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Stochastic Human Exposure and Dose Simulation Model for Multimedia, Multipathway Chemicals

SHEDS-Multimedia Model
Version 3
User Guide

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Version 3
User Guide

Casson Stallings[1]
Valerie Zartarian[2]
Graham Glen[1]

[1]Alion Science and Technology, Inc.

[2]US Environmental Protection Agency
National Exposure Research Laboratory

U.S. Environmental Protection Agency
Office of Research and Development
Washington, DC 20460

TABLE OF CONTENTS

LIST OF FIGURES iv
LIST OF TABLES vi
Acknowledgments vii
Display Issues, Disclaimer, and Support viii
ACRONYMS AND ABBREVIATIONS ix
1 Considerations for New Users of SHEDS-Multimedia 1
1.1 Introduction 1
1.2 Entering Distributions 2
1.3 Configuring SHEDS to the Scenarios of Interest 3
2 Overview 5
2.1 Introduction 5
2.2 Using the Demonstration File 6
2.3 General Interface Hints 8
2.3.1 Display Issues 8
2.3.2 Grayed Out Buttons or Widgets 8
2.3.3 Entering Probability Vectors 8
2.3.4 Distributions Supported 11
2.3.5 Entering Distributions 11
2.3.5.1 Individual Distribution Widgets 11
3 Installation 13
3.1 Requirements 13
3.2 Installation under MS Windows 13
3.2.1 Starting With a CD 13
3.2.2 Starting with a Downloaded File 13
3.2.3 The Standard Installation Process 14
3.2.4 Starting the Model Interface 16
3.2.5 Removing SHEDS-Multimedia 16
4 The SAS User Interface 18
4.1 The SAS Screen 18
5 SHEDS-Multimedia: The Graphical User Interface 21
5.1 SHEDS-Multimedia Main Interface Screen 21
5.2 Specify Run Name and Files 22
5.2.1 Specify Run Name Dialog 22
5.2.1.1 Edit Selected Run 23
5.2.1.2 Copy Selected Run To New Run 23
5.2.1.3 Create a New Run 24
5.2.1.4 View Results of Selected Run 24
5.2.1.5 Delete Selected Run 24
5.2.2 New Run Name Dialog 24
5.2.3 Specify Files Dialog 25

5.3 Specify Population and Sampling 25
5.4 Specify Simulation Information 27
5.4.1 Simulation Length 27
5.4.2 Source-To-Concentration Approach and Application Dates 27
5.4.3 Dermal Exposure Method 28
5.4.4 Soil Ingestion Approach 28
5.4.5 Exposure-To-Dose Method 28
5.4.6 Maximum Diary Event Length 28
5.4.7 Keep Intermediate Variables 28
5.4.8 Save the Log File 29
5.5 Specify Application Scenarios Simulated 31
5.5.1 Specify Exposure Scenarios 31
5.5.2 Specify Exposure Scenario Details 33
5.5.3 Specify Application Dates: Model Determined 34
5.5.4 Specify Application Dates: User Specified 36
5.5.5 Specify Co-Occurrence 36
Specify Application Times 38
5.5.6 Specify Re-entry Times 39
5.6 Specify Concentration-Related Inputs 39
5.6.1 Specify Decay and Dispersion Distributions 40
5.6.2 Specify Decay and Dispersion Distributions: Background 41
5.6.3 Specify Post-Application Distributions 42
5.6.4 Specify Post-Application Distributions: Background 43
5.6.5 Specify Time Series Inputs 44
5.6.5.1 Time Series File Format 44
5.7 Specify General Exposure and Dose Factors 45
5.7.1 Variability Distributions 46
5.7.2 Edit Variability Distributions 47
5.7.3 Correlating Input Variables 50
5.7.3.1 Select Correlated Variables 51
5.7.3.2 Specify Variable Correlations 52
5.7.3.3 Contact Probabilities 54
5.7.3.4 Edit Contact Probabilities 56
5.8 Run Simulation 57
5.9 View Results 59
5.9.1 Additional Outputs and Files 60
5.9.2 View Results for the Population 60
5.9.2.1 Summary Table 63
5.9.2.2 CDF 63
5.9.2.3 Box and Whiskers 65
5.9.2.4 Contribution by Pathway 66
5.9.3 View Results for an Individual 69
5.9.3.1 Time-Series 71
5.9.3.2 CDF 71

5.9.3.3 Box and Whiskers ... 71
5.9.3.4 Contribution by Pathway ... 72
5.9.3.5 Summary Table ... 72
5.9.3.6 Detailed Table ... 72
5.9.4 View Diary Pool Sizes ... 73
6 SHEDS-Multimedia: Batch Mode ... 74
6.1 Installing Batch Capability ... 74
6.2 Defining Inputs for a Batch Run ... 74
6.3 Submitting a Batch Run ... 75
6.4 Uncertainty Runs ... 76
6.5 Sensitivity Runs ... 77
Appendix A. Directories and Files ... A-1
A.1 Directories ... A-1
A.2 Critical Input Files ... A-1
A.3 User Specified Output Files ... A-2
A.4 Other Output Files ... A-2
A.4.1 Diary Related Output Files ... A-2
A.5 Exporting SAS Datasets ... A-3
A.6 Moving Run Files ... A-3
A.6.1 Background on the RunInfo Dataset ... A-3
A.6.2 Moving the Run Directory ... A-3
A.6.3 Integrating the Old and New RunInfo Records ... A-4
A.6.4 Replacing the RunInfo File (Dataset) ... A-4
A.6.4.1 Integrating Records into the New RunInfo File ... A-4
A.6.5 Running the %RunInfoAddDirs Macro ... A-4
A.6.6 Moving a Run: An Example ... A-4
Appendix B. Reference Tables ... B-1
B.1 Variable Names ... B-1
B.2 Media Descriptions ... B-2
Appendix C. Probability Density Functions ... C-1
C.1 Beta ... C-1
C.2 Exponential ... C-1
C.3 Gamma ... C-1
C.4 Lognormal ... C-2
C.5 Normal ... C-2
C.6 Point ... C-3
C.7 Triangular ... C-3
C.8 Uniform ... C-3
C.9 Weibull ... C-3
C.10 Discrete Probability Density Functions ... C-4

LIST OF FIGURES

Figure 2-1. Overview of the SHEDS Multimedia Interface at Version 3. 7
Figure 2-2. Sample of Two Buttons, One Normal and One Grayed Out (Bottom). 8
Figure 2-3. Example of List Box with a Blue Background Indicating There are More Groups to Complete. 8
Figure 2-4. Specify Re-entry Times Screen Containing Two Probability Vectors. 9
Figure 2-5. Example Distribution Widget. 12
Figure 3-1. Setup Screens: Initial Screen. 14
Figure 3-2. Setup Screens: Welcome and Information Screen. 14
Figure 3-3. Setup Screens: Installation. Directory Screen. 15
Figure 3-4. Setup Screens: Shortcut Folder Name. 15
Figure 3-5. Setup Screens: Confirmation Screen. 16
Figure 3-6. Setup Screens: Completion Confirmation. 16
Figure 4-1. The Main Model GUI Interface Screen in the SAS Window on Startup. 19
Figure 4-2. The SAS Menu Bar and the View Menu. 20
Figure 4-3. The SAS Results Window. 20
Figure 4-4. The SAS Explorer Window. 20
Figure 5-1. SHEDS Multimedia Main Screen. 21
Figure 5-2. Specify Run Name Screen. 23
Figure 5-3. Confirm Delete dialog. 24
Figure 5-4. Enter New Run Name screen. 24
Figure 5-5. Specify Files Screen. 25
Figure 5-6. Specify Population and Sampling Screen. 26
Figure 5-7. Specify Simulation Information Screen. 30
Figure 5-8. Specify Exposure Scenarios Screen. 32
Figure 5-9. Specify Exposure Scenario Details Screen. 34
Figure 5-10. Specify Application Dates: Model Determined Screen. 35
Figure 5-11. Specify Application Dates: User Specifed Screen. 36
Figure 5-12. Specify Co-Occurrence Screen. 37
Figure 5-13. Specify Application Times Screen. 38
Figure 5-14. Specify Re-entry Times Screen. 39
Figure 5-15. Specify Decay and Dispersion Distributions. 41
Figure 5-16. Specify Decay and Dispersion Distributions: Background Screen. 42
Figure 5-17. Specify Post-Application Distributions Screen. 43
Figure 5-18. Specify Time Series Inputs Screen. 45
Figure 5-19. Variability Distributions Screen. 46
Figure 5-20. An example of the Edit Variability Distributions Screen. 49
Figure 5-21. Variable with Two Conditions shown. 50
Figure 5-22. Select Correlated Variables Screen. 52
Figure 5-23. Error Displayed if Zero or One Variables are Selected for Correlation. 52
Figure 5-24. Error Displayed if No Variable Pairs are Selected for Correlation. 52
Figure 5-25. Specify Variable Correlations Screen. 54
Figure 5-26. Contact Probabilities Screen. 56

Figure 5-27. Run Simulation Screen. 57
Figure 5-28. Log Screen after Running a Small Simulation. 59
Figure 5-29. View Results Screen. 60
Figure 5-30. View Results for the Population Screen. 62
Figure 5-31. Example Summary Table for a Population. 63
Figure 5-32. Example CDF for a Population. 64
Figure 5-33. Example Population Box and Whiskers Plot. 66
Figure 5-34. Example Pie Chart Showing the Contribution by Pathway for a Population. 68
Figure 5-35. View Results for an Individual Screen. 70
Figure 5-36. Example Time-Series for an Individual. 71
Figure 5-37. Example Pie Chart Showing the contribution by pathway for an individual. 72
Figure 5-38. Example Detailed Table for an Individual. 73
Figure 5-39. Example Diary Pool Size Table. 73

LIST OF TABLES

Table 2-1. Probability Vector Errors Encountered 10
Table 2-2. Supported Variable Distributions 11
Table 5-1. Output Variable Group and Dose/Exposure Terminology Differences..... 62
Table B-1. Variable Names From Distributions File B-1
Table B-2. Media Descriptions And Symbols B-2

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Display Issues, Disclaimer, and Support

Display Issues
It is strongly advised that the SHEDS user maximize windows so that as much as possible of the full dialog is displayed. You may still need to scroll down to see all of some dialogs. Refer to the images in this User Guide to ensure that all components of a dialog are displayed.

Disclaimer
This is SHEDS-Multimedia version 3.15, an aggregate residential version of the EPA's Stochastic Human Exposure and Dose Simulation model for multimedia, multipathway pollutants that includes the inhalation, dermal, hand-to-mouth, object-to-mouth pathways and a graphical user interface. This version also includes a sample database with *hypothetical* inputs for test and demonstration purposes. All input parameters used in the SHEDS-Multimedia model must be determined independently by the researcher and substantiated by references so that the model results can be evaluated based on the validity of the data sources.

The United States Environmental Protection Agency, through its Office of Research and Development, developed and funded the aggregate residential SHEDS-Multimedia version 3.15 model with assistance from contractor Alion Science and Technology. This model has been subjected to Agency and external peer review. Work is underway for development of SHEDS-Multimedia version 4, which will extend the aggregate (single chemical) algorithms to cumulative (multi-chemical), incorporate a dietary (food and drinking water pathway) model, include a case study, and add help screens and other enhancements.

Support
Please contact one of the following individuals with any questions, comments, or specific suggestions related to this beta version of the SHEDS model:

Dr. Valerie Zartarian, (617) 918-1541, zartarian.valerie@epa.gov
Dr. Jianping Xue, (919) 541-7962, xue.jianping@epa.gov

ACRONYMS AND ABBREVIATIONS

CDFs – cumulative distribution functions
CHAD – Consolidated Human Activity Database
EPA – United States Environmental Protection Agency
GI – gastrointestinal
GM – geometric mean
GSD – geometric standard deviation
GUI – graphical user interface
NERL – National Exposure Research Laboratory
ORD –Office of Research and Development
PBPK – Physically-based pharmacokinetic
PDFs – probability density functions
SHEDS – Stochastic Human Exposure and Dose Simulation
ug (in SAS printout or variable names) – microgram

1 Considerations for New Users of SHEDS-Multimedia

1.1 Introduction

SHEDS-Multimedia version 3 (also referred to as 'SHEDS') is a sophisticated but user-friendly aggregate human exposure model for chemicals contacted in a residential setting. It requires the user to select appropriate inputs and to interpret the resulting outputs. Users should therefore be prepared to invest time to configure this model to exposure scenario(s) of their choice. Before attempting to run the model, it is recommended that new users review this User Guide and the Technical Manual to familiarize themselves with the model and the types of information that will be required.

The SHEDS installation package includes the User Guide, Technical Manual, annotated SAS code for use via the graphical user interface (GUI), Consolidated Human Activity Database (CHAD) activity diary and population files, a height/weight data set, and default input distributions. The installation process is explained in this User Guide, which is intended to guide the user through the GUI. The interface has three functions: specifying inputs, executing the model, and storing and viewing the results. The Technical Manual contains a detailed description of the model's structure and algorithms.

The SHEDS model runs on a personal computer and requires that SAS 9.1 or higher be installed prior to the installation of SHEDS. It has been run successfully on various laptops and desktops using Windows XP. It has not yet been tested with Windows Vista. Though hardware requirements are modest, a full-scale model run may take a substantial amount of time. As a rough guide, a variability-only (1-stage Monte Carlo) run takes about 1 hour for every 1000 persons being simulated and a typical run may be several thousand persons. Uncertainty (2-stage Monte Carlo) runs are much slower and may take several days to complete.

SHEDS is a stochastic model in which each simulated individual is different. There are approximately 100 variables that are sampled randomly for each person; many of these variables require multiple samples per person as they change over time throughout the simulation period. Increasing the number of simulated individuals provides a better characterization of the population under study. SHEDS version 3 uses new random number seeds each time the model is run. This has one main benefit and one main drawback. The benefit is that results may be combined across runs with the same input settings: for example, two runs of 5000 persons each (with the same input settings) are equivalent to a single run of 10,000 persons and the outputs from the shorter runs could be directly combined. The drawback is that model runs are not reproducible. (The option to reproduce an earlier run exactly is planned for version 4.)

SHEDS separately constructs time series for the environmental concentrations in each simulated person's house, as well as an activity sequence through time based on the selection of human activity diaries from EPA's Consolidated Human Activity Database (CHAD;

http://www.epa.gov/chadnet1). These are combined, using exposure pathway-specific equations and exposure factors sampled from user-specified distributions, to generate a time series of exposure for each simulated individual. The time step is variable and depends on the event duration from the activity diaries, ranging from one minute to one hour. Therefore, a 1-year simulation will have a very large number of such events (generally 10,000 to 20,000) for each simulated person. These results are automatically aggregated over time to produce (for example) daily exposure totals, although for some purposes the finer time resolution may be useful. Due to their size, the event-level exposure time series are not usually saved as permanent output; as a rule only summary statistics on daily and longer periods are saved.

SHEDS does not attempt to model the exposures of particular individuals. Instead it randomly creates a population of simulated individuals who collectively represent the target population. Thus, an appropriate result of a model run might be the statement 'SHEDS indicates that 5% of the target population receives an exposure in excess of …', but it is not appropriate to say that a specific real-world individual receives any particular exposure.

SHEDS has a graphical user interface (GUI) that guides the user through the various input screens. The GUI comes with a demonstration scenario. It may be useful to copy this under a new name and to make changes to this copy. This is described in more detail later in this manual.

SHEDS version 3 allows only one chemical per model run, although the chemical can effectively be changed by altering appropriate inputs. The user may select several product categories (each containing the same chemical) to be analyzed together in the same run. The model permits the use of co-occurrence factors that control the likelihood of the various products being used together. The human exposure results are automatically aggregated across the products used in the given model run.

1.2 Entering Distributions

Many SHEDS inputs are randomly sampled from user-specified distributions. SHEDS accepts a wide variety of continuous distributions as detailed in Appendix C. Some inputs require probability vectors (see the Appendix and section 4.1.1 of the Technical Manual). For continuous distributions, the user selects the type from a pull-down menu and then specifies the desired parameters. For discrete distributions (probability vectors) the user enters the probability of each outcome.

The GUI will highlight invalid choices with a yellow background. This usually results from numeric parameters being specified that are incompatible with the type of distribution. For example, the lognormal distribution requires a geometric mean greater than zero and a geometric standard deviation greater than one. A missing numeric parameter will also result in the yellow error indicator. For probability vectors, the sum of the probabilities must be one or else an error will be indicated.

The user has the option of truncating distributions at one or both ends by specifying minimum and/or maximum values. If the random number generation produces values outside these limits then the values are automatically reset to the maximum or minimum, depending on which was exceeded.

1.3 Configuring SHEDS to the Scenarios of Interest

The user has the ability and the responsibility to configure SHEDS to a particular scenario(s) of interest. This includes specifying the target population, the simulation period, the chemical and application method(s) of interest, and the distributions for many model parameters. As an example, SHEDS supports three methods of determining the chemical concentrations: user-supplied time series, a decay/dispersion model based on chemical application dates, or a post-application decrease based on time intervals. The user must choose which one is most appropriate for the problem at hand. These three methods are described in more detail in the SHEDS Technical Manual.

The SHEDS installation package comes with example input distributions for demonstration purposes, to help orient users in how to run the model. The user is strongly cautioned that these values were not created with any specific scenario in mind and may not be appropriate for a particular chemical or scenario of interest. These values can be used as a starting point for becoming familiar with the GUI, or modified by the user as appropriate.

