that have a

pretreatment code in PCS that identifies the POTW as having a pretreatment program to treat pollutants in wastewater from industrial (non-domestic) users. All 35 of the other selected industrial categories in E-FAST2 are based on a facility's SIC code.

2.1.3 Probabilistic Dilution Model (PDM)

PDM is available within both options to predict: (1) the probability that a target stream concentration (COC) will be exceeded due to the discharge from a facility; and (2) the number of days per year the exceedence condition will exist. A simple mass balance approach forms the basis of the model; however, the input variables are not single point estimates. Streams follow a highly variable seasonal flow pattern and numerous variables in a manufacturing process can affect the chemical concentration and flow rate of the effluent. PDM uses probability distributions as inputs and calculates the resulting probability distribution of the concentration in the stream. Additional information on PDM is available in the PDM Pathway discussion (Section 4.0).

2.1.4 Revisions to GPE Model

EPA revised the GPE Model to utilize the most current readily available and accurate facility and receiving stream information that would be consistent with data throughout the GPE Pathway, as well as the Down-the Drain and PDM Pathways. These data are contained within the E-FAST2 Main Facility File. In addition, a change in the approach used for statistical calculations ensures that future updates of the GPE Model can be made efficiently and cost-effectively.

As described in the above sections, the GPE Model has two options for performing analyses: (1) site-specific and (2) generic (SIC Code). Input data for each option in the original E-FAST GPE Model included facility discharge information for both direct and indirect dischargers, which was maintained in two separate files.

Updated information for direct dischargers was compiled as part of EAB's new chemical reviews. These data, obtained from a variety of information sources as shown in Figure 2-1 and discussed in Section 2.2, are included in the E-FAST2 Main Facility File.

While the original E-FAST GPE Model used the most complete and readily available data for indirect dischargers on a national level, limitations existed with these data. The

Industrial Facilities Discharge (IFD) file, which was created in 1978 specifically to provide the Office of Water with a comprehensive database of industrial dischargers including indirect dischargers, served as the primary source of indirect discharger information in both the Site-Specific and SIC Code Option of the original E-FAST GPE Model. However, the available data for the indirect dischargers was outdated (i.e., last update in early 1990s and many of the facilities once "active" were now "inactive;" new "active" facilities are not included) and represented only a small fraction of the industrial plants that discharge to POTWs. In addition, IFD is no longer supported by EPA.

EPA investigated alternative sources of indirect discharger information such as State Files and other EPA databases. Limitations in obtaining and using data from these alternative sources precludes their use at this time. Therefore, EPA determined that the use of indirect discharger information in the E-FAST2 GPE Model would no longer be supported. As a result of removing indirect discharger information from the E-FAST2 GPE Model, under the Site-Specific Option, users are now only able to search for direct discharger information within the E-FAST2 Main Facility File. To perform an analysis for an indirect facility, the user needs to know the NPDES number (or some other identifying information such as the name and/or location) of the POTW that receives the discharge.

Removal of indirect discharger information also affects analyses performed using the generic (SIC Code) option in the E-FAST2 GPE Model. SDFP has been revised in the E-FAST2 GPE Model to only include the same data for direct dischargers (Main Facility File) as accessed in the Site-Specific Option and to use an improved method of statistical calculations. As a result, data are no longer available for 4 of the original 40 industries (Building Paper and Board Mills; Photographic Processing; Plastic Products Manufacture; and Textile Dyeing and Finishing (Carpets)). Therefore, the option to choose these industries has been removed from the model. In addition, the "POTWs-Industrialized" category was originally based on POTWs that received discharges from indirect facilities in select industrial categories (defined by SIC codes 1011-1999, 2211-5199, 5511-5599, and 7211-8099). In the E-FAST2 GPE Model, these POTWs are selected based on their pretreatment designation in the Permit Compliance system (PCS).

While the same methodology employed in the original SDFP option is used, the retrieval of receiving stream data, calculation of dilution factors, and ranking of the flow data and dilutions, are now all conducted within the E-FAST2 GPE Model. This will ensure that future updates of the GPE Model will be made efficiently and cost-effectively.

Additional revisions to the E-FAST2 GPE Model have also been made. The user may now also specify up to three chemical concentrations of concern (the original E-FAST GPE model allowed only one) for use in the calculation of days of exceedence.

An additional data search has also been included in the Site-Specific Option of the GPE Model. The user may now search for a list of endangered species in the vicinity of a facility's discharge to surface waters. The E-FAST2 GPE Model utilizes endangered species data obtained from EPA's Endangered Species Protection Program (ESPP) Database (U.S. EPA, 2004) in conjunction with the Main Facility File.

As will be seen in the following sections, the updated Main Facility File in the E-FAST2 GPE Model contains all of the facility information and basic receiving stream information necessary to be used by the two other surface water modules (Down-the-Drain, PDM) of E-FAST2. (PDM and Down-the-Drain do require the use of additional files of statistical stream data that are used in conjunction with the Main Facility File). Therefore, separate files of facility and basic receiving stream information will no longer be used for each module, and when the Main Facility File is updated, all of the surface water modules will be automatically updated.

2.2 Data Sources in GPE

The input data necessary for the GPE Model include (1) facility discharge information and (2) estimated receiving stream flow data. GPE uses data from the E-FAST2 Main Facility File. This file was created in 2002 by extracting various information from six water-related information systems, as well as supplemental information. Three of these systems are no longer being supported by EPA. However, some data elements in these systems are still valid and are included in the Main Facility File as noted below. One additional source of information, endangered species, is used in conjunction with the Main Facility File. Figure 2-1 presents an overview of the surface water discharge information organization and sources for the E-FAST2 GPE Pathway. The basic program methodology used in the statistical calculations are highlighted.

2.2.1 Facility Discharge Information

The information sources used to create the E-FAST2 Main Facility File are described below, along with a description of the ESPP Database. As noted above, some of the systems are no longer being supported by EPA, but, include data elements that are still valid and remain in

the GPE Model. For those data elements available from multiple sources, a hierarchy was established to ensure that the more accurate source of data was used. It is anticipated that primary sources of information will continue to be maintained by EPA into the future. Sources that are no longer supported by EPA have been archived and are available for any future updates of E-FAST2. It should be noted that the date information was extracted from the various sources may differ from the date the information was last updated within the source. This will be especially true with sources that are no longer being supported by EPA. Both dates are presented in the description, where possible, for each information source.

2.2.1.1 *Permit Compliance System (PCS)*

PCS is a national computerized management information system, maintained by the Office of Enforcement and Compliance, that automates entry, updating, and retrieval of NPDES data and tracks permit issuance, permit limits and monitoring data, and other data pertaining to facilities regulated under NPDES. PCS was developed in 1974 and contains information for more than 100,000 discharge permits (of which approximately 67,000 are active) issued to facilities. PCS has extensive records on approximately 7,000 permits which are classified as "major" based on the potential threat to human health or the environment. A separate permit facility record exists for each NPDES number in the database.

PCS serves as the major source of direct discharging facilities in the E-FAST2 Main Facility File. PCS is updated on a regular basis and is expected to continue to be supported by EPA for many years. There are more than 1,400 data elements within PCS which have been collected from State and EPA regions. The following data elements were retrieved and saved for direct dischargers in the select industrial categories.

- NPDES number
- Facility name and location
- Effluent flow
- SIC code
- Discharge status
- Receiving stream name and reach number (limited availability)

Several limitations of PCS should be noted.

- Only facilities that <u>directly</u> discharge to navigable waters and have a NPDES permit are captured by PCS;

- PCS reports the primary SIC code for a facility that represents the principal activity causing the discharge. Other activities may be ongoing at the facility that would not be reflected in this code even if they contribute to the discharge;
- Discharge Monitoring Reports (DMRs), which report facility discharge flow values, are required only from major facilities. Major facilities account for approximately 10 percent of the total number of facilities issued NPDES permits.

Because PCS is updated by States and EPA Regions on a continuous basis, the date of extract may be considered the date of the most recent update of PCS. The most recent version of PCS used in extracting data for the GPE Model is April 2002. Flow data were generated in 1996 using the Effluent Data Statistics System (EDSS) developed by EPA Region II. These data are still considered valid at this time. In general, a facility's discharge flow remains consistent over a period of time.