SHEDS is designed to estimate human exposure in a residential setting, but is not geared to any specific chemical. The user customizes the model run for the chemical of interest by setting appropriate input parameters, for example, product types and usage frequencies, initial application amounts, and concentration decay rates. The model allows the user to select one or more product application methods from a pre-determined list in the GUI (which can be modified in the SAS code).

The SHEDS GUI allows the user to select the gender and age range of the target population. It is worth re-emphasizing that SHEDS is a population-based model. Therefore it would be appropriate for simulating exposure for school-age children in general, for example, but should not be expected to be reliable for simulating a specific child or even a specific set of children. Beyond age and gender, the user may target populations by selecting input distributions that reflect characteristics of those groups. For example, pica children could be simulated by specifying a large soil ingestion rate.

The ‘simulation period’ is the user-specified time over which the exposure is tracked for each simulated individual. The model allows this to range from one day to several years, but the user should be aware of certain considerations. For example, if the user supplies concentration time-series data, then the period is limited to the extent of this data. Note that the model does not change the age of individuals, and therefore simulation periods longer than one year may not be advisable for children. Finally, longer simulations require longer run times.

SHEDS calculates exposure from several different pathways. If desired, the user may restrict the model to selected pathways by judicious specification of inputs. For example, ingestion of chemical via object mouthing can be 'turned off' simply by setting the distribution for object-to-mouth contact frequency to a point value of zero. Similarly, other pathways such as inhalation, hand mouthing, direct soil ingestion, dermal absorption, and GI tract absorption could be eliminated.

There is no facility to supply differing inputs by region within a single run in SHEDS version 3. To model regional variation the user would have to construct a separate model run for each region with distinct input distributions. The distributions for each run would then reflect the variation within the given region (but not across regions). For example, pesticide usage may differ in warm and cold climates. Seasonal variation may be handled in a similar manner. By bypassing the GUI, advanced SAS users have the option of incorporating seasonal variation in distributions within a single model run.

2 Overview

2.1 Introduction

Reliable models for assessing human exposures are important for understanding health risks from chemicals. The Stochastic Human Exposure and Dose Simulation model for multimedia, multiroute/pathway chemicals (SHEDS-Multimedia), developed by EPA's Office of Research and Development (ORD), National Exposure Research Laboratory (NERL), is a state-of-science computer model for improving estimates of aggregate (single-chemical, multi-route/pathway) and cumulative (multi-chemical, multi-route/pathway) human exposure and dose. SHEDS-Multimedia is the EPA/ORD's principal model for simulating human exposures to a variety of multimedia, multipathway environmental chemicals such as pesticides, metals, and persistent bioaccumulative toxins. Exposure is defined in SHEDS-Multimedia as the contact between a chemical agent and a simulated human target at the skin, lung, and gastrointestinal tract exposure surfaces. Dose is defined in SHEDS-Multimedia as the amount of chemical that enters the target after crossing the exposure surfaces.

SHEDS-Multimedia is a physically-based, probabilistic model that predicts, for user-specified population cohorts, exposures incurred via inhaling contaminated air, touching contaminated surface residues, and ingesting residues from hand- or object- to-mouth activities. To do this, it combines information on chemical usage, human activity data (e.g., from time/activity diary surveys and videography studies), environmental residues and concentrations, and exposure factors to generate time series of exposure for simulated individuals. One-stage or two-stage Monte Carlo simulation is used to produce distributions of exposure for various population cohorts (e.g., age/gender groups) that reflect the variability and/or uncertainty in the input variables. While the core of SHEDS-Multimedia is the concentration-to-exposure module, there are various options (built-in source-to-concentration module; user-entered time series from other models or field study measurements) for obtaining concentration inputs, and SHEDS-Multimedia exposure outputs can be used as inputs to physically-based pharmacokinetic (PBPK) models.

For a more detailed technical description of the SHEDS model, please refer to the SHEDS-Multimedia version 3 Technical Manual. The purpose of this User Guide is to assist the SHEDS-Multimedia user in navigating through the graphical user interface to apply SHEDS-Multimedia. Figure 2-1 provides an overview of the SHEDS-Multimedia user interface. The major interface screens are each represented with one box. Not all screens are represented in Figure 2-1. In general, the user will navigate through the interface from left to right and top to bottom as shown on the overview. The exact screens visited will vary depending on the type of run being defined and data required for that run. Typically, the interface will prevent the user from moving ahead unless all data for the current step have been entered.

The user interface guides the user through a set of screens that define the inputs needed for a SHEDS run. When a new run is created, most of these screens contain default choices, or choices from a previous model run, that the user may either edit or accept. The best way to run SHEDS is to carefully prepare the inputs for an initial 'baseline' run; thereafter, one can start

with the baseline run and make a small number of changes from run to run, greatly speeding up the process.

Some sections will need to be revisited a number of times to enter all information. In particular the sections defining application details and dates, and those defining media concentrations will need to be defined for each application or scenario type being simulated. The screens used to enter variability distributions and contact probabilities will need to be revisited for each group of variables being defined.

Every effort has been made to reduce the amount of information entered by the user. For instance, if dermal transfer efficiencies are being used, then the user will not be presented with the opportunity to enter data on dermal transfer coefficients. Likewise, if the decay and dispersion module is being used to model media concentrations, users will only enter information relevant to that and not to time-series or post-application distributions.

2.2 Using the Demonstration File

When installed, SHEDS-Multimedia version 3 comes with a completed sample run. This sample run is named "Demonstration File" and is meant to assist the user in becoming familiar with the interface. The Demonstration File simulates up to four scenarios for each individual. These include a crack and crevice application along with pet, lawn, and garden applications. The simulations last a year for each individual, use decay and dispersion, direct ingestion, transfer coefficients and assume a number of input variables are correlated. The run supplied contains results for 100 people. The user may change this value and re-run the simulation if a different number is desired. A typical production run will require substantially more individuals.

It is very important to note that the default input values defined in the Demonstration File are not meant to represent any specific chemical or situation. They are supplied for demonstration purposes and should not be used for production runs.

The results from the file are available on installation and can be viewed by selecting the View Results of Selected Run button on the Specify Run Name dialog (described on page 22). While the inputs in the Demonstration File are safe when you use the View Results button, changes made after selecting the file with Edit Selected Run will overwrite the original values. It is strongly recommended that the user not edit the original Demonstration File. To view and edit inputs from the demonstration, go to the Specify Run Name dialog (described on page 22), highlight "Demonstration File", and click on Copy Selected Run To New Run. You will be prompted for a new run name. After entering the run name and visiting the Run Files screen you will be free to make any desired changes without affecting the original Demonstration File.

Warning: The data supplied in version 3 of SHEDS-Multimedia is not meant to represent any specific chemical or situation and should be used for demonstration purposes only.

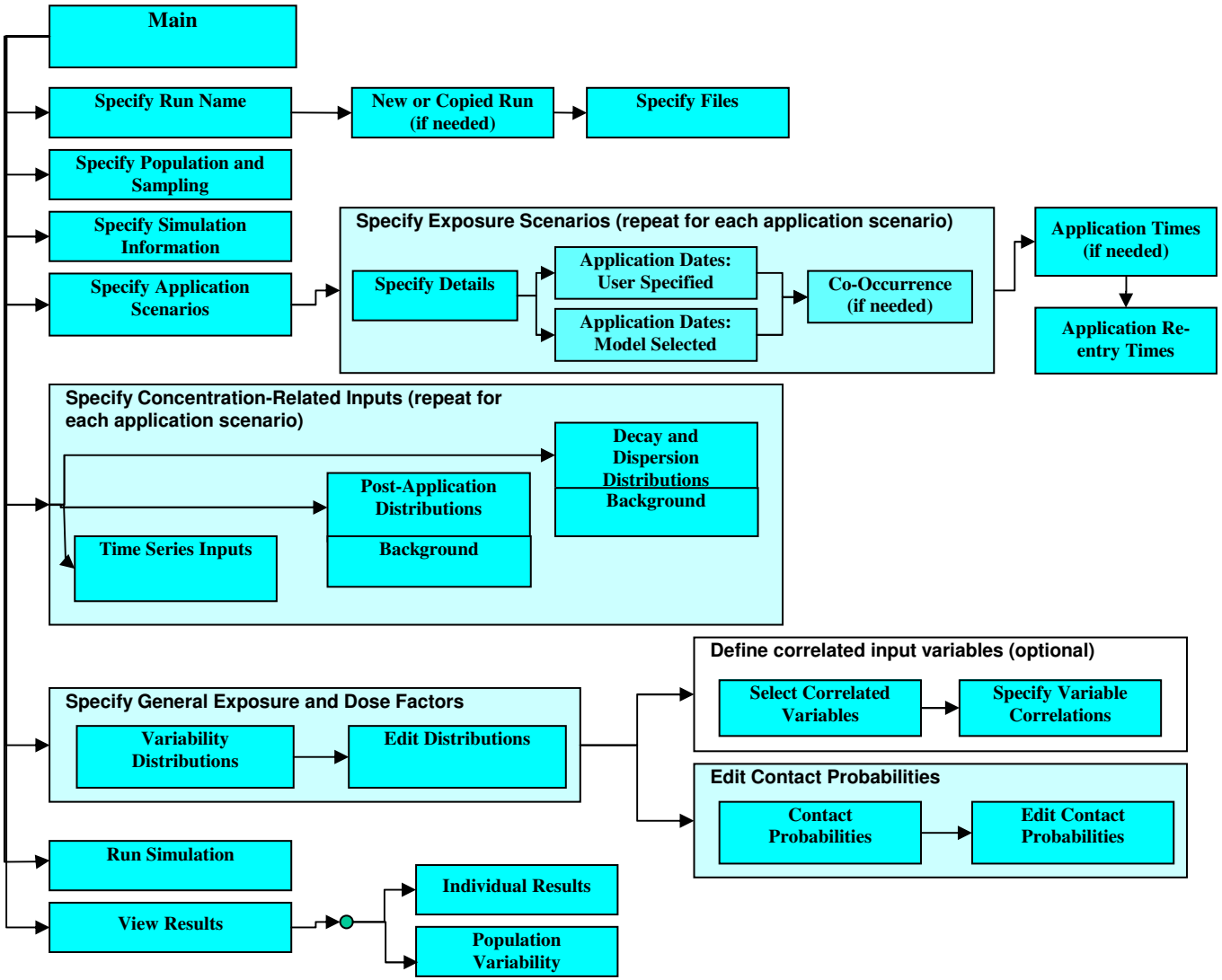


Figure 2-1. Overview of the SHEDS Multimedia Interface at Version 3.

2.3 General Interface Hints

2.3.1 Display Issues

Display issues can arise when SAS does not have room to display the entire dialog. When a screen does not initially draw correctly either the top title text or the bottom left button (Continue, or Return) do not display. If in doubt compare the display to the appropriate figure in this manual. The easiest method of minimizing these issues is to maximize the main SAS window. On smaller monitors some screens may still not display fully. The screen's scroll bars should be used to view the bottom of the screen. Unfortunately, SAS does not always display the scroll bars automatically. Resizing the SHEDS dialog will force SAS to redraw the dialog and include scroll bars if necessary.

2.3.2 Grayed Out Buttons or Widgets

Occasionally buttons will be grayed out (displayed with muted text, see Figure 2-2). This may mean that a function has not been implemented. In version 3 the Help and About buttons have not been implemented.

Figure 2-2. Sample of Two Buttons, One Normal and One Grayed Out (Bottom).

In many cases a grayed out button means that additional steps are required before the user is permitted to enter certain data. This is particularly true on the main screen where data entry must be completed sequentially, by starting at the top button and working down. There are also several screens where the user must complete data entry or editing for each group of variables listed before continuing. In these cases, the groups are listed on the left and all completed groups are listed on the right. If the groups remain uncompleted, the completed list is highlighted in a light blue (Figure 2-3).

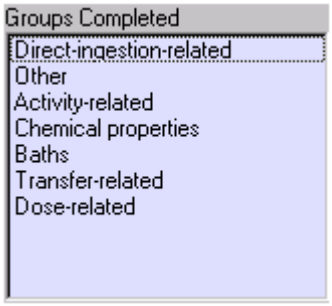


Figure 2-3. Example of List Box with a Blue Background Indicating There are More Groups to Complete.

Another reason a button may be grayed out (Figure 2-2) is due to a current error on the screen. Typically, the user is not allowed to continue or navigate away from a screen when there are data entry errors on the screen. These errors will always be identified by yellow or red highlighting and often accompanied with a more specific error message.

2.3.3 Entering Probability Vectors

There are a number of places in the interface where probability vectors must be entered. These are used to enter probabilities associated with a set of mutually exclusive outcomes. Each uses a similar graphical interface as can be seen on the Specify Re-entry Times screen (Figure 2-4). This

screen contains two probability vectors where the user enters information on how long after a treatment the simulated individual stays out of the treated area. Each probability vector is composed of:

- A container box with a descriptive title. In the case of the top probability vector this title is 'Re-entry Time to Treated Indoor Area (probabilities for hours)';
- A series of labeled text entry boxes. In this case 9 of them. Each is labeled and contains a probability;
- A space below the text entry boxes where error messages may be displayed; and
- An OK button used to validate the entry.

Each text box must contain a probability, thus a number between 0 and 1 inclusive. The total of all probabilities must sum to one. The user can enter values in all but the last box (the one with a bold outline). The last box automatically displays the amount necessary to sum all probabilities in the vector to 1. When an inappropriate value is entered by the user, the background will turn yellow and an error message will be displayed. The probability vector as a whole will be validated, and the sum recalculated every time the user uses the return key or when the OK button is clicked. Examples of possible error messages are shown in Table 2-1. The error messages are not displayed in some contexts. The text boxes are always highlighted in yellow. If there are errors with individual probabilities or with the sum of probabilities, the user will not be allowed to continue to the next screen. The errors must be corrected and the vector validated, or the Cancel button must be used. No values will be saved if the Cancel button is used.

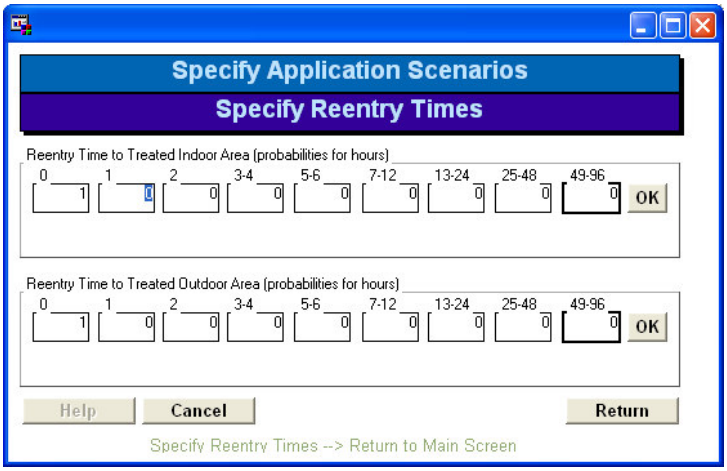


Figure 2-4. Specify Re-entry Times Screen Containing Two Probability Vectors.

Table 2-1. Probability Vector Errors Encountered

Error	Sample Display
The value entered was not a number.	Reentry Time to Treated Indoor Area (probabilities for hours) 0: 1 | 1: 0 | 2: 0 | 3-4: . | 5-6: 0 | 7-12: 0 | 13-24: 0 | 25-48: 0 | 49-96: 0 | OK Invalid Number.
A negative value was entered.	Reentry Time to Treated Indoor Area (probabilities for hours) 0: 1 | 1: 0 | 2: 0 | 3-4: -.1 | 5-6: 0 | 7-12: 0 | 13-24: 0 | 25-48: 0 | 49-96: 0 | OK Invalid Number.
A value outside the range of 0 to 1 was entered.	Reentry Time to Treated Indoor Area (probabilities for hours) 0: 0 | 1: 0 | 2: 0 | 3-4: 1.5 | 5-6: 0 | 7-12: 0 | 13-24: 0 | 25-48: 0 | 49-96: -0.5 | OK Sum of probabilities must be 1.
The sum of all values entered is too large.	Reentry Time to Treated Indoor Area (probabilities for hours) 0: .8 | 1: .1 | 2: .1 | 3-4: .3 | 5-6: 0 | 7-12: 0 | 13-24: 0 | 25-48: 0 | 49-96: -0.3 | OK Sum of probabilities must be 1.

2.3.4 Distributions Supported

Since the SHEDS Multimedia model is a stochastic model, a large number of its input variables are defined by distributions rather than constants. The model supports point values (constants) and 8 distributions. The distributions, parameter names, and rules for the parameters are given in Table 2-2. Detailed information on the distributions and their parameters can be found in the SHEDS-Multimedia Technical Manual.

Table 2-2. Supported Variable Distributions

Distribution	Number of Parameters	Parameter Names	Rules for Valid Distribution
Point	1	Value	
Uniform	2	Minimum, Maximum	minimum < maximum
Normal	2	Mean, Standard Deviation	standard deviation > 0
Log Normal	2	Geometric Mean (GM), Geometric Standard Deviation(GSD)	GM>0, GSD>1
Triangle	3	Minimum, Mode, Maximum	minimum <= mode <= maximum, minimum < maximum
Exponential	2	Minimum, Mean	minimum < mean
Gamma	2	Shape, Scale	shape>0, scale>0
Beta	2	Shape1, Shape2	shape1>0, shape2>0
Weibull	2	Shape, Scale	shape>0, scale>0

2.3.5 Entering Distributions

2.3.5.1 Individual Distribution Widgets

Distribution widgets are an interface object used to enter parametric distributions. They may be found on various interface screens (e.g., Figure 5-15, Figure 5-16, and Figure 5-17 on pages 41, 42, and 43, respectively) and on the Edit Variables screen which also includes visualizations of the resulting distributions (Figure 5-20). The distribution widget (Figure 2-5) is composed of:

- A container box with a descriptive title.
- A pull-down combo box with a list of distributions.
- A series of labeled text entry boxes. The number of text entry boxes varies with the number of parameters required.
- An OK button to force validation.