2.2.1.2 *Task 73 Report*

The Task 73 Report was originally created in the 1980's as a list of select U.S. industrial facilities that manufacture organic chemicals. The list was created to support the efficient and consistent assessments of exposures to PMNs received by OPPT under Section 5 of TSCA. Over the years, the Task 73 Report grew as additional facilities that submitted PMNs were added. In 1992 and 1997, site-specific dilution factors were added. The most current version of the Task 73 Report contains information for 865 facilities including 474 direct discharging facilities and 332 indirect discharging facilities.

Information contained in the Task 73 Report includes facility name and location, discharge type, NPDES permit number (for the facility or the POTW receiving effluent), receiving stream data, and comments/notes. All of the Task 73 Report's direct discharging facilities, along with corresponding information, are included in the E-FAST2 Main Facility File. Direct facilities that are no longer actively discharging are identified based on the discharge status (active or inactive) in PCS. Each Task 73 Report record represents a single facility and is keyed to the facility's or POTW's NPDES permit number. Information in the Task 73 Report was compiled from a variety of sources including IFD, Gage, Needs Survey, SRI Directory of Chemical Producers, State environmental departments, and PMN submitters.

The Task 73 Report was a valuable resource in preparing exposure assessments and serves as a secondary source of information for direct dischargers in the GPE Model. In general, the data in the Task 73 Report were verified by an EAB assessor at the time of collection and all

of the facility names were checked every one to two years in the SRI Directory of Chemical Producers and updated as needed. Because the data maintained in the database are limited (outdated and missing many data points), PCS is used as the primary source of facility information. Information from PCS has been incorporated into the E-FAST2 Main Facility File for all of the Task 73 direct discharging facilities (active or inactive status). The Task 73 Report data used in the GPE Model were compiled in November 1998. Data in the Task 73 Report were last updated in 1997.

2.2.1.3 *Industrial Facilities Discharge (IFD) File*

IFD is an automated database of industrial and municipal point source dischargers to surface waters in the United States. IFD was created in 1978 specifically to provide OW with a comprehensive database of industrial dischargers including indirect dischargers. The last version of IFD contains information for approximately 120,000 facilities, of which nearly half are POTWs. There are approximately 130 data elements within IFD which have been collected from various sources. Primary data sources in 1978 included:

- PCS - PCS was used to identify NPDES permitted facilities;
- NPDES Permit Files - Permits were accessed at the Regional EPA offices. Discharge and location information was obtained for both direct and indirect point source dischargers. States and local agencies provided additional and more recent information; and
- Needs Survey Data Files - The Needs Survey was used to add information on existing POTWs identified by an NPDES number.

When a new NPDES number was issued, the facility was added to IFD. However, many of the associated data elements (e.g., receiving stream information) were not completed for these entries. Weekly review of reported gaps or errors were made. Updates were not performed in a scheduled manner.

Facilities in IFD are keyed to the NPDES permit number. IFD also associates facilities with waterways receiving their discharge by assigning U.S. Geological Survey (USGS) hydrologic unit numbers and EPA's segment number (i.e., REACH number). Because some of the information in IFD is out of date when compared to other source databases (e.g. PCS) and is no longer supported by EPA, the Site-Specific Option of the GPE Model primarily uses IFD only to identify the receiving stream name and reach number for direct dischargers. Complete information (e.g., reach number) is not available for all facilities of interest. IFD is also used as

a secondary source of effluent facility flow data. While the data may not accurately reflect current conditions, approximately 24 percent of the effluent flow data used in E-FAST2 are obtained from IFD. The most recent version of IFD used in the E-FAST2 Main Facility File is November 1998 (extract date). Data in IFD were updated continuously until the early 1990s when support of IFD was discontinued. IFD consisted of data extracted from other EPA databases that were already scheduled for permanent retention.

2.2.1.4 *Needs Survey*

The Office of Wastewater Management (OWM) conducts the Clean Water Needs Survey (CWNS) on a periodic basis. It is a joint effort between States and EPA conducted in response to Section 205(a) and 516(b)(1) of the CWA. The CWNS has information on POTWs, facilities for control of sanitary sewer overflows (SSOs), combined sewer overflows (CSOs), stormwater control activities, nonpoint sources, and programs designed to protect the nation's estuaries. Information obtained from the survey is maintained in an automated database and serves as the basis for EPA's Report to Congress.

The last survey, available at the time of the data extract, was conducted in 1996. The 1996 CWNS database contains information on 16,024 wastewater treatment facilities. Information for each POTW includes location and characteristics, construction cost estimates, populations served, flow capacity, effluent characteristics, and treatment processes. Each facility in the database is keyed to the NPDES permit number. The CWNS serves as a primary and supplemental source of POTW information in the E-FAST2 Main Facility File. Information in the CWNS that has been incorporated into the E-FAST2 Main Facility File includes the POTW NPDES permit number, existing flow data (total and domestic), and populations served. The most recent extractions of data from the 1996 CWNS were November 1998, and July 2004.

2.2.1.5 *Supplemental File*

In 2000, EPA generated a database containing locational data for all POTWs (identified from PCS) in the United States. POTWs that did not have an assigned reach number (~9,300) were identified and ranked by discharge flow. EPA then identified and assigned reach numbers, using hydrologic unit maps, USGS topographic maps, and on-line digitized maps, to POTWs that met the following criteria:

- Missing an assigned reach number

- POTW discharge flow ≥ 1MLD
- Available latitude/longitude coordinates
- Available receiving stream name

As a result of this effort, reach numbers and receiving stream flow values (as appropriate) were identified and assigned to 315 POTWs. These data are included in the E-FAST2 Main Facility File.

In addition, updated facility information was compiled as part of EAB's new chemical reviews. These data were also updated into the E-FAST2 Main Facility File.

2.2.2 Receiving Stream Information

2.2.2.1 *Gage File*

The Gage File is an automated data file developed by OW to provide flow data on river segments (reaches) that have been assigned a U.S. EPA reach number. The Gage File was derived from the National Water Data Exchange, the Master Water Data Index, the Basic Characteristics File, and the STORET Daily Flow System, which in turn is supplied by USGS. There are approximately 36,000 records in the file. The stream flow data stored in the Gage File include mean annual stream flow, 7Q10 (7-day-10-year) low flow, and flow velocities. Some of the stream flow data in the Gage File are measured flows from USGS gaging stations which can be located anywhere in the reach. Most of the stream flow data in the Gage File, however, are estimated flow values. These estimated stream flows represent the downstream endpoints (discharge) of reach segments, and are based on the best available measured flow data and on drainage areas. The most comprehensive set of stream flow data were estimated by W.E. Gates and Associates in 1982 (W.E. Gates, 1982) and account for approximately 99 percent of the estimated flow values in the Gage File. Other estimated flow values in the Gage File (GKY, IAS, GLCW) were developed for special studies conducted for streams of interest (i.e., not specifically developed for the Gage File) or for connecting waterways within the Great Lakes Region (e.g., Niagara River). (Versar, 1990) Some overlap may exist with the estimated flows for a specific reach, however, the flows estimated by W.E. Gates and Associates are preferred, based on their completeness.

The following data elements were retrieved (extracted) from the Gage File in March 1997/November 1998:

- WEG Station ID
- Estimated mean annual and 7Q10 low flows
- Receiving stream reach number

The Gage File is no longer an EPA supported database. However, the estimated flows are still valid unless significant modifications have been made that affect the stream hydrology. The W.E. Gates estimated flows are currently the only comprehensive set of flows available for the national hydrologic database of stream segments (Reach File 1 - see below) which is used in the E-FAST2 Main Facility File.

2.2.2.2 *Reach File*

The Reach File, developed by the Office of Water Regulations and Standards and currently maintained by the Office of Wetlands, Oceans and Watersheds (OWOW), is a series of national hydrologic databases of surface water features in the United States. It uniquely identifies and divides each surface water into segments called reaches. Each reach is uniquely identified by an eleven-digit REACH number. The three versions of the Reach File that currently exist, known as Reach File 1 (RF1), RF2, and RF3, were created with increasingly detailed sets of digital hydrography data. RF1 is used as the basis of many water quality modeling applications today. RF1 contains information for 68,000 reaches covering approximately 700,000 miles of streams. Information maintained for each reach includes:

- Hydrologic structure, such as reach name, type, upstream and downstream connections;
- Reach trace, giving latitude and longitude coordinates along reaches; and
- Open waterbody characteristics, such as surface area and perimeter.