Enter a distribution by clicking on the pull-down arrow and making a selection from the list that is displayed. Then enter values for each parameter. Pressing the tab key will move from parameter to parameter. However, you will need to either press the enter key or click the OK button to force the values to be validated. If the one or more of the values are incorrect when validated, the background of the container box will turn yellow and you will not be permitted to go to the next screen. Truncation minimum or maximums[3] may be left undefined. The text box containing these values will indicate an error, but the distribution as a whole will still validate.

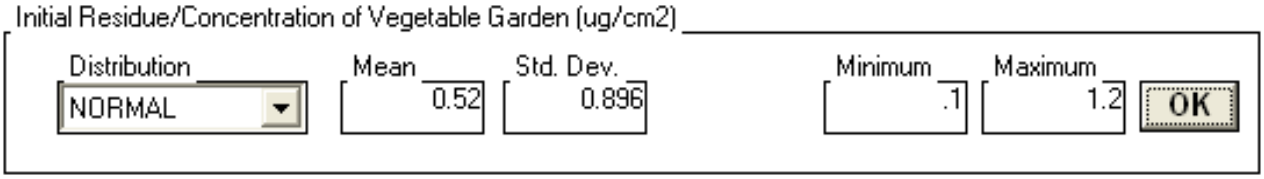


Figure 2-5. Example Distribution Widget.

After entering corrections hit return or click on the OK button to force validation and clear errors. In some contexts specific error messages will be displayed.

3 Truncation minimums and maximums are not part of the distribution definition. These include the minimum and maximum on the normal distribution and the maximum on the Log Normal, Exponential, Weibull, and Gamma.

3 Installation

3.1 Requirements

SHEDS Multimedia was developed under SAS version 9.1 on machines running MS Windows 2000 and XP Professional.

To install and use SHEDS-Multimedia, you will need a computer running SAS version 9.1 or higher. SAS must be installed prior to installing SHEDS. Your computer hardware needs to be adequate to run SAS and MS Windows. Additionally you should have:

a 600 MHz processor,
64 MB of RAM, and
100 MB of free disk space.

However, it is recommended that you have:

a faster processor,
128 MB or more RAM, and
more than 200 MB of free disk space.

The software should run on other systems where SAS is implemented, but this has not been tested.

Each run will consume about 16MB + (0.28*N) MB where N is the number of people simulated for 1 year. So a run of 200 people will take up 72 MB of disk space.

3.2 Installation under MS Windows

Installation has been designed so that administrative privileges are not required.

WARNING: If you wish to save the results from model runs, copy the affected results files from the installation directories to another location before uninstalling or reinstalling SHEDS.

3.2.1 Starting With a CD

If you have a CD, do the following:

1. Insert the CD into your CD reader.
2. Use Windows Explorer to navigate to the top level files on the CD.

Double click on the SHEDS_Multimedia_Setup.exe file to initiate the installation. The installation may have version numbers after the "Setup". For instance …Setup_3.14.exe.

3.2.2 Starting with a Downloaded File

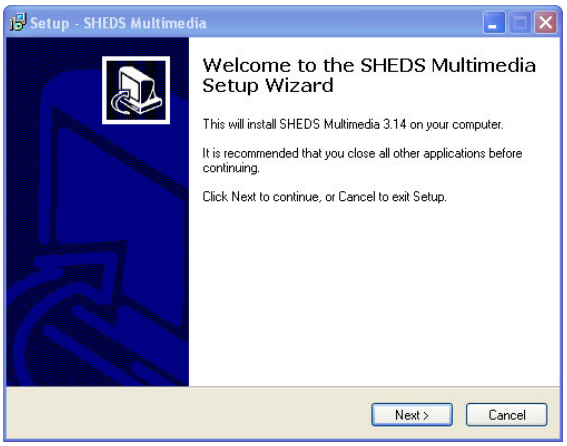
You may obtain the setup file via FTP or another electronic means.

1. Save the attachment to a local or network hard drive. The method you use to do this will vary depending on the program you use obtain the file.
2. Use the Windows explorer to navigate to the saved file.
3. Double click on the saved file to start the installation.

3.2.3 The Standard Installation Process

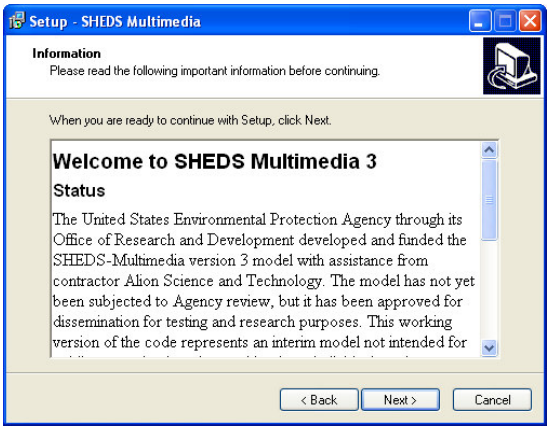
Once the installation wizard is initiated, simply follow the instructions. This will install the necessary program and data files, create a program group on the Start menu, and create an icon on the desktop. The desktop icon will execute the interface within SAS. The program group will contain an additional shortcut (menu item) to uninstall the model and program data.

The screens encountered during install, and an explanation of each, are shown in the following figures. For a default install, users should simply continue to click the Next buttons until the final screen.



The initial screen informs the user what version will be installed. Click the Next button to continue.

Figure 3-1. Setup Screens: Initial Screen.



This screen provides some information about the current state of the program and how to get support.

Figure 3-2. Setup Screens: Welcome and Information Screen.

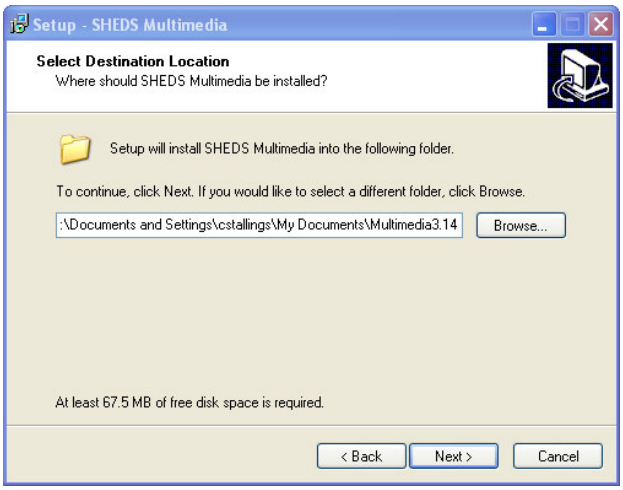


Figure 3-3. Setup Screens: Installation. Directory Screen.

The user may elect to install the files somewhere besides the default location. The default location is in the user's My Documents directory. If the user desires, the Browse button can be clicked and a dialog allowing the choice of an alternate location will come up. The main reason one might want to install somewhere else is that the user generated simulation results are large and by default are stored under the install directory. Note that the user may redirect the output to another location.

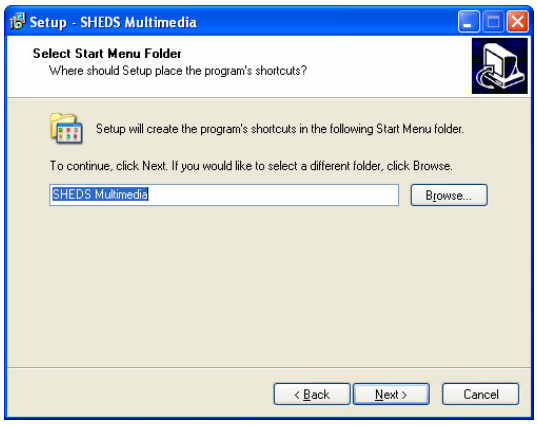


Figure 3-4. Setup Screens: Shortcut Folder Name.

Figure 3-4 shows the final window before install begins. Allows the user to set the name of the program group in the Start Menu. The user should not need to change this.

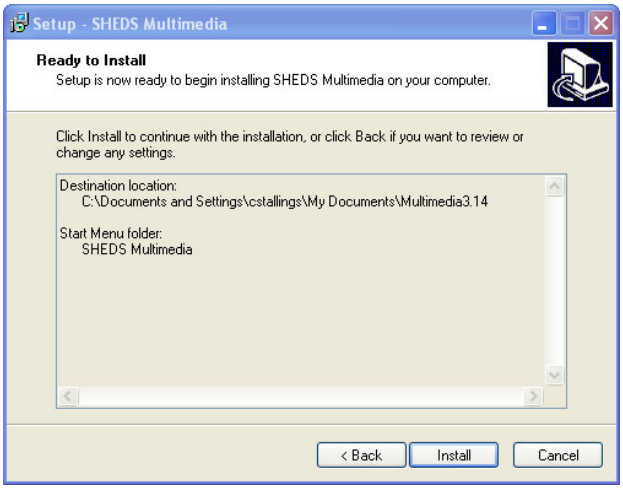


Figure 3-5. Setup Screens: Confirmation Screen.

The user has the chance to review installation specifications on this screen before the installation begins.

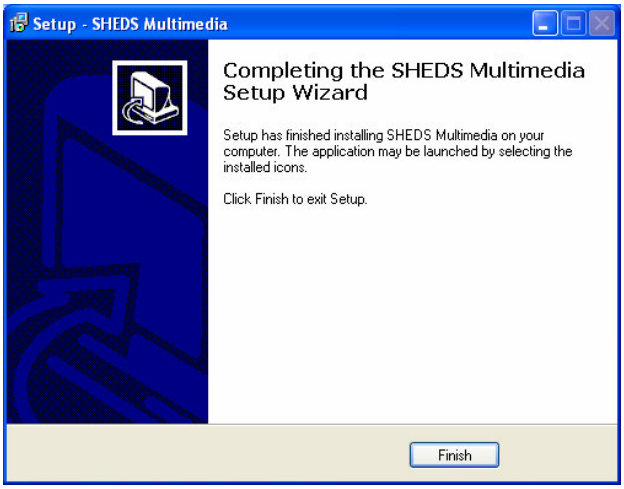


Figure 3-6. Setup Screens: Completion Confirmation.

After the files have been extracted and placed in the specified install directory, and the desktop icon has been placed, the final screen will indicate that the installation is complete.

3.2.4 Starting the Model Interface

The installation will place an icon on your desktop. The icon should appear as the standard SAS icon, with the label "SHEDS Multimedia 3". However, this varies depending on the version of SAS the user is running. It will typically include an inverted triangle as part of the icon. Double click on the icon (figure at right) to start SAS and the main screen of the SHEDS Interface.

Figure 3-7. SHEDS Multimedia Desktop Icon.

3.2.5 Removing SHEDS-Multimedia

If SHEDS was installed using the installation wizard, the user can uninstall it in a manner similar to other Windows programs. **Removal of the program will**

remove all of the user's simulation output files unless these were saved elsewhere. To start the removal process, click on the "Uninstall SHEDS Multimedia" choice in the SHEDS Multimedia group of the Programs menu.

4 The SAS User Interface

Most of the SAS user interface provides detailed fine-tuning capabilities that are usually not necessary for typical model use. The average user may still find a brief review of this section useful. If the user is unfamiliar with SAS and wishes to explore raw datasets used by the model, then it is a good idea to read this section more carefully.

4.1 The SAS Screen

Assuming one uses the link in the MS Windows Programs menu or the screen icon to start the model, the main GUI screen will start inside the main SAS window (Figure 4-1). By default, the SAS log window also starts.

The SAS window is split into a number of distinct areas. The main area for viewing documents, forms, data sets, and graphs is in the middle. This area may have multiple windows active at one time. The user may activate a particular window by clicking on the title of the window. The bar immediately below this area contains one button for each window in the main area. The buttons indicate which window is active, and allow one to activate a different window. In Figure 4-1, the main SHEDS screen is active as can be seen by the colored title bar and the depressed appearing button. Note that since the main SHEDS screen does not have a title on the title bar, its button is unlabeled. As the SHEDS GUI and model are run, informational and error messages will be displayed in the log window. The pull-down menus are on the top of the screen, just under the title. The toolbar is below this. At the very bottom of the SAS window is a status bar.

Additional SAS windows can be opened using the SAS View menu (Figure 4-2). The Graph window displays all graphical output generated. The interface uses a separate output window for this purpose so the Graph window will generally not be needed. It should also be noted, that since the model interface overwrites images of the same type, SAS's graph window may appear unreliable.

The SAS output window is where any tabular output generated is written by default. Generally, the model does not provide this type of output.

The Results window (Figure 4-3) provides a list of tabular and graphical results generated and printed to the graph and output windows. It is generally locked on the left side of the SAS window. If additional windows are locked in this area, they are accessed with tabs that appear below. The Results window may be used to navigate among the different outputs. However, it will not open the output or graph windows; this must be done manually.

The Explorer window (Figure 4-4) is used to navigate through SAS libraries and files, data sets, forms, and programs. It can be used to access the raw files used as input or output to the model. This screen may float in SAS's main area or it may be locked on the left side of the SAS window and be accessed via a tab on the bottom of this area. This screen may be toggled between tree mode (shown) and a single pane, similar to MS Windows Explorer.

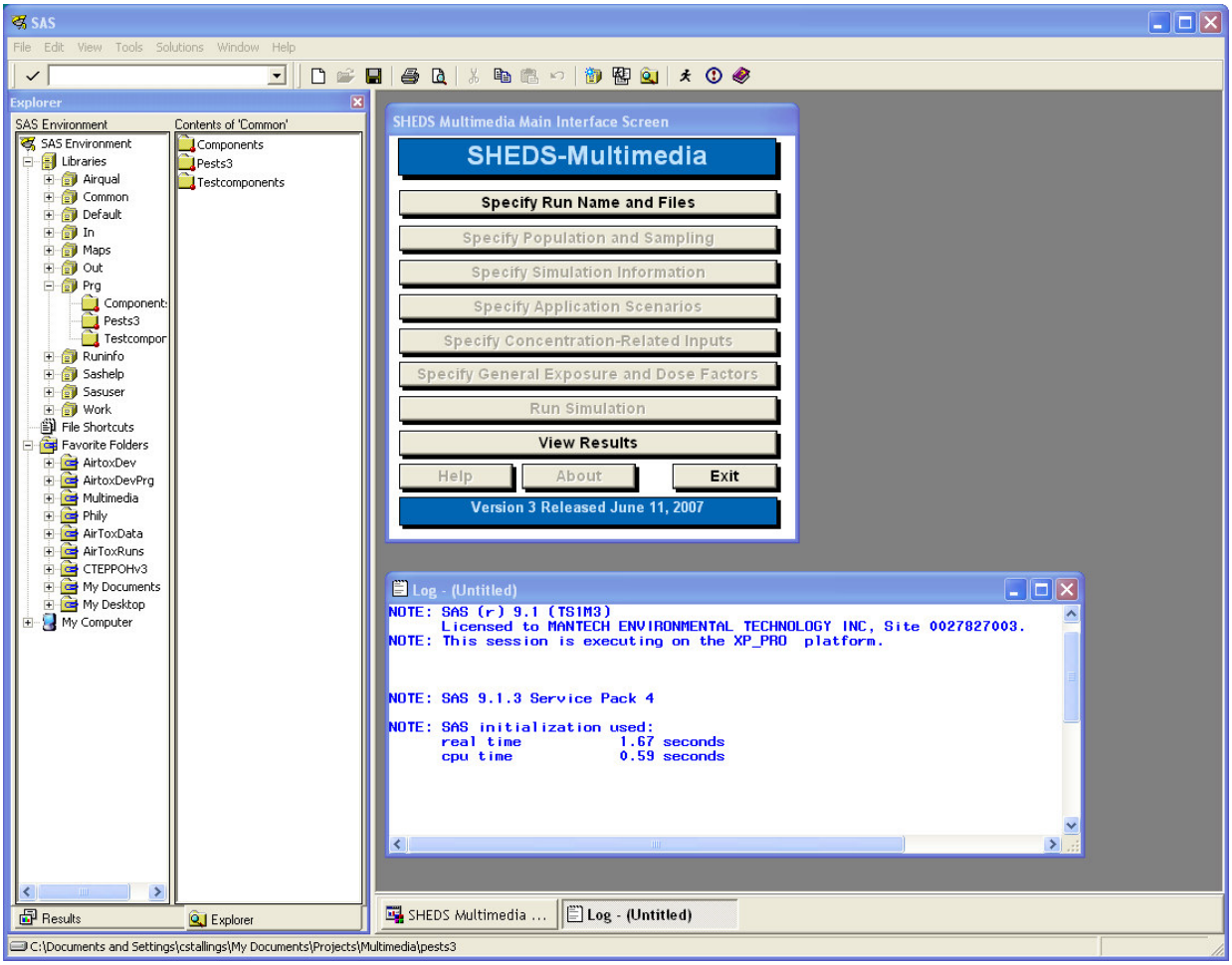


Figure 4-1. The Main Model GUI Interface Screen in the SAS Window on Startup.

Figure 4-2. The SAS Menu Bar and the View Menu.

Figure 4-3. The SAS Results Window.

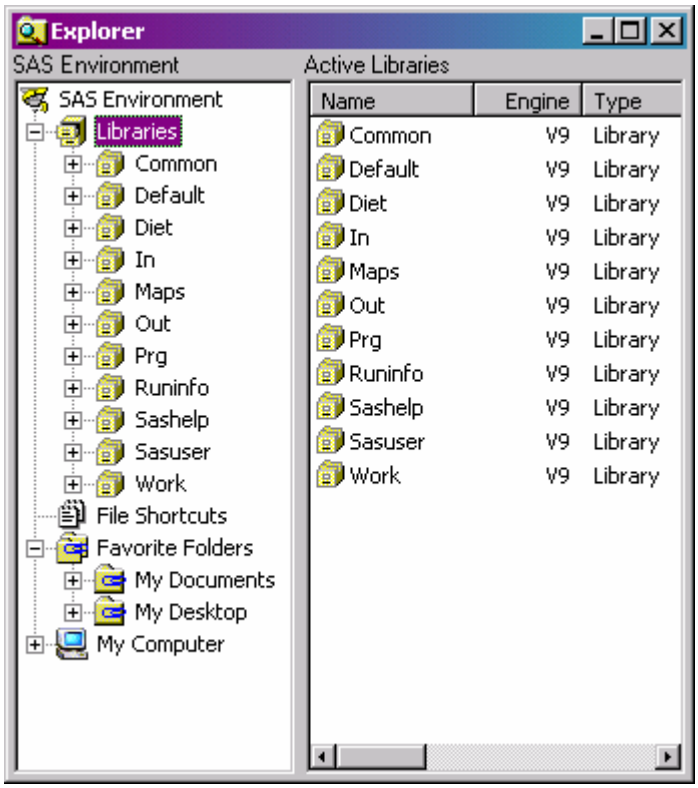


Figure 4-4. The SAS Explorer Window.

5 SHEDS-Multimedia: The Graphical User Interface

5.1 SHEDS-Multimedia Main Interface Screen

When SHEDS Multimedia is started the main screen will be displayed (Figure 5-1). This is the main interface window that you will be returned to after completing each main step. It contains the following buttons.

Specify Run Name and Files: Choose or define a new run name, identify existing input files

Specify Population and Sampling: Define basic information for the run, number of people sampled, variability or uncertainty (only variability is active in the GUI for version 3), ages of interest

Specify Simulation Information: Define the length of simulations, source-to-concentration approach, and a number of other global simulation variables

Specify Post-Application Exposure Scenarios: Define the dates and times of applications, re-entry times, and relationship between application dates

Specify Concentration-Related Inputs: Specify decay and dispersion inputs, or post-application distributions, or time-series data

Specify General Exposure and Dose Factors: Specify all other inputs including transfer variables, use groups, contact probabilities, input variable correlations, etc.

Run Simulation: Run the current simulation

View Results: View results from previous runs

Help: Bring up the contents for the help screens (to be implemented)

About: Bring up the help screen describing

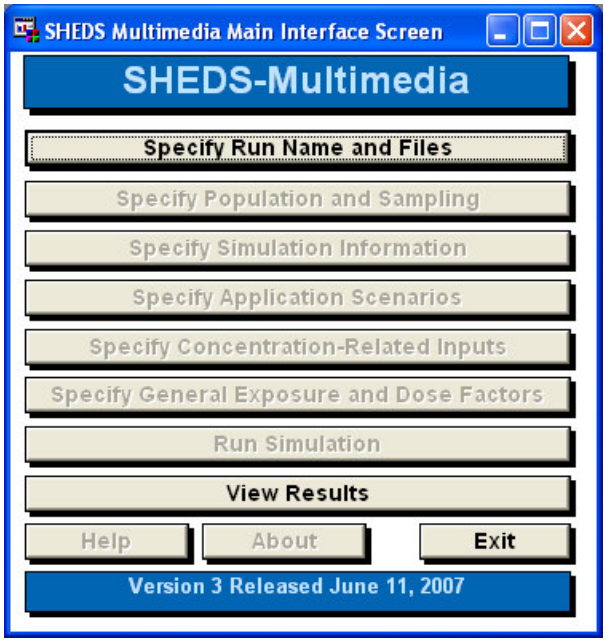


Figure 5-1. SHEDS Multimedia Main Screen.

this version of the model (to be implemented)

Exit: Close the SHEDS user interface

These buttons allow the user to move through the proper sequence of steps to conduct a new model run, or to view results and manage files from previous SHEDS simulations. Initially only a few of the buttons are enabled. Buttons that are not enabled are displayed with a slight gray tint to the font. The initially enabled buttons are Specify Run Name and Files and Exit.

Before beginning to specify the inputs for a new simulation run, editing the inputs for an existing simulation, or viewing the results of a previous run, the user will need to specify the run name. The run name is simply a title for a simulation run that references all input files for and output files from a run.

Clicking on the "Specify Run Name and Files" button will bring up a screen allowing the user to enter the run name. After specifying the run name and if necessary, the files (see below), the user will be returned to the Main Window. If setting up a new run the Specify Population and Sampling button will now be enabled. If viewing the results of a previous run, then the View Results button will be enabled. The appropriate buttons will be enabled as the user completes each step, and returns to the main menu.

5.2 Specify Run Name and Files

The first step in SHEDS-Multimedia version 3 is to click on the "Specify Run Name and Files" button. The run name is like a file folder that keeps together all the information specific to a simulation. In technical terms, it relates to a directory where files are stored and a record in a database that stores information about a run.

5.2.1 Specify Run Name Dialog

The Specify Run Name dialog (Figure 5-2) allows the user to do several things:

Edit Selected Run: Restore the contents of a previous run for editing.

Copy Selected Run To New Run: Restore the contents of a previous run into a new run name and allow them to be edited.

Create a New Run: Enter a new run name and begin defining inputs

View Results of Selected Run: Select run so that the user can view its results (edits will not be allowed)

Delete Selected Run: Delete an existing run.

The "Specify Run Name" dialog is composed of three main parts: The first is a list box containing the names of previously defined simulation runs. The currently selected run name is highlighted in this box. Below the list box, the description of the currently selected run name is displayed. This provides additional information on the run. The user enters it when the run is created. On the right of the dialog are the action buttons. These perform an action, usually on the selected run name. As in other dialogs the "Help" button (when implemented) will bring up a help screen for this dialog. The Cancel button closes the screen without selecting a run name.

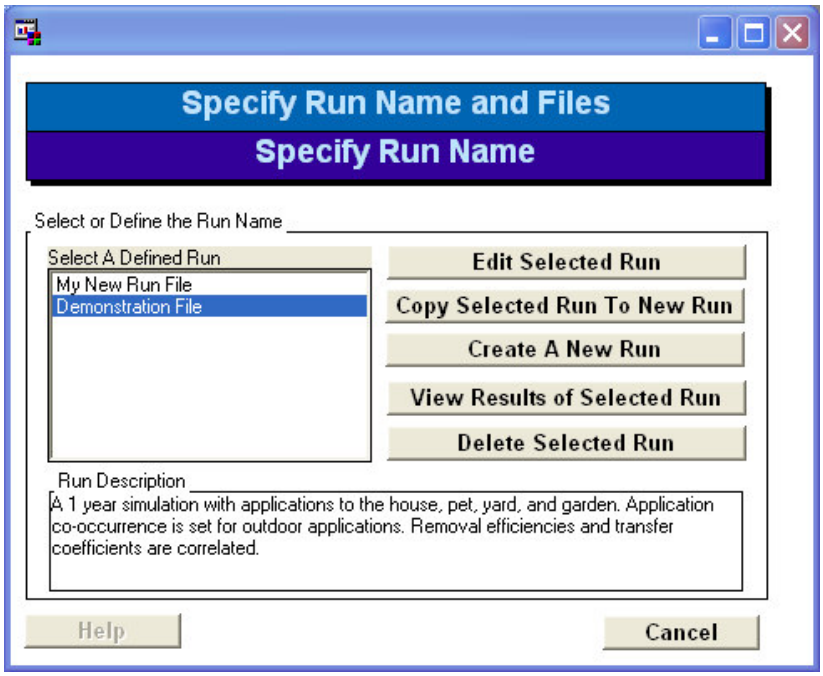


Figure 5-2. Specify Run Name Screen.

To select an existing run name simply click on that name in the Select A Defined Run list box. In most cases the user will need to select a run name before clicking on the action button.

5.2.1.1 Edit Selected Run

This button allows the user to continue editing an existing run. The user will be taken to the "Specify Files" screen (Figure 5-5). After that the user will be returned to the main menu. This feature is useful, for example, if one is interrupted in the process of creating a run. The inputs already entered may be saved and SHEDS exited. To finish creating the run, one selects the incompletely specified run, chooses this "Edit" button, and continues defining the run. This button is also useful in changing inputs on a previously completed run, if the user is willing to overwrite the previous inputs and the resulting output. When becoming familiar with the model using the Demonstration File it is recommended that you use the Copy Selected Run to New Run since any changes made using this button overwrite the original file.

5.2.1.2 Copy Selected Run To New Run

A run name should be selected before clicking on this button. The information for that run will be copied. The user will be allowed to define a new run name using the "Enter New Run Name" screen (Figure 5-4) and will then be taken to the Specify Files Dialog and allowed to edit information there. As distinct from the "Edit Selected Run" button, this button is used to modify

inputs from a previous run, save the changes into a new run name, and still maintain the original run.

5.2.1.3 Create a New Run

To create a new simulation from scratch, click on "Create A New Run". The "Enter New Run Name" screen (Figure 5-4) will appear allowing the user to enter the new run name and description. After this is completed, the "Specify Files" screen will be displayed (Figure 5-5). Initially, defaults for all values will be used. Note that the default input values provided in SHEDS-Multimedia version 3 are not intended to represent any specific chemical or situation.

5.2.1.4 View Results of Selected Run

Clicking this button chooses the currently selected run name and returns the user to the main menu where the "View Results" button will be enabled. This will allow the user to view output from the selected run. The user will not be allowed to view or edit run inputs in this model.

5.2.1.5 Delete Selected Run

Clicking this button deletes the selected run name from the database. After a dialog confirming that the user wants to delete the run information (Figure 5-3) the user is returned to this dialog.

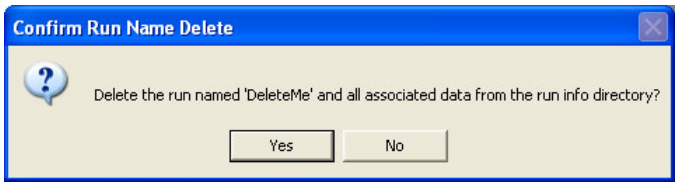


Figure 5-3. Confirm Delete dialog.

5.2.2 New Run Name Dialog

The dialog shown in Figure 5-4 allows the user to enter a new run name and a directory path in which to store the results. This screen is accessed when the user clicks on either "Create A New Run" or "Copy Selected Run To New Run" from the Run Name Dialog. There are three cases for the directory path. When copying from another run, this box shows the location of the prior run and the user can change this. When creating a new run, this box displays the storage location of the last run. If there is no prior run (immediately after the installation), this box displays the default run location.

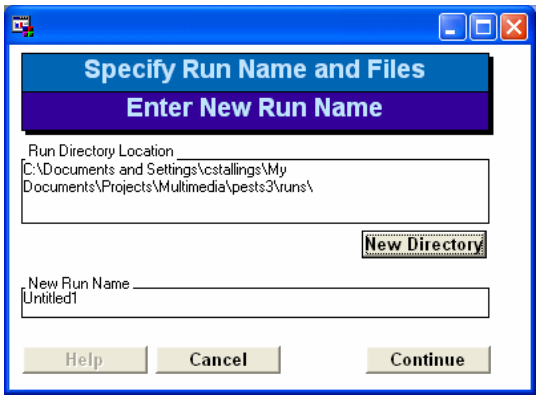


Figure 5-4. Enter New Run Name screen.

The default run name is "UntitledN" where N is the next integer after the last stored untitled run. The user may enter any valid Windows file names. After entering the run name, press return and then click on the Continue button. If the name is the same as a previously used name an error will be displayed and the user will be allowed to enter a new name. Clicking on continue will in general take the user to the "Specify Files" Screen.

5.2.3 Specify Files Dialog

When creating, copying, or editing a run, the user will reach this dialog (Figure 5-5). This dialog allows the user to verify the main directories and specify alternate dietary inputs.

The very top of the dialog simply displays the current run name and run directory. The run directory should be similar to the run name, but altered so that it is a valid directory name. The input and output files from the simulation run will be stored in this directory. The default data directory is where the basic model input data is stored.

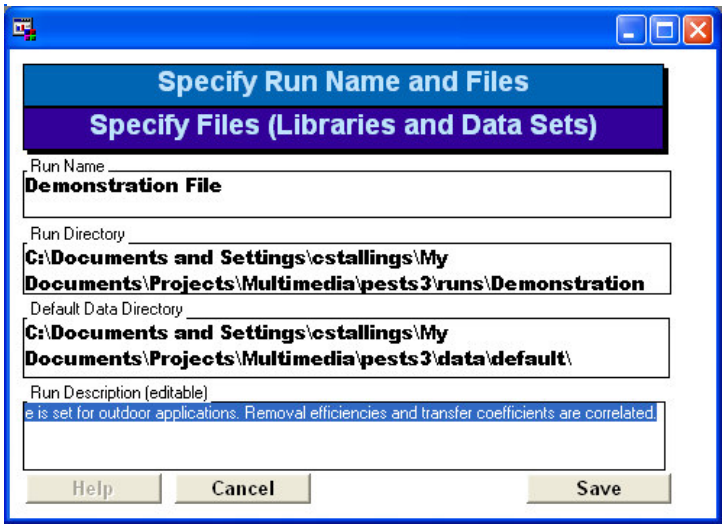


Figure 5-5. Specify Files Screen.

The run description will be displayed and may be edited in the next box down.

The "Cancel" button will leave the dialog without saving any changes. The user will return to the Specify Run Name Dialog. The "Save" button will save any changes, and return the user to the main menu.

When the Specify Files dialog is initialized, the SAS libraries are also set up for the simulation run or simulation results. If setup was for some reason not carried out correctly upon installation, various errors may occur at this point. As of this current version, very little can be done to correct these errors. In this case, reinstallation is recommended.

5.3 Specify Population and Sampling

Clicking on this button of the Main Window displays the related screen (Figure 5-6). Currently only variability runs can be made through the interface. See the Technical Manual and the Batch Mode section of this User Guide for information on doing sensitivity and uncertainty runs using batch mode.

In the "Population: Age Groups and Sample Size" box, the user selects gender(s) and age(s) of interest in the simulation (all ages, or some subset of those ages are available for selection). The "Population Size" option allows the user to specify the sample size for the 1-stage simulation.

Clicking on either “Males Only” or “Females Only” will clear all of the other gender allowing the user to specify a single gender simulation. Once cleared, cohorts can be added back by clicking on them.

The time taken to carry out the simulation increases linearly with the Size of Population and Number of Populations selected. There is a lesser increase in run time if longer time-periods are chosen. Depending on the computer hardware, a run of 1000 persons will typically take about an hour to complete.

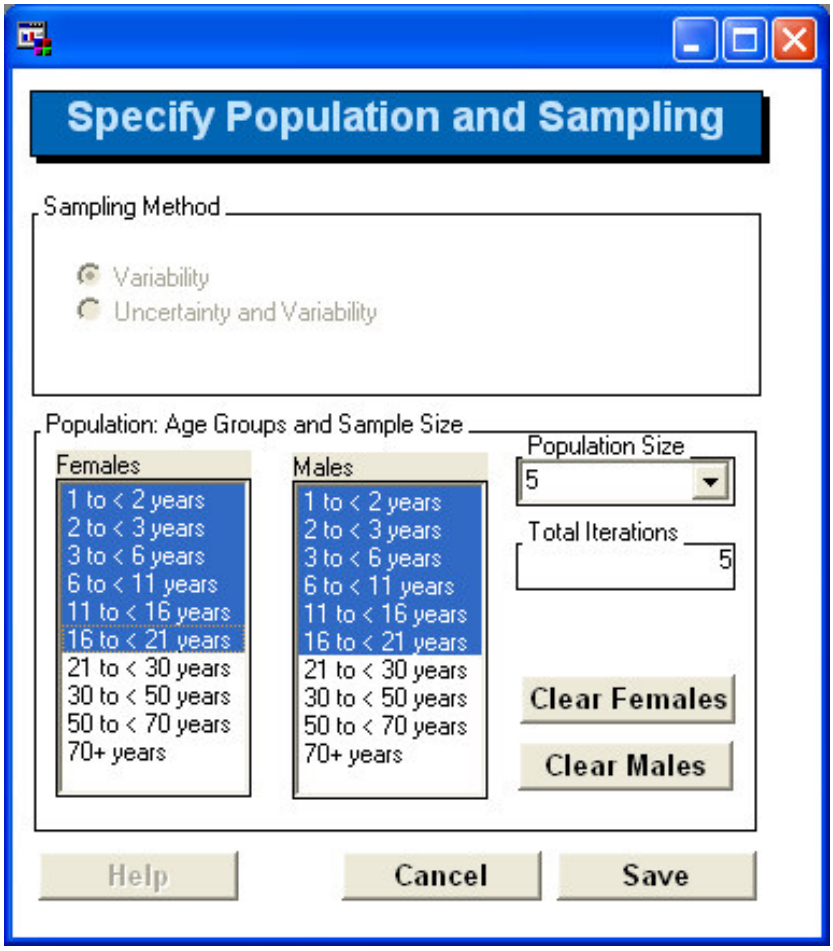


Figure 5-6. Specify Population and Sampling Screen.

5.4 Specify Simulation Information

This screen (Figure 5-7) allows the user to select a number of options that determine overall simulation variables; each is discussed shortly. Clicking the "Save" button commits any changes. The "Cancel" button prevents changes from being saved.