Information in RF1, which was created in 1982, was based on NOAA aeronautical charts and cataloging unit boundaries from the USGS. Data elements incorporated into the E-FAST2 Main Facility File include reach name and number and waterbody type. The Reach File currently serves as the only source of data for surface water features. All information has been verified by EPA with graphical and automated software tools. However, while most major rivers and streams have been assigned a REACH number, there are waterways that have not been divided into reaches.

A successor to the Reach File is the National Hydrography Dataset (NHD) Database. The NHD is being developed as a joint effort between EPA and the USGS, and is being designed to

accommodate and encourage the development of the higher resolution data needed by many software applications (e.g., GIS). The OW is planning to use the NHD as a common framework for interrelating data contained in the many EPA environmental databases such as PCS, and the Safe Drinking Water Information System (SDWIS), and USGS Flow Data. All of the data from the NHD are not yet available. The OW anticipates that flow values will be incorporated in NHD in the near future. Several pilot projects are currently underway which would link data to NHD including the OW models RiverSpill and PipelineNet. RiverSpill is a GIS based tool developed to calculate the travel time, decay, and dispersion of a pollutant introduced into the surface waters of a public water supply. PipelineNet is a companion model to RiverSpill and has been developed to trace the path and concentration of toxic substances within a water pipeline network. In addition, pilot studies are underway to assign estimated stream flows to the NHD reaches and to develop a cross reference from NHD to RF1. Once NHD has been completed, EPA will no longer support the Reach File.

2.2.3 Stream Dilution Factor Program (SDFP)

SDFP was originally developed by OW to obtain effluent and stream flow frequency distributions for a given industrial category or SIC code(s). SDFP was revised in 1987 to meet the needs of OPPT. Since 1987, the program has been periodically revised to include updated data, new variables, as well as changes in the program logic. The major purpose of SDFP is to: (1) retrieve receiving stream flow data for facilities in a particular industry or SIC code(s); (2) calculate dilution factors for each facility (receiving stream flow divided by effluent flow); and (3) rank the flow data and dilution factors and report the results in terms of percentiles. SDFP calculates these values, for all of the selected industries, based on the facility and receiving stream information in the E-FAST2 Main Facility File. When an SIC code or industry-based analysis is performed, GPE uses the 10th and 50th percentile receiving stream flows to estimate flows for a representative facility in the selected industry.

2.2.4 Endangered Species Database

The Endangered Species data in E-FAST2 is used to identify the endangered species known (or possible) to exist in the vicinity of streams and rivers that receive wastewater discharges containing the chemical of concern. The location of endangered species is correlated with the facility location via FIPS State and county codes in the E-FAST2 Main Facility File. The endangered species information includes common name, county and State, taxonomic group

(e.g., mammals, birds, fish, plants, reptiles, amphibians, clams, etc.), listing action (listing, proposed, delisting), and occurrence. The data were extracted from EPA's Endangered Species Protection Program (ESPP) Database (February 2004 release). The ESPP is a cooperative effort between the U.S. Fish and Wildlife Service (FWS), EPA Regions, States, and pesticide users. ESPP is located in the Field and External Affairs Division (FEAD) of the Office of Pesticide Programs (OPP).

2.3 Hierarchy Used in Selection of Data Elements

Twenty-three data elements for direct discharges were compiled from the various water-related environmental systems to be included in the E-FAST2 Main Facility File. Since the same data element(s) may be available from more than one database, a hierarchy was established to ensure that the more accurate sources of data are used. Table 2-1 presents a list of the various data elements compiled for direct dischargers for use in E-FAST2. For a given data element, sources are presented based on the hierarchy established for the Main Facility File in E-FAST2. Not all of the data elements were compiled directly from the various sources. The estimated mean and 7Q10 (lowest 7-consecutive day average flow that occurs every 10 years) flow values extracted from the Gage File were used to estimate the harmonic mean (inverse daily flow), 1Q10 (lowest 1-day average flow that occurs every 10 years), and 30Q5 (lowest 30-consecutive day average flow that occurs every 5 years) flow values.

Table 2-1 - Data Elements Included in E-FAST2 Main Facility File of Direct Dischargers*

Data Element	Source	Comments
NPDES Number	PCS, Task 73	Serves as major linkage between databases
Company Name	PCS, Task 73	
City	PCS, Task 73	
State	PCS, Task 73	
State/County FIPS Code	PCS	
Zip Code	PCS	
SIC Code	PCS	Facility Level
Discharge Type	PCS, Task 73	Direct
Discharge Status	PCS	Inactive (I) or Active (A)
Facility Flow	NEEDS, PCS, IFD	Total Facility Flow/Domestic POTW Flow
Receiving Stream Name	Task 73, IFD, PCS	
Reach Number	Task 73, IFD, PCS	Serves as linkage between databases
Reach Name	REACH	
HIT Code	IFD	Located on Reach - Yes, No or Unknown
Water Body Type	REACH	River or Estuary/Lake
Mean Flow	GAGE	Estimated WEG flow
Harmonic Mean Flow	Calculated	Calculated
7Q10 Flow	GAGE	Estimated WEG flow
30Q5 Flow	Calculated	Calculated
1Q10 Flow	Calculated	Calculated
Acute Dilution Factor	Task 73	Mixing Zone Critical Dilution Factor
Chronic Dilution Factor	Task 73	Mixing Zone Critical Dilution Factor
Population Served	NEEDS	Population serviced by POTW

* Additional data elements are available but are not currently included in E-FAST2.