5.4.1 Simulation Length

The box labeled "SIMULATION START AND LENGTH" allows the user to specify the beginning date (month, day, and year) and the number of days the simulation will track each individual. One common choice of simulation period is to start on January 1st and continue for 1 year (365 or 366 days). However, the model allows a great deal of flexibility. A simulation may begin on any day of the year and can be as short as one day or as long as desired and may cross calendar years. However, caution should be exercised when specifying very long periods as they take longer to run and the model does not alter many personal variable settings (including age) over the simulation period.

5.4.2 Source-To-Concentration Approach and Application Dates

There are three options to generate residues and concentrations for scenario-relevant media:

- **Decay/Dispersion Model:** Specific applications leave a residue on surfaces, in the soil, and in the air. These residues decay with time and are moved to untreated areas.

- **Post-Application Distributions:** Specific applications leave residues on various media. The concentrations on the media are determined by distributions that change with the time since the application.

- **User-Specified Concentration Time Series:** The user supplies a time series of concentrations for each medium.

The Decay/Dispersion model is a built-in source-to-concentration model that requires the user (in subsequent screens) to enter application and decay rates, and the ratio of residue concentrations in untreated to treated media for indoor applications. Additionally, background distributions can be defined for the various media when Decay/Dispersion is used.

The Post-Application Distributions selection will require the user (in subsequent screens) to enter distributions of relevant media residues and concentrations for discrete post-application time periods (<1 day, 1-7 days, 8-30 days, 31-365 days).

The User-Specified Concentration Time Series option will require the user (in subsequent screens) to enter time series of residues and concentrations for each medium of interest (e.g., from a measurement study or outputs from an external source-to-concentration model).

If either Decay/Dispersion or Post-Application Distributions are chosen, a box will appear (to the right of the Source-To-Concentration radio box in Figure 5-7) that allows the user to specify whether the application dates will be User-Specified or Model-Determined. Details will be input on subsequent screens. For user specified dates, the user will enter specific day numbers for each application type, where day 1 is the first day of the simulation period. Applications will always occur on the dates given. For modeled dates, the user will specify probability vectors for month, day of week, number of applications, and time of applications.

5.4.3 Dermal Exposure Method

For dermal exposure, the user can select the Transfer Coefficient approach or the Transfer Efficiency approach. These two methods are described in the SHEDS-Multimedia version 3 Technical Manual. Changing this value on a previously defined run will result in the user having to visit the Specify General Exposure and Dose Inputs screen to define related variables.

5.4.4 Soil Ingestion Approach

For soil ingestion, the user can select the Direct or Indirect approaches, both of which are described in the SHEDS Technical Manual. Changing this value on a previously defined run will result in the user having to visit the Specify General Exposure and Dose Inputs screen to define related variables.

5.4.5 Exposure-To-Dose Method

SHEDS-Multimedia version 3 allows the user to either use a built-in pharmacokinetic model (discussed in the SHEDS Technical Manual) to compute absorbed dose, or to export SHEDS exposure time series so that the files can be read by an external PBPK model.

5.4.6 Maximum Diary Event Length

The Maximum Diary Event Length box allows the user to break CHAD diary events into smaller intervals, if desired. Diary events cannot exceed 1 hour. Average event duration while awake is about 30 minutes. While carrying out simulations many stochastic decisions are made for each event (e.g., which surface the individual contacts). The decisions apply to the entire event. To force these decisions to be made more often, the diary can be broken up into more pieces, by setting the Maximum Diary Event Length to a value smaller than 60 minutes. Using a smaller value will slightly increase the run time for the simulation (see Technical Manual).

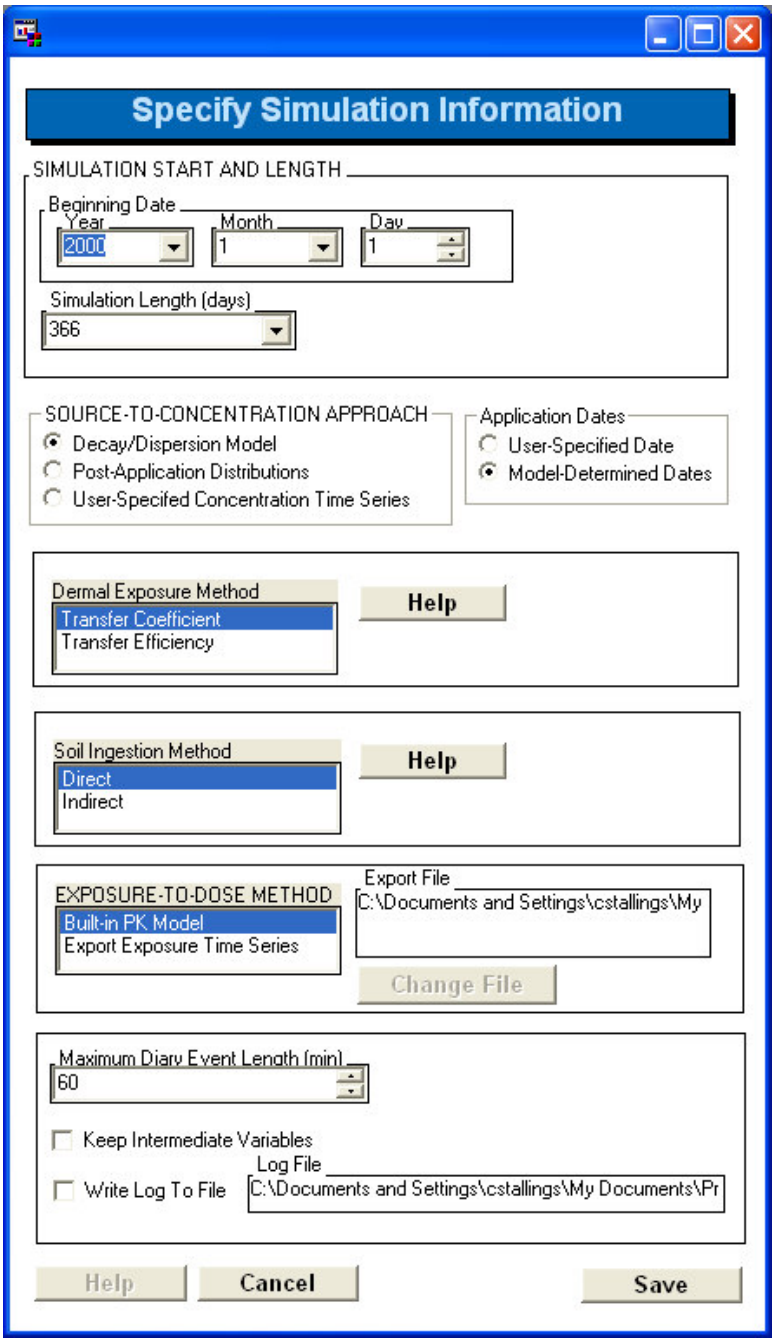
5.4.7 Keep Intermediate Variables

If the user checks the “Keep Intermediate Variables” box, SHEDS will retain variables used in intermediate calculations for simulated individuals. This is useful to check the internal workings of the model.

5.4.8 Save the Log File

To save the log that is generated during the simulation run, the user can click on "Write to Log File" which saves the log to a permanent file outside SAS, thus ensuring the log is saved even if SAS crashes during the run. Unfortunately, under this option the standard SAS log screen is not used, and the user cannot track the progress of the run.

If the log file is not saved, a line of output is written to the log window before each individual is simulated, and this is the best way to tell how the simulation is proceeding. If the log is written to a permanent file, the user can open the file with a text editor from time to time to check the status of the run. The name of the log file is fixed. It is stored in the output library.



Note: To utilize the co-occurrence option, the user must select Model-Determined Dates on this screen. The user must also select Specify Parameters before clicking the Specify Inputs button on the Specify Exposure Scenario Details screen (Figure 5-9) for each scenario for which co-occurrence inputs are to be specified. Application co-occurrence is explained in section 5.5.5.

Figure 5-7. Specify Simulation Information Screen.

5.5 Specify Application Scenarios Simulated

Clicking on "Specify Application Scenarios" on the main screen begins a series of screens through which the user must navigate in their entirety before returning to the main screen. The exact screens vary depending on options selected. The following screens may be visited:

The first screen is used to identify the scenarios to be simulated.

Specify Exposure Scenarios (Figure 5-8)

The second screen is used to specify details for each scenario and is used to get to the Application Dates and Co-Occurrence screens for each scenario.

Specify Exposure Scenario Details (Figure 5-9)

These screens are visited once for each scenario, after which the user is returned to the Specify Exposure Scenario Details screen.

Specify Application Dates (Figure 5-10 and Figure 5-11. The version visited depends on date types specified)

Specify Co-Occurrence (Figure 5-12. Only visited if the user chooses this option)

Clicking the Continue button on the Specify Exposure Details screen takes the user to these screens. They are visited once for each simulation.

Specify Application Times (Figure 5-13. Only visited for model determined application dates)

Specify Re-entry Times (Figure 5-14)

5.5.1 Specify Exposure Scenarios

The specific scenarios or applications to be simulated are specified on this screen if the user is simulating chemical applications. In the later screens, additional information will need to be entered for each scenario defining the probability, dates and co-occurrence of applications, and re-entry times. The exact screens visited will depend on options chosen by the user. If the user is becoming familiar with the interface, it is recommended that only one or two scenarios be chosen.

This screen will not be shown (the button on the main screen will be grayed out) if the User-Specified Time Series was chosen as the source-to-concentration method. If the user is simulating a multimedia measurements study then specific applications are not specified.

Each scenario chosen is assigned a priority. The priority becomes important when application co-occurrence is of interest. That is, when one is interested in using the dates of one scenarios' applications to influence the dates of applications in other scenarios. The dates of an application can only be influenced by applications occurring in scenarios given a higher priority.

The left most list box, titled "Application Type" indicates the supported application types or scenarios. Clicking on an application in this list box copies it to the list of "Selected Scenarios" in the middle of the screen. The scenarios are prioritized from top (1st) to bottom in the Selected Scenarios list. Click on a scenario description to select it. Use the up and down arrows on the right to change the priority of the selected scenario. Clicking on the "Delete Selection" button will delete the currently selected scenario from the Selected Scenarios list.

When all desired scenarios are selected and prioritized, clicking on the Continue button will take the user to the remaining screens.

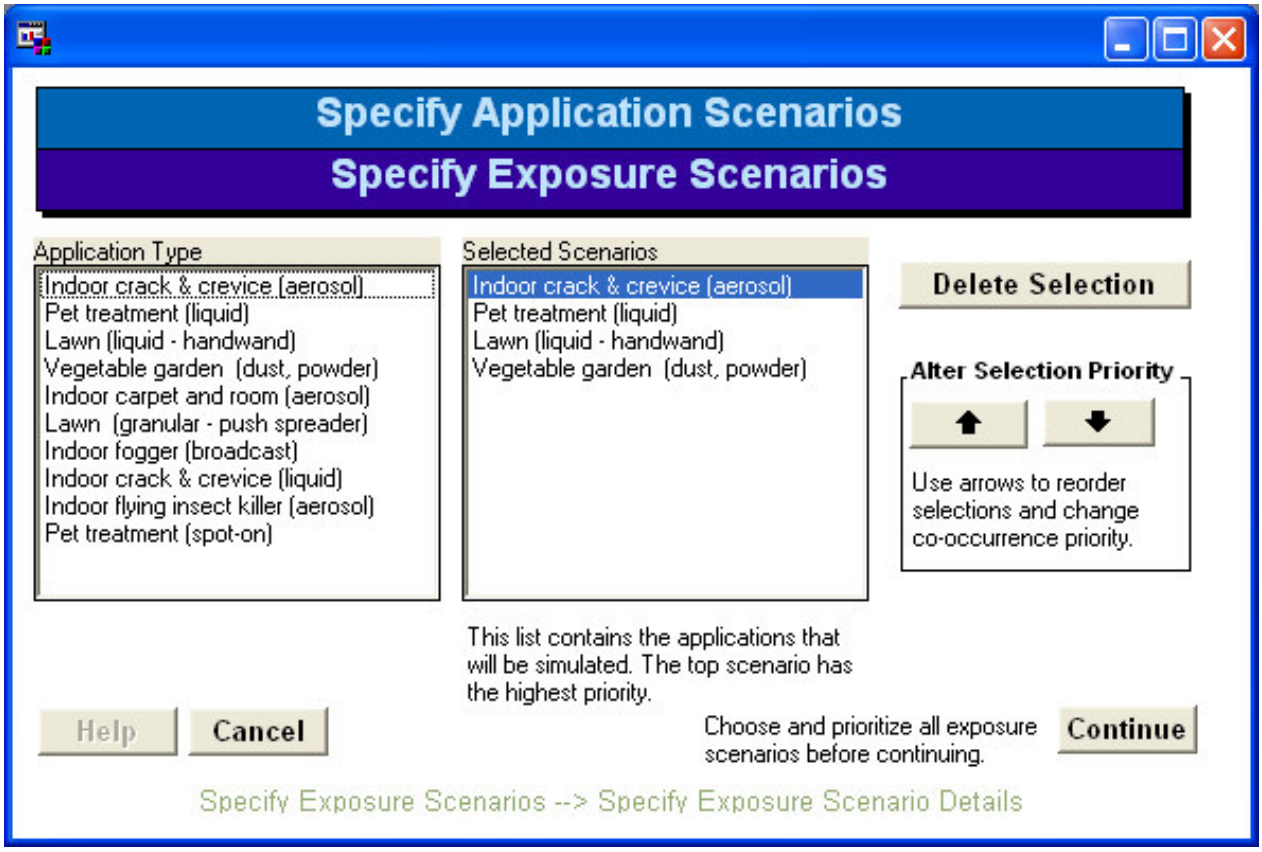


Figure 5-8. Specify Exposure Scenarios Screen.

5.5.2 Specify Exposure Scenario Details

The list box on the left of Figure 5-9, "Scenarios", displays the scenarios chosen by the user in the previous screen. Clicking on one of these entries selects that scenario as the current one (and highlights it). Once selected, the user needs to do the following for each scenario:

1. Specify or edit the application probability.
2. Specify whether co-occurrence will influence this scenario's dates.
3. Click the Specify Inputs button to enter application dates, times, and co-occurrence.

Only when these have been completed for each scenario will the user be permitted to continue. If the existing values for probability and co-occurrence are acceptable, the user is not required to edit these values.

When highlighted, the application's probability and co-occurrence status are displayed. The Application Probability is the probability that this application will be used by an individual that is in the use group (e.g., has a garden for a garden application).

If Specify Parameters is selected in the "Scenario Co-Occurrence" radio box, then the application dates of other scenarios will be allowed to influence the application dates of this scenario. Selecting this here will cause the "Specify Co-Occurrence" screen to be displayed at the appropriate time. The "Specify Co-Occurrence" radio box will be grayed out for the application with the highest priority since no other scenarios are allowed to influence it.

Note: Co-occurrence can only be selected in SHEDS if the chemical application dates are supplied by the model. If user-supplied chemical application dates are used in the Simulation Information Screen, then the co-occurrence radio button selection will be grayed out.

For each selected exposure scenario, the user should enter the Application Probability and specify whether Co-Occurrence should be used. Then clicking on the "Specify Inputs" button will take the user to the Specify Application Dates and Specify Co-Occurrence screen for the selected scenario. After completing the information on these screens the user will be returned to this screen to work on the remaining scenarios.

Scenarios that have been completed are shown in the list box on the right. The user will not be allowed to continue (click on the Continue button) until the application date and co-occurrence information has been filled out for all selected scenarios. Clicking on the Continue button will take the user to the "Specify Re-entry Times" and possibly the "Specify Application Times" screens.

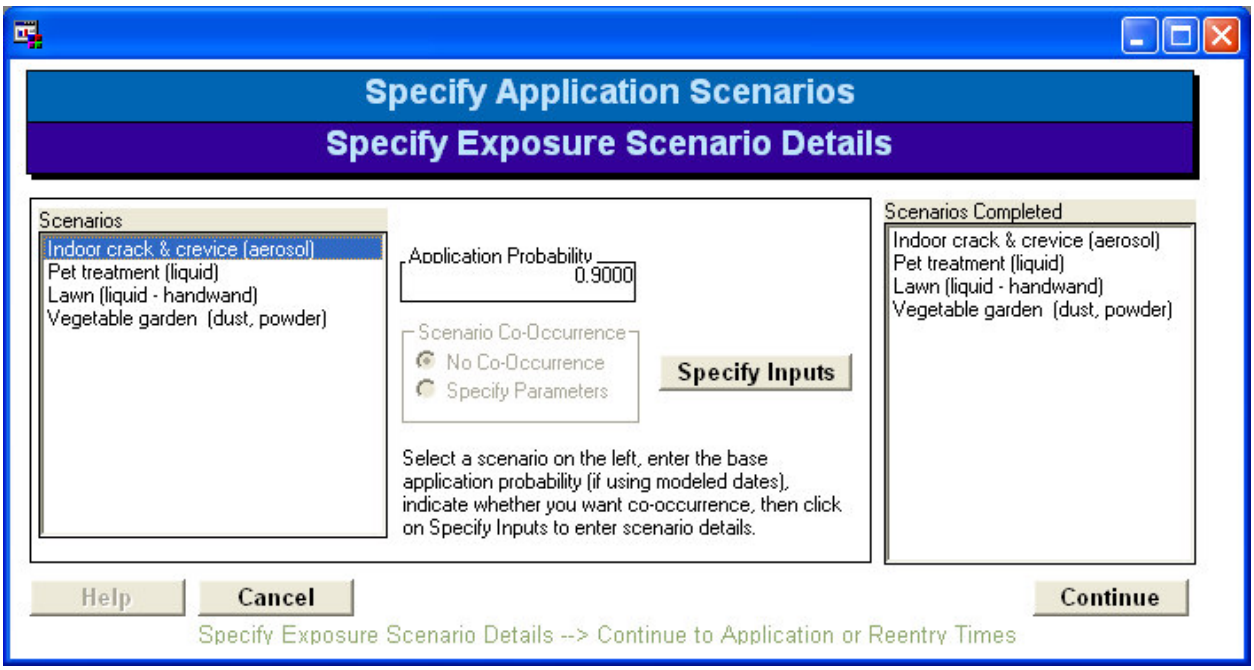


Figure 5-9. Specify Exposure Scenario Details Screen.