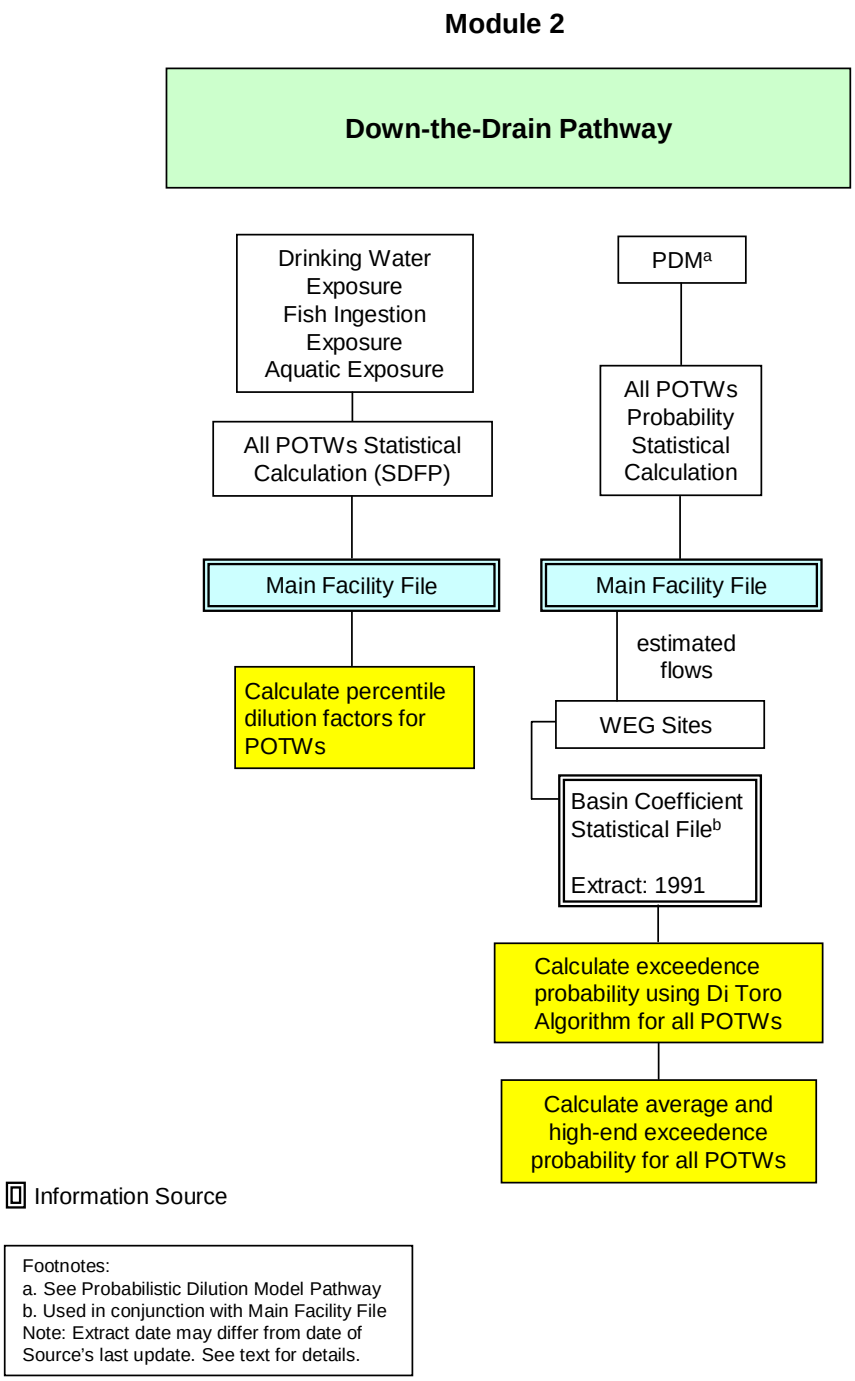

Figure 3-1
Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2)
Down-the-Drain Pathway
(Surface Water Discharge Information Organization and Sources)

3.0 DOWN-THE-DRAIN PATHWAY

3.1 Background

The Down-the-Drain Pathway is a screening level model for estimating concentrations of chemicals in surface waters that may result from the disposal of consumer products into household wastewater. The model assumes that household wastewater undergoes treatment at a local wastewater treatment facility and that treated effluent is subsequently discharged into surface waters. The model provides estimates of aquatic exposure and human exposure from ingestion of drinking water and fish that may become contaminated by these household wastewater releases. In addition, a user may select PDM to estimate the number of days per year that the concentration of a chemical in surface water exceeds the level of concern for aquatic life. The Down-the-Drain model was originally developed for EPA in 1989 as the software program entitled FLUSH. Revisions were made in 1991 and 1992.

Chemical constituents of some household products (e.g., detergents) are expected to end up in household wastewater. Chemical constituents of other household products are not likely to enter wastewater (e.g., fragrance in an air freshener). The physical-chemical properties and the functional role of the chemical in a product should always be evaluated prior to implementing Down-the-Drain because these properties could preclude the presence of the chemical in household wastewater.

Based on user-specified annual production volume (mass of chemical produced annually or discharged annually to wastewater by consumers) and the U.S. population, Down-the-Drain estimates the total daily per capita release of a chemical in household wastewater. The household daily release and stream dilution factors, along with the user-specified wastewater treatment efficiency, are then used to calculate a screening-level estimate of the time-averaged surface water concentration (high-end and median) of a chemical substance released by a wastewater treatment facility receiving household wastewater (assuming all wastewater entering a treatment facility is from residential sources). Surface water concentrations are estimated under four receiving stream flow conditions (1Q10 low flow, 7Q10 low flow, 30Q5 low flow, and harmonic mean flow) as described below, using the mean stream dilution factors for all wastewater treatment facilities based on 10th and 50th percentile values.

Surface water concentrations are estimated in rivers and streams under the four receiving stream flow conditions as recommended in the *Technical Support Document for Water Quality-*

based Toxics Control (U.S. EPA, 1991). Harmonic mean flows are used to generate estimates of chronic human exposure via drinking water and fish ingestion. EPA defines the harmonic mean flow as the inverse mean of reciprocal daily arithmetic mean flow values. EPA recommends using the long-term harmonic mean to assess potential human health impacts because it provides a more conservative estimate then the arithmetic mean flow. The 30Q5 flows (lowest consecutive 30-day flow during any five-year period) are used to generate estimates of acute human exposure via drinking water. To estimate potential acute and chronic aquatic life impacts, the model uses 1Q10 and 7Q10 flows, which are the lowest 1-day and the lowest consecutive 7-day average flows during any 10-year period, respectively. The stream data used are estimated flows at the downstream end of specific stream segments (reaches), and presumably include the discharge flow from any facility on that reach. Stream flows used in Down-the-Drain are corrected in the same manner as those in the GPE pathway (See Section 2.1).

Down-the-Drain incorporates PDM to predict the number of days a COC will be exceeded due to the discharge from a POTW. A simple mass balance approach forms the basis of PDM; however, the input variables are not single point estimates. Streams follow a highly variable seasonal flow pattern and numerous variables affect the chemical concentration and flow rate of the effluent. PDM uses probability distributions as inputs and calculates the resulting probability distribution of the concentration in the stream. Additional information on PDM is available in Section 4.0 of this report. The version of PDM in Down-the-Drain uses a typical per capita release (instead of discharge loading) to generate POTW loadings by multiplying estimates of population served by estimates of per capita household releases. Not all of the POTWs listed in the Main Facility File have the population and stream flow values required for this version of PDM, so the subset of 8,304 facilities with both values serves as the data source.

As seen in Figure 3-1, Down-the-Drain has two analyses available to the user: (1) estimating the surface water concentrations (SDFP) and (2) estimating the number of days a chemical concentration exceeds a COC (PDM). Revisions to both of these analyses were recently completed and are described in the following section. The data sources used in Down-the-Drain are described in Section 3.2.

3.1.1 Revisions to Down-the-Drain

EPA revised Down-the-Drain to utilize the most current readily available and accurate facility and receiving stream information that would be consistent with data used throughout all pathways of E-FAST2. This data is contained within the E-FAST2 Main Facility File. In addition, a change in the approach used for statistical calculations has been made. The improved

method of statistical calculations and use of the E-FAST2 Main Facility File ensures that future updates of Down-the-Drain can be made efficiently and cost-effectively.

In the original E-FAST Down-the-Drain, IFD served as the major source of POTW information in estimating surface water concentrations. However, IFD, which was created in 1978 specifically to provide OW with a comprehensive database of industrial dischargers, is an outdated database and is no longer supported by EPA. The E-FAST2 Down-the-Drain uses the most current information for POTWs that is readily available from the E-FAST2 Main Facility File. Updated information for direct dischargers was compiled as part of EAB's new chemical reviews. These data, obtained from a variety of information sources as shown in Figure 2-1 and discussed in Section 2.2 of the GPE Pathway, are included in the E-FAST2 Main Facility File. Only information for POTWs are used in Down-the-Drain. In addition, retrieval of receiving stream data, calculation of dilution factors, and ranking of the flow data and dilutions are all now conducted within Down-the-Drain in E-FAST2. The same methodology employed in the original SDFP is used.

The POTW information and method of statistical calculations used in the probability calculations (PDM) in Down-the-Drain has also been revised in E-FAST2. POTW information and basic receiving stream information are now obtained from the E-FAST2 Main Facility File. One additional file (the Basin Coefficient Statistical File) is used in conjunction with the E-FAST2 Main Facility File. Direct calculation of exceedence probability is conducted as described in Section 4.0 of this report.

3.2 Data Sources in Down-The-Drain

In estimating surface water concentrations (SDFP) and the probability of exceeding concentrations of concern (PDM), Down-the-Drain uses facility and basic receiving stream information from the E-FAST2 Main Facility File, SDFP, and the Basin Coefficient Statistical File. Figure 3-1 presents an overview of the surface water discharge information organization and sources for the E-FAST2 Down-the-Drain Pathway. The basic program methodology used in the statistical calculations are highlighted.

3.2.1 E-FAST2 Main Facility File

The E-FAST2 Main Facility File contains facility information and basic receiving stream information for over 27,000 direct discharging facilities. The file was created in 2002 by

extracting various information from six water-related information systems (PCS, Task 73 Report, IFD File, Gage File, Reach File, Needs Survey), as well as supplemental information (Supplemental File). Three of these systems are no longer being supported by EPA. However, some data elements in these systems are still valid. The file is used by all three surface water modules (GPE, Down-the-Drain, PDM) of E-FAST2. Separate files of facility and basic receiving stream information are no longer used for each module and when the Main Facility File is updated, all of the surface water modules will be automatically updated. More information on the data sources used to create the E-FAST2 Main Facility File is available in Section 2.2 of this report.

The per capita household wastewater volume (Q_H in units of volume/person/time) was derived from the 1996 Clean Water Needs Survey (CWNS or Needs) data contained in the Main Facility File. Using the same selection method as the original Down-the-Drain module, the following data were selected:

- POTW domestic (residential-source) flows that were less than or equal to total flows
- Resident population served by the POTW.

After correcting for data outliers– those values above the 95th percentile (1,003 liters per capita per day)-- the distribution of Q_H values was calculated, based on data from 12,019 POTWs. The 50th percentile of this data set– 388 L/person/day– was selected as the representative daily per capita wastewater volume (Q_H) released in Down-the-Drain.

3.2.2 Stream Dilution Factor Program

Surface water concentrations are estimated using the 50th and 10th percentile stream dilution factors for streams to which wastewater treatment facilities discharge. The stream dilution factor is equal to the volume of the receiving stream flow under the four flow conditions divided by the volume of the wastewater treatment facility effluent flow. These values are calculated within the Down-the-Drain model for all active POTWs using SDFP.

SDFP was originally developed by the OW to obtain effluent and stream flow frequency distributions for a given industrial category or SIC code(s). SDFP was revised in 1987 to meet the needs of OPPT. Since 1987, the program has been periodically revised to include updated data, new variables, and changes in the program logic. SDFP is designed to: (1) retrieve receiving stream flow data for facilities in a particular industry or SIC code(s); (2) calculate

dilution factors for each facility (receiving stream flow divided by effluent flow); and (3) rank the flow data and dilution factors and report the results in terms of percentiles. In Down-the-Drain, SDFP calculates these values from 9,619 POTWs in the E-FAST2 Main Facility File that have both effluent and stream flow information. This SDFP use is consistent with the use of SDFP for SIC categories in the GPE module (see Section 2.1.2).

3.2.3 Basin Coefficient File

The USGS has divided the U.S. into 18 hydrological river basins or watersheds, subdivided into 204 sub-basins. The flow behavior of streams within each sub-basin is unique, and requires statistical coefficients of variation specific to each sub-basin. The Basin Coefficient File contains coefficients that allow stream flow variation to be calculated for a given sub-basin, mean stream flow, and low (7Q10) flow.

The basin coefficients were derived from measured coefficients of variation, estimated (WEG) mean flow, and low (7Q10) receiving stream flow, obtained from the Gage File in 1991. Data were analyzed by basin and sub-basin, identified by the first four digits of the 11-digit reach number of a POTW's receiving stream. Coefficients of variation for the stream flows were then calculated for each basin/sub-basin using regression analyses. The coefficients are then used in the probability calculations to account for the flow variability that may occur in a particular stream when estimated flows are used.

Module 4

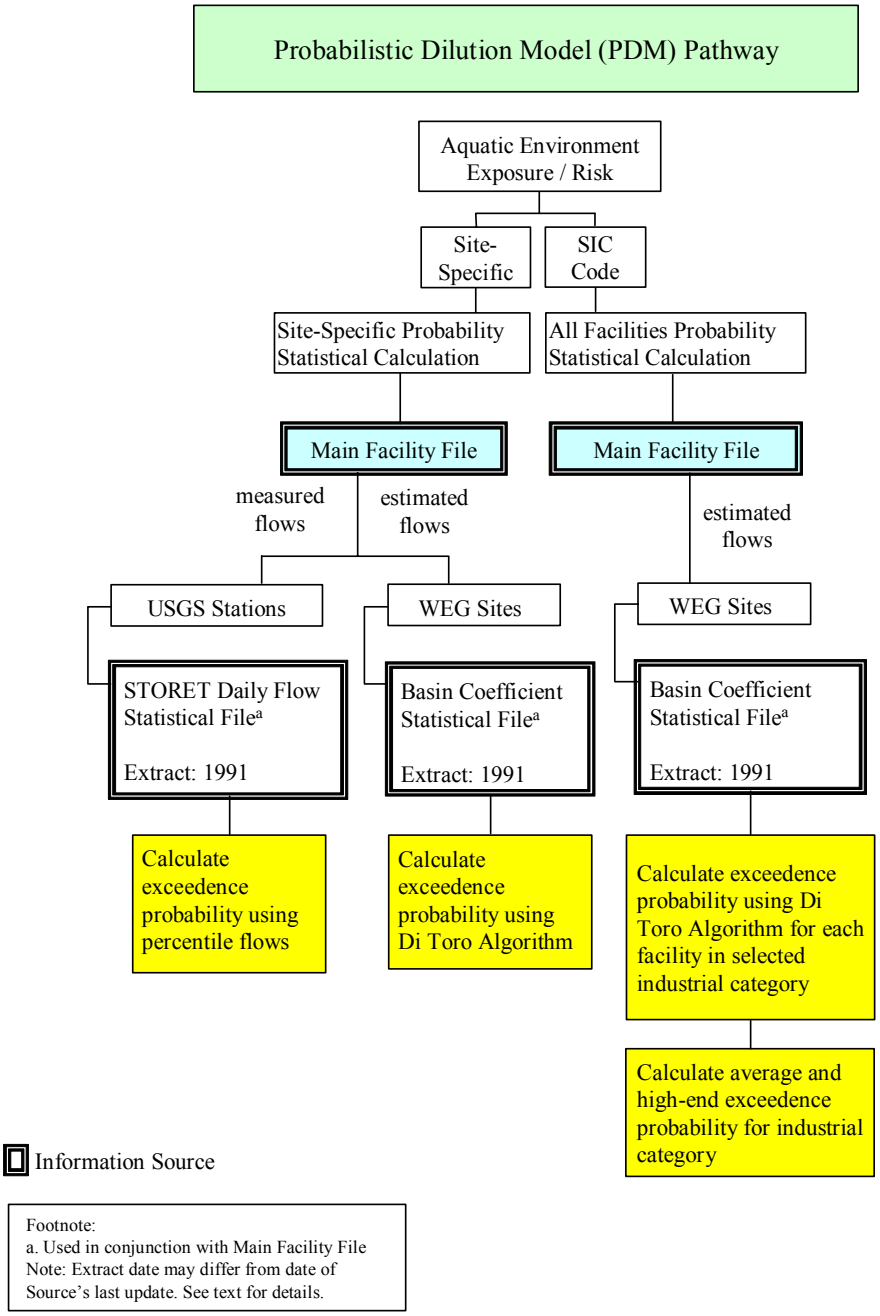

Figure 4-1
Exposure and Fate Assessment Screening Tool, Version 2.0 (E-FAST2)
Probabilistic Dilution Model (PDM) Pathway
(Surface Water Discharge Information Organization and Sources)

4.0 PROBABILISTIC DILUTION MODEL (PDM) PATHWAY

4.1 Background

The Probabilistic Dilution Model (PDM) is used for predicting downstream chemical concentrations from an industrial discharge. It calculates the probability that a given target stream concentration will be exceeded, and the number of days per year the exceedence condition will exist. PDM was originally developed for EPA in 1986 with revisions made in 1987,1988 (Versar, 1988), and 1991. PDM was included as part of the original E-FAST in 1999 and was revised for E-FAST2. A simple mass balance approach forms the basis of the model; however, the input variables are not single point estimates. In reality, these variables are not constant; streams follow a highly variable seasonal flow pattern and numerous variables in a manufacturing process can affect the chemical concentration and flow rate of the effluent. PDM uses probability distributions as inputs and calculates the resulting probability distribution of the concentration in the stream. See Appendix C for an explanation of PDM's statistical framework.

The calculation of probability assumes that receiving stream flow, effluent flow, and effluent concentration are log-normally distributed. The statistics involve both the arithmetic and logarithmic forms of the mean and coefficient of variation (i.e., standard deviation/mean) for the flow and concentration of both the stream and the effluent. PDM utilizes default values for the coefficients of variation for effluent flow and concentration from EPA's Technical Guidance Manual for Performing Waste Load Allocations, Book VII: Permit Averaging Periods (U.S. EPA, 1984). PDM can predict frequency of exceedence of the concern concentration in streams that have a record of flow data from gaging stations as well as in streams without gaging stations. As seen in Figure 4-1, PDM has two options available for performing analyses, depending on the data available. The first option addresses site-specific cases. The second option allows for a high-end or average-case analysis of potential exceedence for an unspecified facility in an industrial category or specific SIC Code(s). This option serves as a screening level analysis to assess the impacts of potentially thousands of facilities in a given SIC Code. The following sections briefly describe the two options, as well as revisions to PDM.