5.5.3 Specify Application Dates: Model Determined

Model determined dates are determined stochastically during the simulation. The dates will typically vary for each individual simulated. The user enters the blackout period, the probability vectors for month, day of week, and number of applications. These are used together to determine the application date or dates. During a simulation the actual dates chosen may be influenced by other scenarios if co-occurrence was specified.

Typically, the weekday probabilities will be used to specify Mon-Fri for professional applications or another configuration, possibly Sat-Sun, for home owner applications. The Monthly probabilities can be used to ensure that lawn or garden applications occur during the appropriate season. The number of applications can be fixed for each individual by specifying a 1 for the probability in the appropriate box.

Taken together the probabilities define the likelihood of an application occurring on each day of the year. For multiple applications the blackout period comes into play. The blackout days indicate how many days must pass before an additional similar application is allowed.

The probabilities for each vector (weekday, monthly, and number of applications) must total 1.0. The user can enter probabilities in the first boxes of each probability vector. The last box of the vector, with a darker border, will always contain the remainder and cannot be edited by the user. Additional information about entering probability vectors is given in the section “Entering Probability Vectors” on page 8.

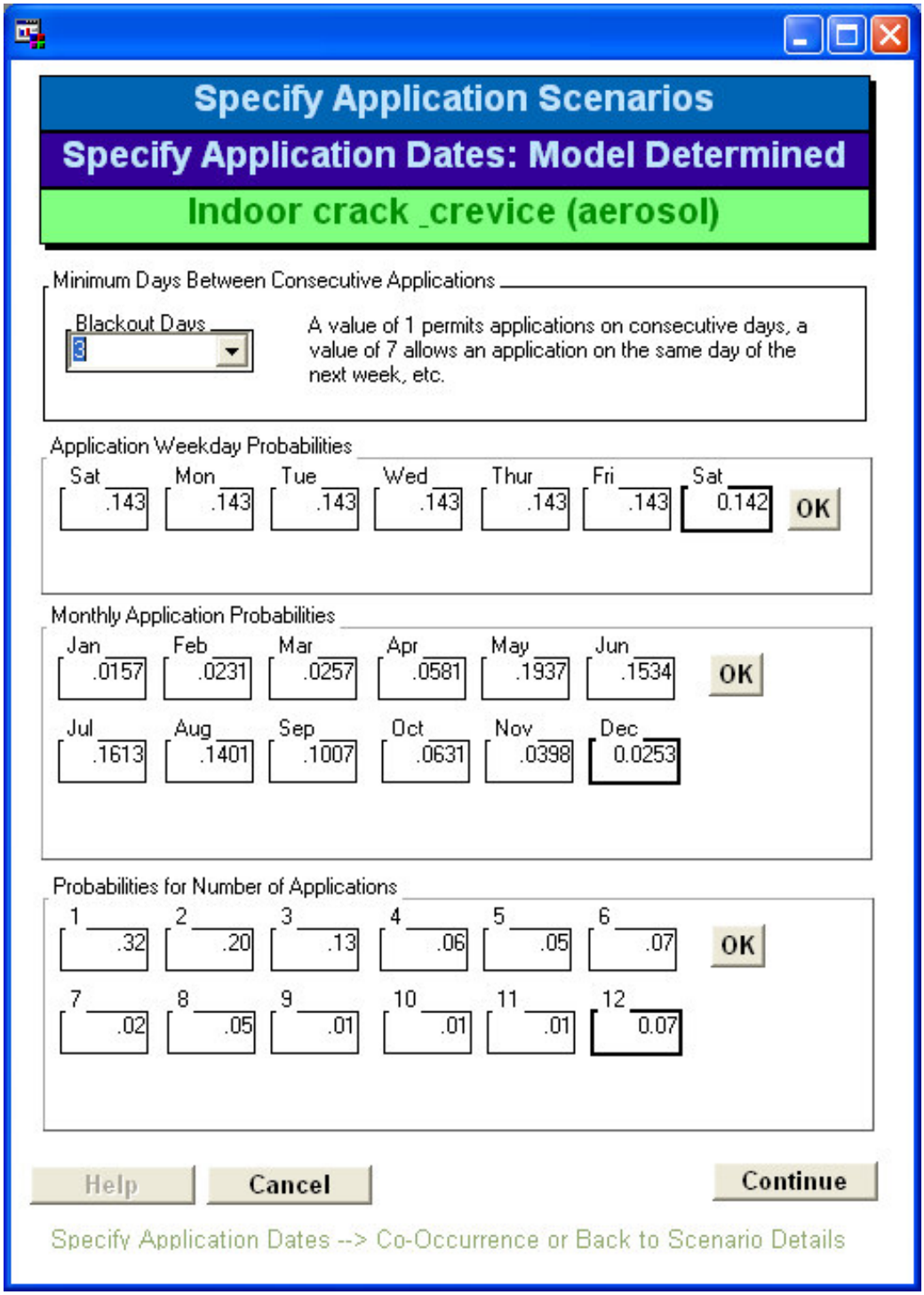


Figure 5-10. Specify Application Dates: Model Determined Screen.

5.5.4 Specify Application Dates: User Specified

This screen (Figure 5-11) is used to enter user specified application dates. These dates are specified by day number (with 1 being the first day of the simulation period). There is no probability associated with these application dates as an application will be made on each of these dates for all users in the appropriate use groups. That is, all lawn applications will be made if the individual being simulated has a lawn, and so on for pets and gardens. In addition to the days of application, the user should select the time. All applications in a scenario will be made at the same time of day.

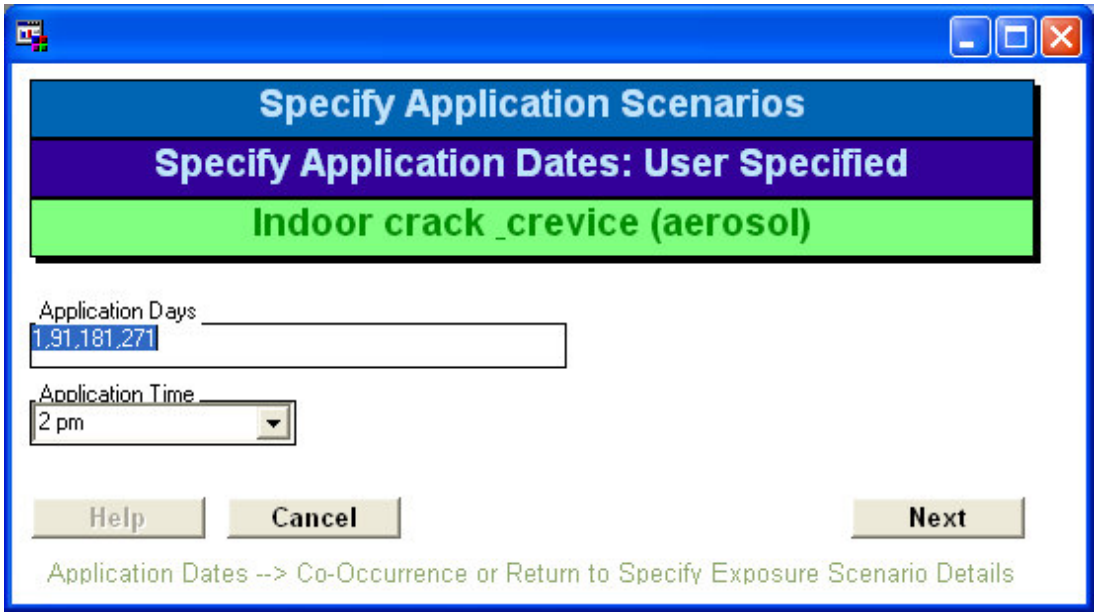


Figure 5-11. Specify Application Dates: User Specifed Screen.

5.5.5 Specify Co-Occurrence

This screen (Figure 5-12) is used to specify how the application dates of other scenarios affect the application dates of this scenario. Scenarios must have been specified as being of a higher priority in the Specify Exposure Scenarios screen (page 32) to affect a scenario. Only those scenarios of a higher priority are listed in "Application Types of Influence". For purposes of discussion let us call the scenario we are working with the "current" scenario, and let us call applications from scenarios with higher priority "previous" applications. In the model code the dates of the previous applications will be determined first. Note that 'previous' in this context refers to the order in which the application dates are determined; it does not mean that the 'previous' dates necessarily occur earlier in the simulation.

The probability of an application from the current scenario occurring on any day of the year is determined based on the probability vectors entered earlier for month and day of week. When working on the current scenario, the application dates for the higher priority scenarios will already have been determined. The probabilities for the current scenario are altered (multiplied) by the influence factor for all days within the influence width of previous applications. This obviously has no effect for those days whose probability is already 0. The influence factor, also called the co-occurrence probability is discussed and illustrated in the "Application Dates and Co-occurrence" section of the Technical Manual.

If the influence factor exceeds one, then the likelihood of the current scenario happening near in time to a previous scenario is increased. If the influence factor is less than one, the likelihood is decreased. An influence factor of zero means that a 'blackout window' is created around each of the dates for the previous scenarios, so that the current scenario cannot occur on those dates. The two scenarios become mutually exclusive for that period of time around an application.

The user must choose an effective combination to continue. That is, at least one application type must be highlighted and the influence factor must be different from 1. If the user wants to turn off co-occurrence for this scenario, then enter an effective combination and return to the Specify Scenario Details screen. On that screen click the No Co-Occurrence choice for this scenario. This will turn off co-occurrence.

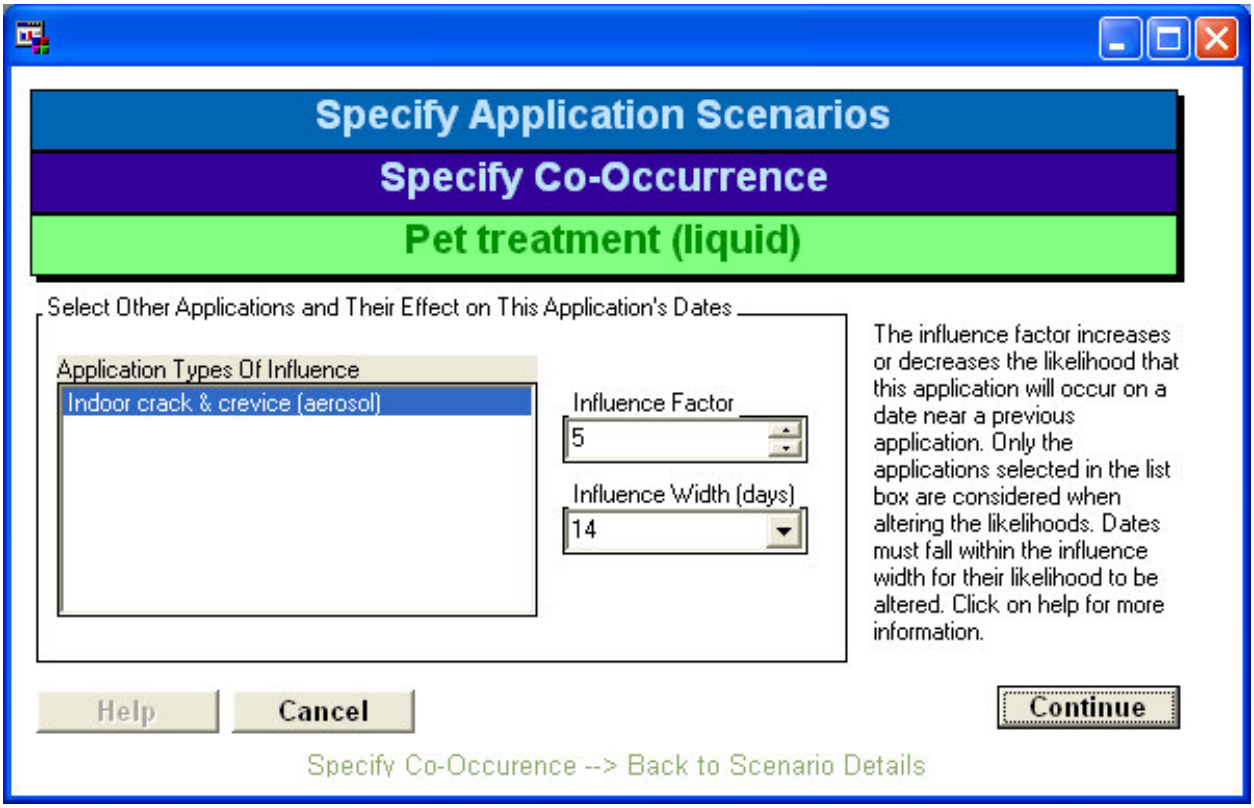


Figure 5-12. Specify Co-Occurrence Screen.

Specify Application Times

When model-determined dates are specified, the user will also need to specify probability vectors for the application times. This screen (Figure 5-13) allows the user to enter one probability vector for all applications occurring inside and one probability vector for all applications occurring outdoors. For a fixed application time for each simulated individual simply enter a probability of 1 in the appropriate box. For general information on entering data in probability vectors see the section "Entering Probability Vectors" on page 8.

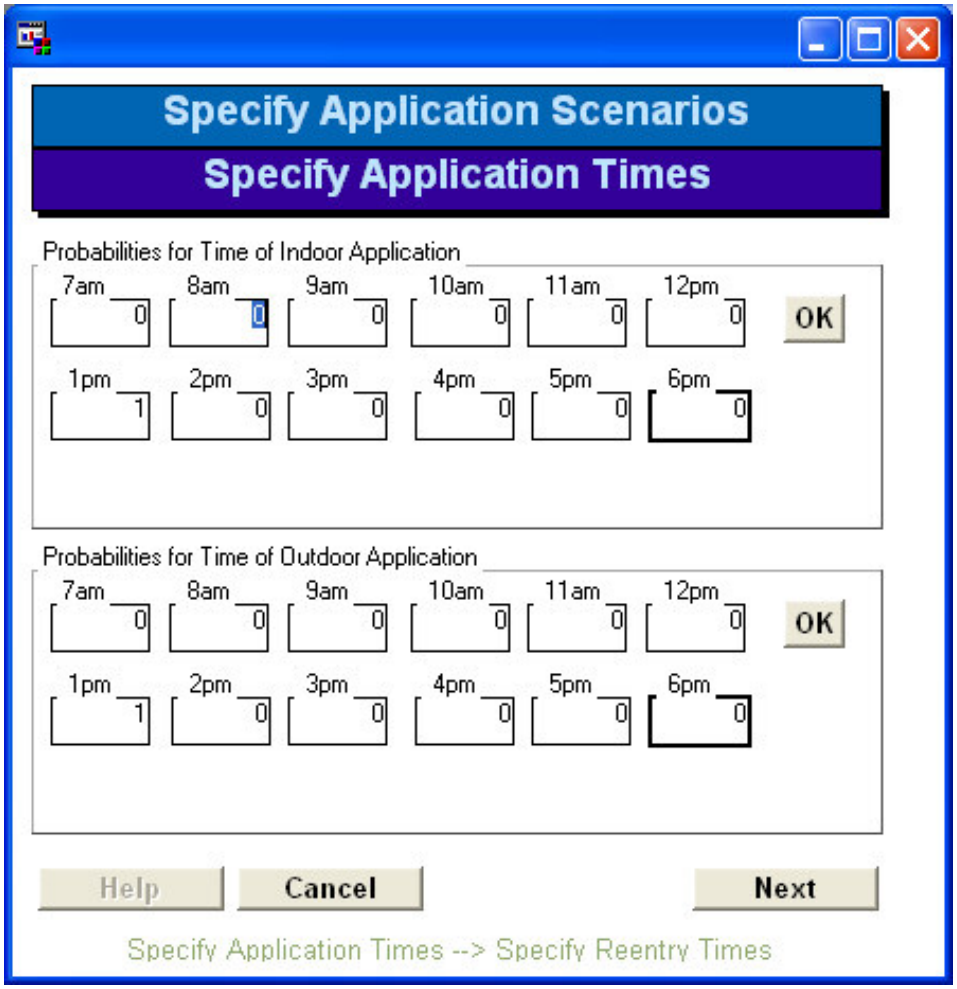


Figure 5-13. Specify Application Times Screen.

5.5.6 Specify Re-entry Times

Simulated individuals may be restricted from entering treated areas for a specified number of hours. This restriction is split into indoor areas and outdoor areas. Within each area the probability of re-entry is the same for all scenarios affecting that area. The probabilities are entered on the Specify Re-entry Times screen (Figure 5-14). For general information on entering data in probability vectors see the section "Entering Probability Vectors" on page 8.