4.1.1 Site-Specific Option

The Site-Specific Option is selected when the NPDES number of the discharging facility is known. PDM locates the facility in the E-FAST2 Main Facility File and then determines whether the associated receiving stream has measured (USGS gaging station), estimated (W.E.

Gates and Associates), or no flow data. Upon entering the number of release days, loading (i.e., mass of chemical discharged per day), and a COC for the protection of aquatic life, the model determines the frequency (i.e., number of days per year) that the receiving stream's concentration will exceed the concern level.

For reaches with gaging stations, daily flow data from the STORET Daily Flow Statistical File are ranked and flows representing the 1st to 100th percentiles (in 1 percentile increments; N=100) are selected for each station (if a gaging station has less than 100 daily flow values, percentiles are not calculated). PDM reports the station ID number, number of observations, period of record, 50th and 10th percentile flows, and the number of stations on each receiving reach. The concentration for each percentile flow is calculated by dividing the loading rate by the percentile flow. The COC is then compared with the 100 calculated concentrations and the highest percentile flow that yields a concentration greater than the COC is selected. The percent of year, as well as the days per year, the COC is exceeded are calculated based on the selected percentile.

For reaches without gaging stations, PDM calculates the exceedence probability using a stochastic procedure developed by Di Toro (1984). This approach requires the means and coefficients of variation of stream flow, effluent flow, and effluent concentration as input. Mean stream flow and mean effluent flow are provided by the E-FAST2 Main Facility File. The stream flow coefficient of variation is estimated using the mean stream flow, low stream flow (7Q10, also available in the E-FAST2 Main Facility File) and empirically-derived coefficients specific to each subbasin that are available in the Basin Coefficient Statistical File. The coefficients of variation of effluent flow and concentration are assumed to be 0.24 and 0.85, respectively (U.S. EPA, 1984). Following entry of chemical loading and the COC, the probability of exceedence is calculated by PDM using the Di Toro algorithm.

4.1.2 SIC Code Option

The SIC Code Option is selected when the location (i.e., facility and receiving stream) of a chemical loading is unknown and only the representative industrial category is known. This option uses the same calculation as the Site-Specific Option (estimated flows only) except that the calculations are performed for numerous facilities to calculate an average-case or high-end probability of exceedence in an industrial category. This analysis represents the average and high-end 10% exceedence probability of facilities for the industrial category, COC, and loading rate.

4.1.3 Revisions to PDM

EPA revised PDM to utilize an approach that would be more transparent and flexible. Such an approach uses the most current readily available data and is consistent with data used in the other pathways of E-FAST2 (GPE and Down-the-Drain). The approach developed ensures that future updates of PDM can be made efficiently and cost-effectively.

As described in the above sections, PDM has two options for performing an analysis: site-specific and generic (SIC Code). The most current information for direct dischargers was compiled as part of EAB's new chemical reviews and are contained within the E-FAST2 Main Facility File. These data were obtained from a variety of sources as discussed in Section 2.2 of this report and were updated into the Site-Specific Option of the original E-FAST PDM Model in April 2002.

IFD (extract 1991) served as the major source of facility information in the SIC Code Option of the original E-FAST PDM. However, IFD is an outdated database (i.e., many of the facilities once "active" are now "inactive"; new "active" facilities are not included). Data for indirect facilities is outdated and represents only a small fraction of the industrial plants that discharge to POTWs. In addition, IFD is no longer supported by EPA. The SIC Code Option of the E-FAST2 PDM now uses the most current direct facility information that is readily available from the E-FAST2 Main Facility File. Data for the industrialized POTW category are now based on a POTWs pretreatment designation in PCS rather than POTWs that receive discharges from indirect facilities in select industrial categories.

The original E-FAST PDM required statistical "matrix files" when calculating probability of exceedence by SIC code. The matrix files were created by performing many thousands of stochastic calculations and storing the results in "look-up" tables. The matrix files were created using facility data from the SIC code groups in 1992 and included both direct and indirect facilities. Although this original method increased the speed of PDM, it required that the matrix files be modified each time an update was made to the SIC code database. Updating the data in the SIC Code Option caused the matrix files to be out of date. Additionally, the data stored within the matrix files had to be interpolated before they were used by PDM. The E-FAST2 PDM performs the probability of exceedence calculations within PDM rather than using a matrix probability/ratio/interpolation method, and makes the use of matrix files obsolete. The internal data structures within E-FAST2 have been updated to accept the revised PDM code.

Another revision to PDM involves how the 7Q10 stream flow is corrected. In some cases, the mean effluent flow from a facility is greater than the estimated 7Q10 flow of the receiving reach. This may be a case where the facility effluent flow is intermittent, and the 7Q10 flow for the reach represents the stream flow at the time of zero or low effluent flow. In E-FAST2, to represent the stream flow in the vicinity of the facility, the greater of the following two flows is used: (1) the effluent flow for the facility of interest or (2) the stream flow (Personal communication from Russell Kinerson, U.S. EPA/Office of Water, to Conrad Flessner, U.S. EPA/OPPT, March 2005).

The PDM portion of the original E-FAST follows this convention and sets the 7Q10 and/or mean stream flows equal to the effluent flow if they are less than the effluent flow. Next, waste-load correction factors are applied and a corrected COC is determined, prior to calculating the exceedence probability. Previously, for the waste-load correction factors, if the 7Q10 flow was greater than the effluent flow, the corrected COC was based on the 7Q10 flow only. Otherwise, the corrected COC was based on the 7Q10 flow plus the effluent flow. However, for those cases where the 7Q10 flow was already set equal to the effluent flow (i.e., if the 7Q10 flow was originally reported as less than the effluent flow, as described above and in Section 2.1), the 7Q10 flow was artificially high, and the corrected COC was essentially based on twice the effluent flow. This second set of stream flow modifications was removed from PDM, such that the corrected COC is based solely on the first modification made to the 7Q10, with no additional flow corrections made in PDM.

4.2 Data Sources in PDM

The input data necessary for PDM include: (1) facility information and estimated receiving stream flow data from the E-FAST2 Main Facility File, values which are also currently used in both the GPE and Down-the-Drain Pathways of E-FAST2, (2) percentile stream flow values (where available), and (3) coefficients of stream flow variations.

4.2.1 E-FAST2 Main Facility File

The E-FAST2 Main Facility File contains facility information and basic receiving stream information for over 27,000 direct discharging facilities. The file was created in 2002 by extracting various information from six water-related information systems (PCS, Task 73 Report, IFD File, Gage File, Reach File, Needs Survey), as well as supplemental information

(Supplemental File). Three of these systems are no longer being supported by EPA. However, some data elements in these systems are still valid. The file is used by all three surface water modules (GPE, Down-the-Drain, PDM) of E-FAST2. Separate files of facility and basic receiving stream information are no longer used for each module—so when the Main Facility File is updated, all of the surface water modules are automatically updated. More information on the data sources used to create the E-FAST2 Main Facility File is available in Section 2.2 of this report.

4.2.2 STORET Daily Flow Statistical File

The STORET Daily Flow System (DFS) serves as the source of daily flow values for the Site-Specific Option in PDM. The STORET Flow File was an automated database that was maintained by OW and was one of the three main information areas of STORET. It contains daily observations of stream flow and miscellaneous water quality parameters collected at gaging stations belonging to the U.S. Geological Survey's National Network. The DFS contains essentially the same information as the USGS Flow Files and serves as an alternative source for the information and simplifies linkages to other, non-USGS water databases. The system contains information for more than 700,000 records, each representing a single water year's worth of information, for over 29,585 gaging sites. USGS supplied new flow data into the file on a biannual basis. The file currently used by PDM contains data up to February 1991. With the modernization of STORET and Y2K, all data owned by USGS has been removed from STORET and is now only available directly from USGS.

Several limitations of the STORET DFS should be noted:

1) Information is out-of-date when compared to other source databases (USGS). Daily stream flow data since 1991 are not included; however, the data collected from 1966 to 1991 are still valid unless significant modifications have been made that affect the stream hydrology.
2) Only 12 percent of the facilities of interest to EAB are located on receiving streams with available daily flow values.
3) STORET DFS is no longer an EPA supported database. The most recent version of DFS used in extracting data for PDM is 1991.

4.2.3 Basin Coefficient File

The USGS has divided the U.S. into 18 hydrological river basins or watersheds, subdivided into 204 sub-basins. The flow behavior of streams within each sub-basin is unique, and requires statistical coefficients of variation specific to each sub-basin. The Basin Coefficient File contains coefficients that allow stream flow of variation to be calculated for a given sub-basin, mean stream flow, and low (7Q10) flow.

The basin coefficients were derived from measured coefficients of variation, estimated (WEG) mean flow, and low (7Q10) receiving stream flow obtained from the Gage File in 1991. Data were analyzed by basin and sub-basin, identified by the first four digits of the 11-digit reach number of a facility's receiving stream. Coefficients of variation for the stream flows were then calculated for each basin/sub-basin using regression analyses. The coefficients are then used in the probability calculations to account for the flow variability that may occur in a particular stream when estimated flows are used.

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Appendix C

Statistical Framework of Probabilistic Dilution Model (PDM)

THE PROBABILISTIC DILUTION MODEL

Introduction

The Probabilistic Dilution Model (PDM) predicts the likelihood that a chemical concentration downstream of a discharger will exceed a target concentration of concern (COC). PDM estimates stream concentration for a given flow condition using a simple dilution model, then predicts the exceedence probability based on the variability of stream or effluent flow. PDM may be applied to a single facility or for all facilities within an industrial category. If the user selects the all facilities option, PDM predicts the exceedence probability for each facility in an industrial category and then reports the 50th and 10th percentile results. The current version of PDM (PDM 4) calculates exceedence probability in a fashion similar to previous versions. However, increases in desktop computer speed allow exceedence probability to be directly calculated for all facilities within an industrial category; previous versions of PDM required a mainframe computer to calculate intermediate matrix files that were stored within PDM for use by desktop computers. This revised approach is both simpler and more accurate than previous versions because it automatically reflects updates to the facility data source, the E-FAST2 Main Facility File (see Appendix B), without the need for the intervening matrix files. The specific approaches employed by PDM for the three options (single facility with actual flows, single facility with estimated flows, and all facilities in an industrial category) are described below.

Case I: Exceedence Probability for a Single Facility with Actual Flows

PDM uses actual flow statistics to calculate the exceedence probability for facilities that discharge to stream reaches containing gaging station data. PDM first calls the E-FAST2 Main Facility File to identify the reach associated with the facility, then searches the database to determine if flow statistics are available for that reach. The database stores 100 percentile daily flows (in 1-percentile increments) for the entire record of each gaging station. PDM then calculates the concentration for each percentile flow as:

$$C_s = L / P(Q_s) \qquad \text{Eq. 1}$$

where C_s is the concentration downstream of the discharging facility, L is loading, and Q_s is the stream discharge rate associated with the percentile, $P()$. PDM then finds the critical percentile flow at which the COC is exceeded, and reports this value as the exceedence probability.

Results are more likely to be accurate by this approach because actual (not estimated) flow data are used. In addition, this method does not assume that stream flow follows a particular stochastic distribution. Unfortunately, actual flow data are available for fewer than 1% of reaches in the United States, so this approach is rarely an option.

Case II: Exceedence Probability for a Single Facility with Estimated Flows

For cases where actual flow data are unavailable, PDM estimates the exceedence probability using the Di Toro (1984) method. The Di Toro approach is based on a simple dilution governing equation:

$$C_s = C_e / (1 + R) \qquad \text{Eq. 2}$$

where C_e is the facility effluent concentration and R is the dilution ratio. This equation may be used to calculate C_s directly if C_e and R are known. However, to be used as a predictive tool, the variability of each of these parameters should be considered. PDM accounts for variability by assigning stochastic distributions to these parameters. PDM assumes that these parameters are lognormal, and can be represented by their logarithmic means (μ_{Ce} and μ_r) and standard deviations (σ_{Ce} and σ_r), respectively. Once these are known, the probability that the stream concentration will exceed the concentration of concern, $P(C_s > COC)$, may be calculated as:

$$P(Cs > COC) = 1 - \int_0^1 Q\left(\frac{\ln(COC_{CORRECTED}) + \ln\left[1 + \exp(\mu_r + \sigma_r Q^{-1}(x))\right] - \mu_{ce}}{\sigma_{ce}}\right) dx \qquad \text{Eq. 3}$$

where $Q(x)$ is the standard normal cumulative distribution function (CDF) and $Q^{-1}(x)$ is the inverse standard normal CDF.

PDM solves Equation 3 using numerical integration (32-point Laguerre quadrature) and polynomial approximations of the normal and inverse-normal CDFs.

The following input parameters are required to run PDM using estimated flows:

- Reach basin and sub-basin, available from the Reach ID in the E-FAST2 Main Facility File;

- Arithmetic mean effluent flow rate, μ_{Qe}, available in the E-FAST2 Main Facility File;
- Arithmetic mean stream flow rate, μ_{Qs}, available in the E-FAST2 Main Facility File (originally derived from the W.E. Gates & Associates study, 1982);
- Arithmetic low stream flow rate, Q_{s_7Q10}, available in the E-FAST2 Main Facility File (originally derived from the W.E. Gates & Associates study, 1982);
- Arithmetic coefficient of variation of effluent flow rate, v_{Qe}, default set to 0.24 (from US EPA, 1984);
- Arithmetic coefficient of variation of effluent concentration, v_{Ce}, default set to 0.85 (from US EPA, 1984);
- Arithmetic daily loading rate, L, provided by the user; and
- Arithmetic concentration of concern, COC, provided by the user.

Several of these parameters require correction factors and transformation before they may be utilized by Equation 3, as outlined below:

Step 1: Modify mean and low stream flow if they are less than mean effluent flow

PDM checks to assure that mean and low stream flow (μ_{Qs} and Q_{s_7Q10}) are equal to or greater than the mean effluent flow (μ_{Qe}). If the low or mean stream flow value is less than μ_{Qe}, the low or mean stream flow value is set equal to μ_{Qe}, respectively (Personal communication from Russell Kinerson, U.S. EPA/Office of Water, to Conrad Flessner, U.S. EPA/OPPT, March 2005).

Step 2: Estimate the coefficient of variation for stream flow

The coefficient of variation for stream flow (v_{Qs}) is determined from an empirical relationship between μ_{Qs}, Q_{s_7Q10}, and two coefficients (a and b) specific to the reach's sub-basin as follows:

$$v_{Qs} = exp\,(a - b\,(Q_{s_7Q10} / \mu_{Qs})) \qquad \text{Eq. 4}$$

These basin coefficients (a and b) were established for each sub-basin in the United States by Versar in 1988, and are currently stored within the source code of PDM. If the sub-basin or basin are unknown, PDM supplies basin- or nation-wide basin coefficients.

Step 3: Apply the waste-load correction factors

PDM employs a normalization scheme using the modified (corrected) 7Q10 from Step 1. The corrected COC is calculated as follows:

$$COC_{CORRECTED} = \frac{COC(Q_{S_7Q10_CORRECTED})}{L} \qquad \text{Eq. 5}$$

Step 4: Calculate the log-transformed means and standard deviations of effluent concentration and dilution ratio

In this final step, the corrected variables are log-transformed to estimate μ_{ce}, σ_{ce}, μ_r, and σ_r as follows:

$$\mu_{ce} = \ln\left(\frac{1 + Q_{S_7Q10_CORRECTED} / \mu_{Qe}}{\sqrt{1 + v_{Ce}^2}}\right) \qquad \text{Eq. 6}$$

$$\sigma_{Ce} = \sqrt{ln(1 + v_{Ce}^2)} \qquad \text{Eq. 7}$$

if ($\mu_{Qs} = \mu_{Qe}$) **then** $$\mu_r = \ln\left(\frac{\mu_{Q_s}}{\mu_{Q_e}}\right) + \ln\left(\sqrt{1 + v_{Q_e}^2}\right) - \ln\left(\sqrt{1 + v_{Q_s}^2}\right) \qquad \text{Eq. 8}$$

else $$\mu_r = \ln\left(\frac{\mu_{Q_s} - \mu_{Q_e}}{\mu_{Q_e}}\right) + \ln\left(\sqrt{1 + v_{Q_e}^2}\right) - \ln\left(\sqrt{1 + v_{Q_s}^2}\right) \qquad \text{Eq. 9}$$

$$\sigma_r = \sqrt{ln\left(1 + v_{Q_s}^2\right) + ln\left(1 + v_{Q_e}^2\right)} \qquad \text{Eq. 10}$$

These parameters may now be used in Equation 3 to calculate exceedence probability.