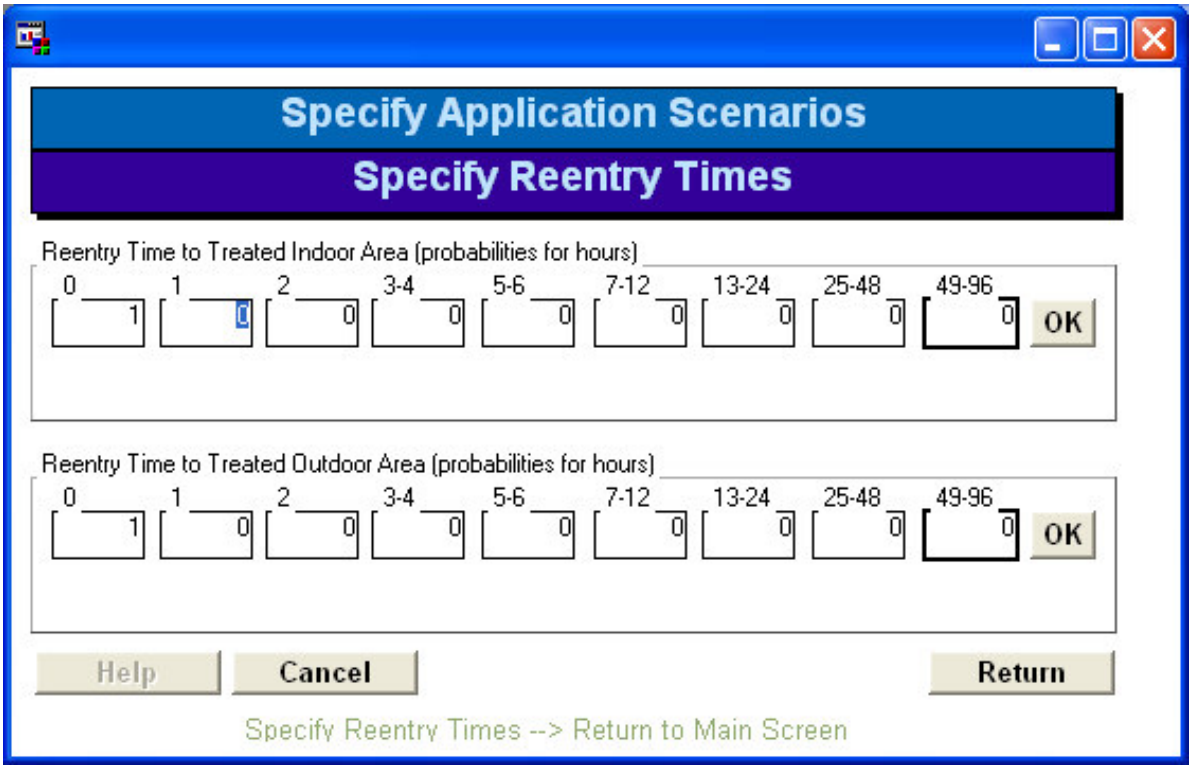


Figure 5-14. Specify Re-entry Times Screen.

5.6 Specify Concentration-Related Inputs

Clicking on "Specify Concentration-Related Inputs" from the main screen begins a series of screens through which the user must navigate in their entirety. The exact screens vary depending on the source-to-concentration options selected earlier. Since these screens may have to be revisited for each scenario, the scenario being edited is always displayed in the third (blue) title at the top of the screen. The following screens may be visited:

WARNING: Different surface residue collection devices are available (e.g., aluminum plates, rollers, sleds, hand presses, hand wipes); some collect dislodgeable residues and some collect total residues. These methods, as well as current methods for obtaining dermal transfer efficiencies and dermal transfer coefficients, have inherent uncertainties. Thus, it is important to consider matching the correct type of surface loading with the corresponding transfer factor (i.e., transfer efficiency or transfer coefficient) when developing inputs for modeling dermal exposure.

Please see the technical manual (section on Dermal Exposure to Surface Residues) for a discussion of entering compatible concentrations and transfer factors (e.g., to prevent double counting of residue transfer from surfaces to skin).

The following screens will be visited once for each scenario selected, depending on the overall method used. The exception is the Background screen which is only visited once and only for the Decay and Dispersion and Post-application methods.

Decay and Dispersion: **Specify Decay and Dispersion Distributions** (Figure 5-15)
Specify Decay and Dispersion Distributions: Background (Figure 5-16)

Post-application: **Specify Post-Application Distributions** (Figure 5-17)
Specify Post-Application Distributions: Background (Figure 5-16)

Time series: **Specify Time Series Input** (Figure 5-16)

5.6.1 Specify Decay and Dispersion Distributions

Use of the decay and dispersion method requires that at least two distributions be defined for each medium affected by a scenario's applications. These distributions define the initial residue or concentration and the decay rate of the chemical for the medium. These are the first two distributions given on the screen (Figure 5-15). Additionally, for indoor media the rate of dispersion to the untreated part of the house must be calculated. To do this, SHEDS requires as input the distribution for the untreated to treated concentration ratio at the time of maximum concentration in the untreated area. (See the Technical Manual for more details.) If the user chooses to ignore dispersion into the untreated area, then this ratio should be set to a point value of zero.

These distributions need to be specified for each of the media in the simulation. The list of media will vary depending on the scenario being worked on. Clicking on a specific medium in the "Media Affected" list box will display the distributions associated with that medium. The two or three distributions can be edited while their associated medium is highlighted. The third

distribution will only be displayed for indoor media. A complete list of media is shown in the list box on Figure 5-16 and in Table B-2.

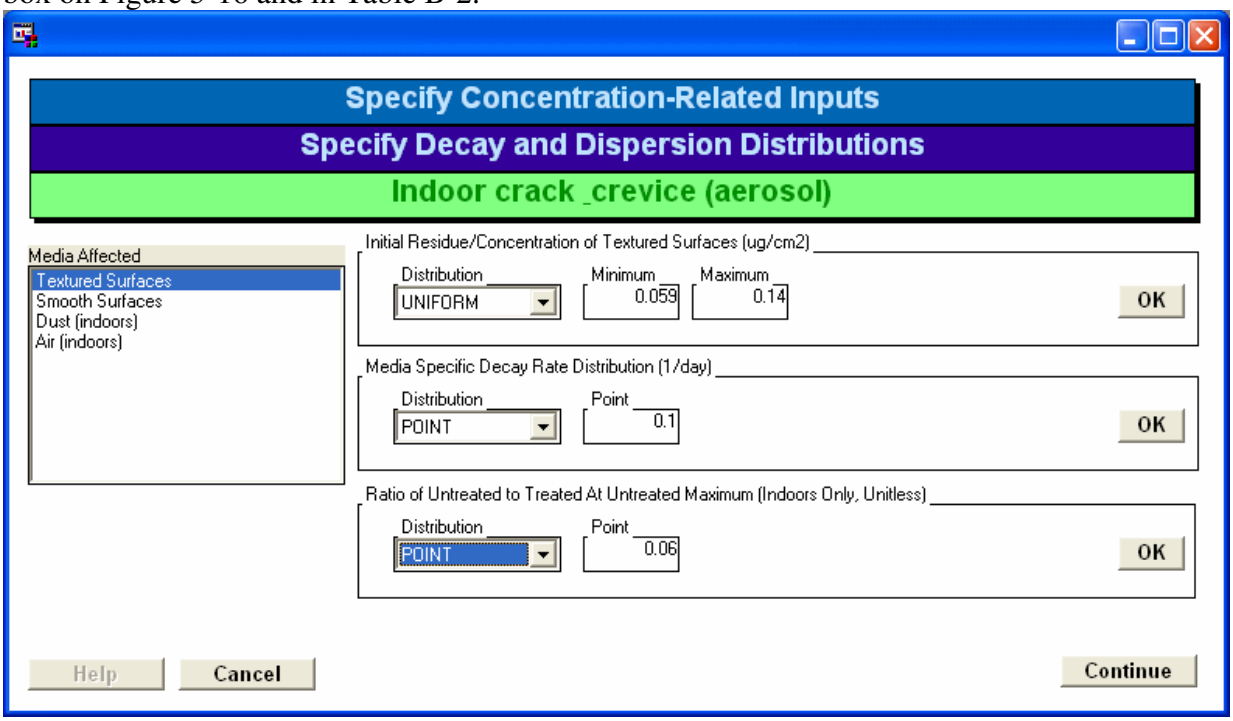


Figure 5-15. Specify Decay and Dispersion Distributions.

5.6.2 Specify Decay and Dispersion Distributions: Background

The background values define distributions of the chemical added to each medium over the course of the entire run. The background concentrations are added to any chemical on the media resulting from a chemical application. The chemical concentrations from applications persist from one time period to the next (altered by decay and dispersion). In contrast, the background values are estimated daily and used for only that day.

The background concentration for each medium is defined by a single distribution. This same distribution is used throughout the simulation. Background values can be added to all media that the model understands, not just those involved in a scenario. The user may disable the addition of background concentrations by setting each distribution to a point value of 0 (their default value).

The same screen is used for both Decay and Dispersion and Post-application backgrounds.

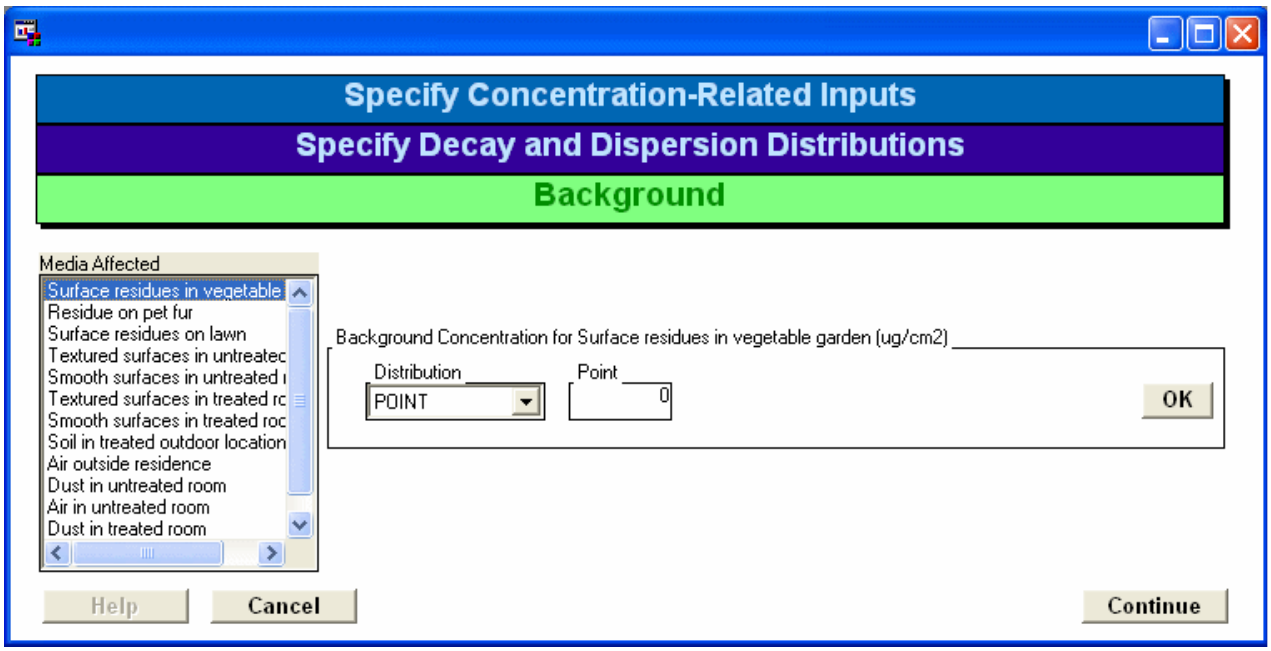


Figure 5-16. Specify Decay and Dispersion Distributions: Background Screen.

5.6.3 Specify Post-Application Distributions

Post-application distributions might be used when measurement studies have determined the actual concentrations over time after applications. SHEDS uses four time periods:

1. The day of application (< 1 day).
2. The day after application to 7 days after application (1-7 days).
3. The 8th day after application to the 30th day (8-30 days).
4. The 31st day after application and the remainder of the simulation period.

The user must define these four distributions for each medium affected by each scenario. Once an application is made for a scenario, these distributions will determine the concentrations on each medium. When another application is made in the same scenario, the first distribution is used once again; there is no persistence of chemical from the previous application. The concentrations on a medium from different scenarios are added when determining exposure of an individual. It is assumed that background values are included in the distributions; the user cannot define background concentrations on media not included in the scenarios.

As on the previous screens, the third title, in blue, indicates the current scenario. Clicking on a medium in the Media Affected list box selects and highlights that medium. The distributions displayed are related to that medium for the current scenario. The user is not forced to enter data for each media. Any distributions not entered by the user will retain their previous values whether desirable or not. Once the distributions have been edited as desired, the user should click on Continue to go on to the next scenario. If the user is working on the last or the only scenario, then Continue will take the user back to the main screen.

The user is not forced to edit the distributions for all media. Those not edited will maintain the previously defined values. The Continue button will be active unless one of the distributions contains an error. Click on Continue to go to the screen to enter data for the next scenario. If this is the only or last scenario, then the next screen will be used to define background values for all media.

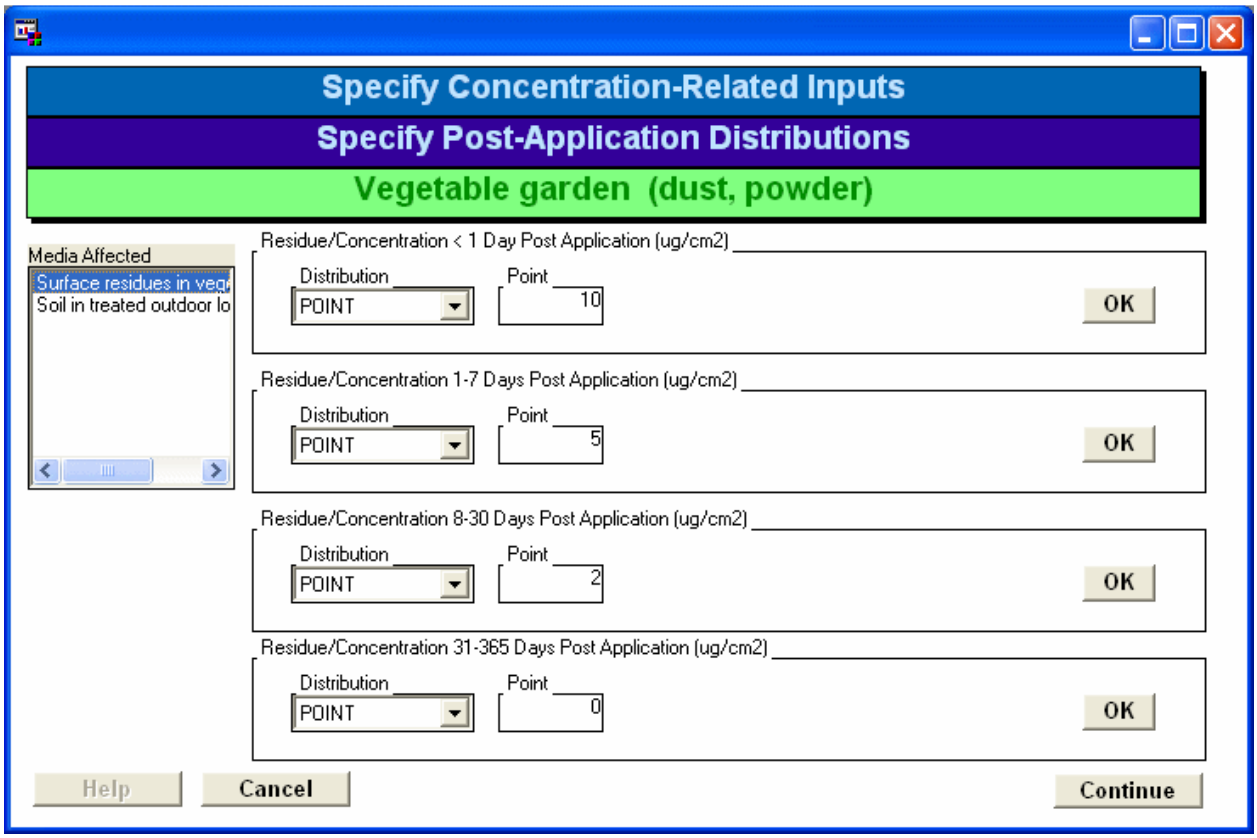


Figure 5-17. Specify Post-Application Distributions Screen.

General information on distributions are provided in section "Distributions Supported" on page 11 and information on entering distributions on this screen are discussed in "Individual Distribution Widgets" on page 11.

5.6.4 Specify Post-Application Distributions: Background

Entering distributions for background concentrations works the same as entering the background concentrations for decay and dispersion (page 41). In the case of post-application concentrations, the assumption is that background values for any media with a defined concentration are built into the concentration distributions. So one is only allowed to enter background concentration distributions for those media that do not have application related concentrations defined. Media

that have post-application concentrations defined will not be listed in the Media Affected list box.

5.6.5 Specify Time Series Inputs

Time series inputs allow the user to specify the exact concentrations on each medium for specific dates. This is a convenient method of using data derived from studies of multiple households. Details on the file format required are discussed in the next section (Time Series File Format).

The burden is on the user to create the file containing time series for all affected media. The interface expects to be given a single SAS dataset which is copied into the input directory for the run. The dataset is specified by clicking on Copy Time Series Dataset (Figure 5-18) and then using the explorer to identify the dataset.

When using time series inputs the Specify Application Scenarios button on the main screen is grayed out. The model does not simulate specific applications in this case.

5.6.5.1 Time Series File Format

The SAS dataset must contain one variable named Date containing the date in SAS date format. The rows must contain sequential values for the date from the first specified to the last. The remaining columns define a time series of concentrations for each of the media. Multiple time series may be supplied for each medium. If multiple time series are supplied, the model will choose them at random for each individual. Corresponding time series are always used; if the first time series is chosen, then the first time series for each medium will be used.