Case III: Exceedence Probability for an Industrial Category

PDM is often used to estimate exceedence probability for the general case where a chemical is released to multiple facilities in an industrial category rather than a single facility. For this situation, PDM calculates the exceedence probability (using estimated flows) for all facilities in the Main Facilities File that belong to the industrial category of interest. PDM then sorts the results and reports the "average case" (the mean exceedence probability) and "high-end" (the mean of the worst-case 10% exceedence probabilities) of all facilities in the industrial category.

Previous versions of PDM resorted to using matrix files to decrease computation time. This is no longer necessary using a contemporary PC, which can perform these calculations for industrial categories containing 20,000 facilities in 20 seconds or less, depending on the computer.

Converting from Exceedence Probability to Number of Days per Year Exceeded

Strictly speaking, PDM reports the "probability that the downstream concentration will exceed the *COC* on any given day." PDM uses this as a surrogate to estimate the percentage of release days that the COC will be exceeded. For example, if a release occurs 100 days/year, and the probability of exceedence is 30 percent, PDM reports that the COC will be exceeded 30 days (8 percent) of the year.

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Appendix D

Issues Pertaining to Inhalation Exposure Estimation Conducted in CEM

ISSUES PERTAINING TO INHALATION EXPOSURE ESTIMATION CONDUCTED IN CEM

Introduction

This appendix provides further discussion on issues pertaining to the inhalation exposure modeling algorithms used in CEM. The issues covered are not all inclusive, but elaborate on topics discussed in Section 3.3 of the EFAST2 Documentation Manual.

1. Inhalation Modeling Duration

In CEM, air releases are modeled for 60 days, regardless of the scenario. This choice, considered adequate to cover all scenarios, was dictated largely by the "Product Placed in Environment" scenario, which has a default central-tendency duration of use of 30 days. This duration was doubled to ensure that time-integrated concentrations and doses, used in LADC/LADD calculations, would account for the vast majority of the concentration/dose for such an event. Although the default high-end duration of use for this scenario is 90 days, CEM only uses this high-end duration for estimation of short-term exposure measures (ADR and Cp), which generally occur near the beginning of the modeling period. Even in the event that a steady-state condition were reached, such a condition would occur well before 60 days had elapsed. CEM calculates all possible ADRs, over the 60-day modeling period, as running 24-hour integrations (i.e., hours 1-24, 2-25, etc.), and then reports the highest of these computed values as the ADR.

The user should also understand that, for scenarios that use a constant emission rate (i.e., product placed in environment), while the model may run the exposure and concentration algorithms for a 60-day period, there may be instances where the emissions will be truncated at or before 60 days. From Section 3.3.7.2, the evaporation time is defined as a function of molecular weight and vapor pressure. If the evaporation time is less than the 60 days of modeling time, then CEM assumes that the source is no longer emitting after the evaporation time and sets the emission rate to zero at that point. For evaporation times longer than 60 days, CEM assumes that the source has been removed from the environment after 60 days and is no longer emitting.

2. Exposure Events

When estimating exposure dose and concentration, CEM models a single exposure event for the given scenario, over a period of 60 days, and computes the time-integrated concentration and dose for that event. The model results can appear somewhat misleading in situations where exposure events occur more frequently than every 60 days. For instance, in the General Purpose Cleaning scenario, the default exposure frequency is 300 times per year, indicating that an exposure event occurs roughly every 1.2 days. This might lead the user to assume that the exposure is governed by the activity pattern in the Day of Use, plus the first few hours in the Day After Use. However, this type of approach to modeling the exposure would not account for the cumulative release of material newly applied and the material still remaining from previous uses. Figure D-1 depicts the situation where an individual is repeatedly exposed to material that is applied before the material from the previous application has completely evaporated. The dotted line depicts the cumulative concentration or dose that occurs in these situations. It should be apparent that if CEM modeled only the duration from the start of an event to the start of the next event, then the exposure

concentration or dose would be much less than the cumulative amount under the curve (i.e., the solid line corresponding to the first event). CEM, however, models a single release until most, if not all, of the material has evaporated, and takes the product of the time-integrated concentration or dose per event and the number of events in a year to estimate the exposure concentration or dose for the year. The exposure estimated using this technique more accurately accounts for overlapping periods of use and cumulative releases.

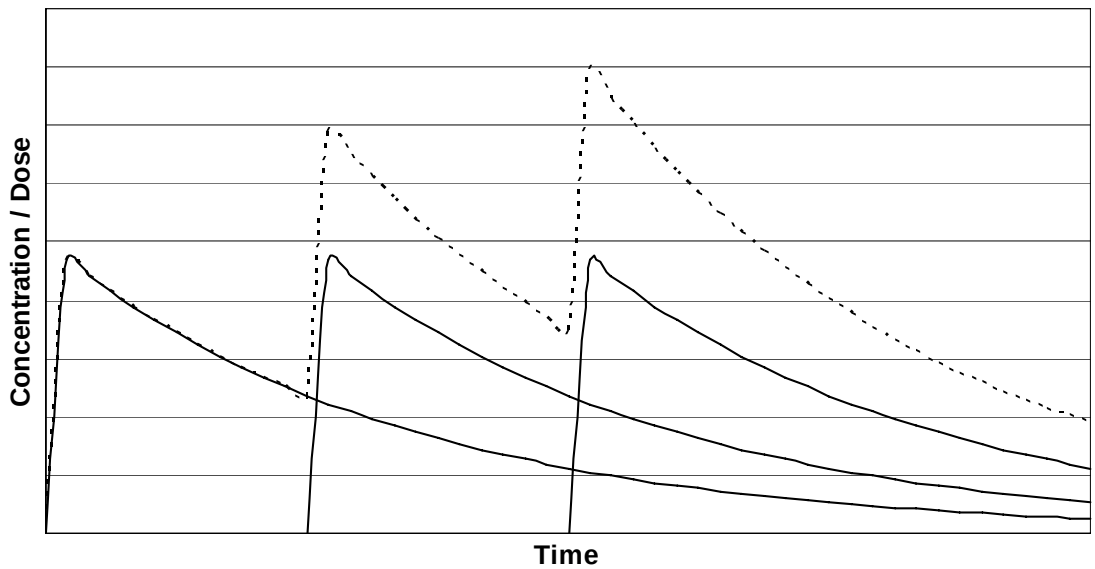

Figure D-1. Exposure of Overlapping Events

It should be noted that this approach, however, will underestimate the ADR and Cp for cases where events overlap and the modeled concentration has not returned to zero prior to the start of the next event. This possibility was recognized in the early days of CEM design, but the chosen approach was considered a reasonable compromise to avoid excessive modeling and source-code complexities.

3. Model Usage of Activity Patterns

In modeling a release over 60 days, CEM uses the Day of Use activity pattern from the exposure event Start Time through midnight of the first day. CEM uses the Day After Use (Non-Use Day) activity pattern for the remaining time. Therefore, Day of Use activity patterns prior to the exposure event Start Time do not factor into the exposure estimate. Additionally, the Day After Use (Non-Use Day) activity pattern plays a fairly significant role in estimating exposure.

It should be noted that CEM is a screening model, and as such has not been designed to accommodate events where the duration of the event continues into the Day After Use (e.g., an exposure duration that lasts 4 hours and begins at 10:00 PM). Users who wish to model such an event are instructed to select a Start Time that allows for the event to be completed during the Day of Use (e.g., move the Start Time of the previously discussed event to 8:00 PM). Otherwise, the model will not function properly.