A SAS variable name designates each individual time series. The variable name indicates the medium by text and an appended number indicates the position in the set for the medium. For example, ATair_3 is the SAS variable name for the time series for the air in the treated portion of the third house. A complete list of text names for the media is given in Appendix B, Table B-2.

These time series cannot contain internal gaps, but they may begin after the start of the simulation period or stop prior to the end of the simulation period. Alternatively, the time series may begin before the start of the simulation period or extend beyond it. Time series with different numerical indices may have different start and stop dates, but time series with the same numerical index must all have the same start date (and the same stop date).

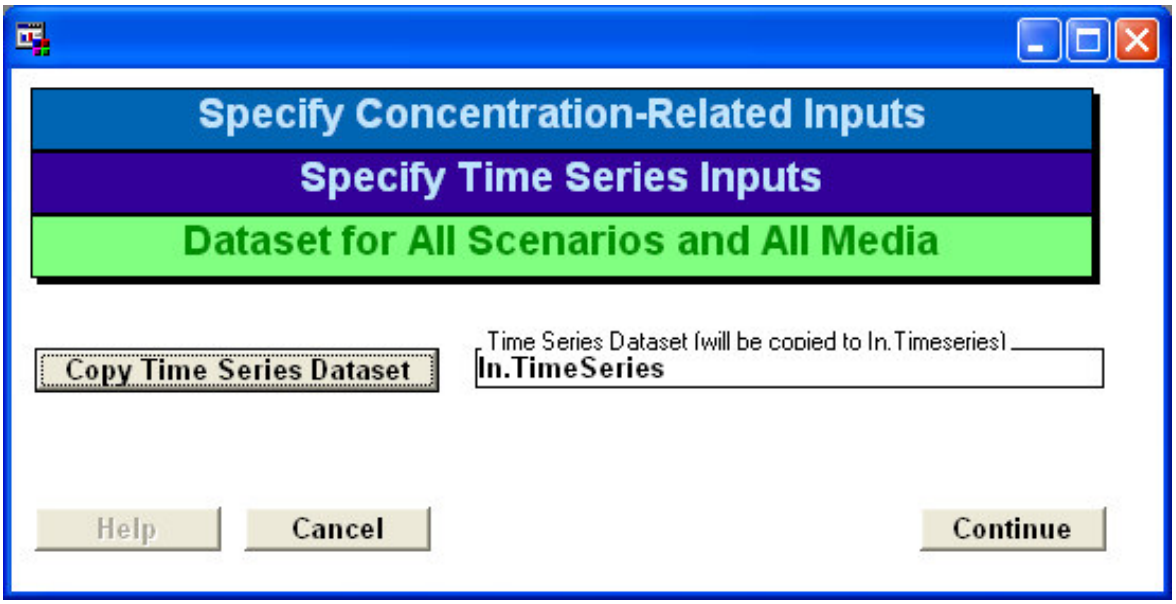


Figure 5-18. Specify Time Series Inputs Screen.

5.7 Specify General Exposure and Dose Factors

Clicking this button on the main screen begins a sequence of screens allowing the user to enter or edit the remaining inputs. These inputs fall into three broad categories:

1. Individual exposure and dose factor variables, typically defined by a distribution.
2. Contact probabilities, defining how frequently an individual comes into contact with specific media.
3. Correlation between input variables (optional).

Each of these categories is discussed in the sections below.

Initially the user is taken to the **Variability Distributions** screen (Figure 5-19). From this screen the user repeatedly visits the **Edit Variability Distribution**s screen (Figure 5-20).

If the user desires to define correlated inputs, clicking on Define Correlated Input Variables will lead to the following two screens: **Select Correlated Variables** (Figure 5-22), and **Specify Variable Correlations** (Figure 5-25). The first "Select Correlated Variables" screen is used to select which variables are to be correlated; the "Specify" screen is used to specify the correlation values defined.

When the previous screens have been visited, the user clicks on the Continue button on the Variability Distributions screen and is taken to the **Contact Probabilities** screen (Figure 5-26).

This screen is used to repeatedly visit the **Edit Contact Probabilities** screen (Figure 5-26. Contact Probabilities Screen.) where the user can specify contact probabilities for the various media.

5.7.1 Variability Distributions

The variables set using the first two screens in this series are grouped as follows:

- Activity-Related (Probabilities related to lawns, gardens, and pets)
- Dose-Related (GI and dermal absorption rate, elimination rate, etc.)
- Transfer-Related (skin adherence, non-dietary ingestion, etc)
- Removal-Related (hand washing frequency, removal efficiencies, etc.)
- Baths (time between baths)

Each variable is defined by a distribution, except for the time between baths which is a probability vector.

The initial Variability Distributions screen (Figure 5-19) is used as a jump point. The user selects a variable group by clicking on the group name in the Variable Groups list box. The group is highlighted and the descriptions of each variable in the group are displayed in the center list box. Clicking on the Specify Inputs button will take the user to the next screen where individual distributions can be edited. After clicking on Save, the user will be returned to this screen. The

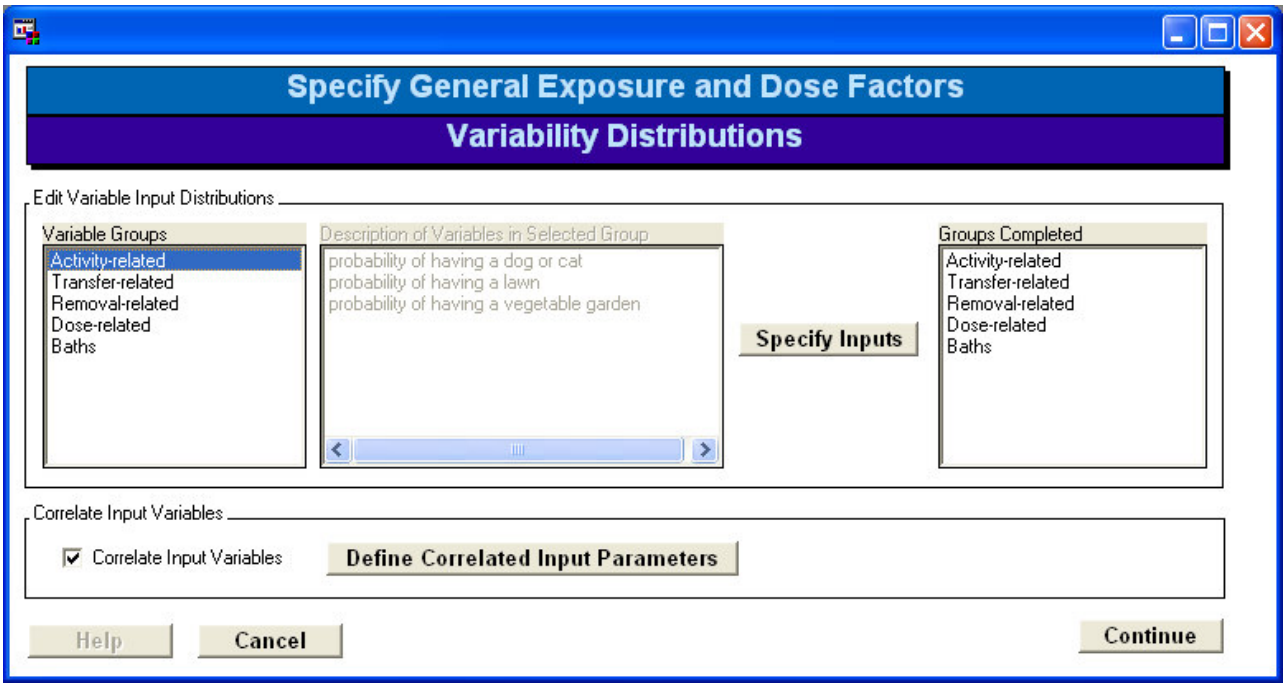


Figure 5-19. Variability Distributions Screen.

variable group just edited will be added to the Groups Completed list box if it was not already there. While one or more variable groups remain to be edited, the background of the Groups Completed list box will be light blue (Figure 2-3 on page 8) and both the Define Correlated Input Variables and the Continue button will be disabled. When all groups have been completed the user may continue contact distribution screens.

If the user returns to the Simulation Information screen and changes options, she will be forced to return here and enter values for any variables not previously defined. For example if the simulation options are switched to Transfer Coefficients, the user will need to return here to edit the Transfer-Related group. Only then will the user be able to continue and run the simulation.

Once all groups are completed, the user will be able to define correlated inputs. By default correlated inputs are turned off; no input variables are correlated. To turn correlation on click on the check box labeled Correlate Input Variables. This will enable the Define Correlated input Variables button. Click on the button to proceed to the two screens used to select and define correlated inputs. After defining correlated inputs, the user will be returned to this screen. If the definition of correlated inputs is not completed, input correlation will be turned off when the user returns to this screen.

Only when all variable groups have been completed will the user be allowed to continue. If correlation was turned on, the correlated pairs must be defined or correlation must be turned off before the user may continue. Once enabled, clicking on the Continue button takes the user to the screens used to define contact probabilities.

5.7.2 Edit Variability Distributions

The user comes to this screen (Figure 5-20) when the Specify Inputs button is clicked from the Variability Distributions Screen. The screen will always have the same basic layout, but the specific variables that can be edited will change based on the variable group highlighted when the Specify Inputs button was clicked. The second title will always indicate the variable group being edited.

The variable to be edited is chosen in the left hand list box. If the variable has several distributions associated with it, for different ages perhaps, then a list of conditions will be listed on the right (see Figure 5-21). A variable is selected by Clicking on the variable description, or the condition if present. When selected, the current distribution parameters for that variable will be loaded into the widget. The title of the box surrounding the distribution widget will show the actual variable name, a vertical bar, and then the description for that variable. Use of the distribution widget is covered on page 11.

Whenever a valid distribution is loaded or redefined a frequency histogram will be drawn showing a representative sample for the distribution as defined. To turn this off uncheck the histogram check box on the right. The mean and standard deviation of the sample will also be

shown in the box on the right. It should be emphasized that the sample shown is not used in the model. The distribution will be sampled during the model run to generate values used in the run. Some features, particularly due to truncation, are easier to see if the number of bins are increased using the spin box on the right.

The Print Plot button will route a copy of the plot to the default printer.

To accept the current values click the Continue button. If any of the parameter values are in error, they will be highlighted in red or yellow and the Continue button will be disabled. Clicking on the Cancel button returns the user to the Variability Distributions screen without saving any changes.

More detailed information on editing distributions is given in “Individual Distribution Widgets” in Section 2.3.5.

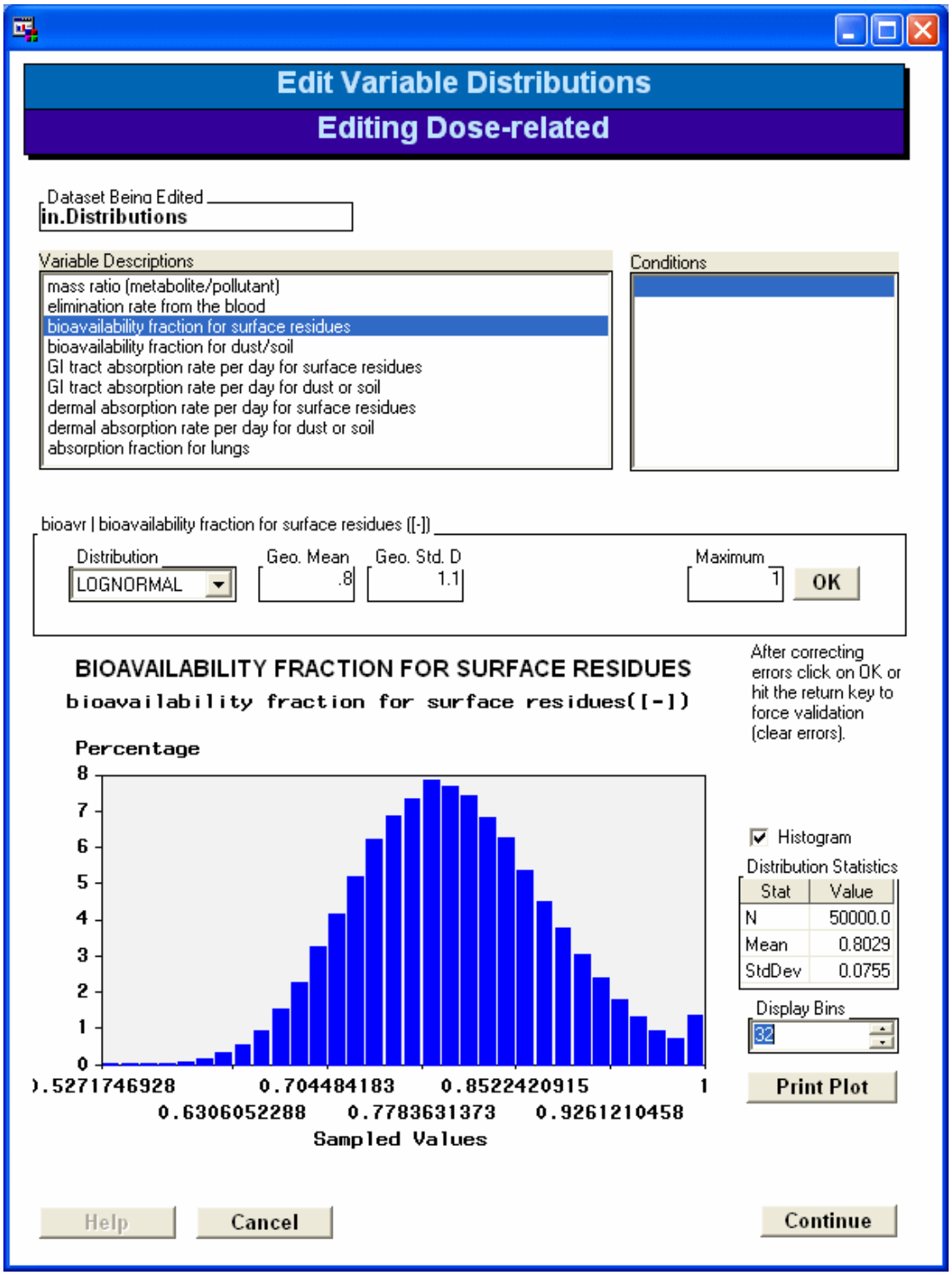


Figure 5-20. An example of the Edit Variability Distributions Screen.

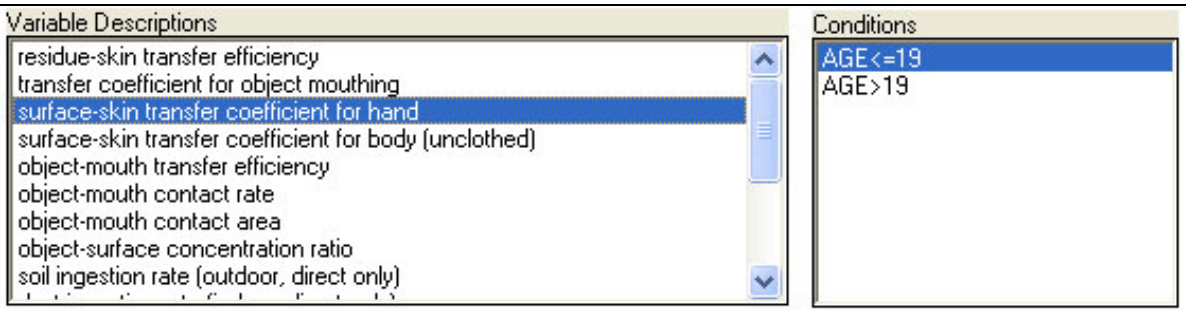


Figure 5-21. Variable with Two Conditions shown.

5.7.3 Correlating Input Variables

All of the variables in this section (General Exposure and Dose Factors) are randomly sampled from the specified input distributions. In certain cases, the user might want some of these variables to be correlated with each other. For example, perhaps the hand-to-mouth transfer efficiency and the object-to-mouth transfer efficiency should have a tendency to track each other, since the physical/chemical properties should be similar in both cases. This can be achieved in SHEDS by requesting that these inputs be correlated.

Any of the variables in the General Exposure and Dose Factors section (with the exception of probability vectors) may be correlated with others. The user selects the subset of input variables that will be subject to correlation, and then specifies the pair-wise Spearman correlations. If 'N' variables are selected for correlation, there are N(N-1)/2 distinct pairs. The user does not have to specify all pairs; any that are not given a definite target correlation are assumed to have a target correlation of zero.

SHEDS uses a modified NORTA[4] method to generate the correlations. The random values for the selected set of variables are first generated from a multivariate normal distribution with the correct Spearman correlations. Each normal variate is then transformed to the specified distribution using a rank-preserving transformation function. Since Spearman correlations depend only on rank, the Spearman correlations are preserved. The result is that the inputs will pair-wise exhibit the desired correlations, but will also have the marginal distributions requested by the user.

It is possible to specify correlations that cannot be achieved. As an example, if two variables are to have a perfect correlation of 1.0, then each must have the same correlation as the other with any third variable. Mathematically, a correlation matrix is valid if and only if all its eigenvalues are non-negative; however, SHEDS-Multimedia requires strictly positive eigenvalues. If the set of requested correlations is not allowed, a message is printed on the SAS log when the model is run.

4 The NORTA method is described in the SHEDS technical manual.

To be correlated on input, a variable must:

- be defined in the distributions file (these are the variables edited through the Variability Distributions screen and given in Appendix B, Table B-1), and
- it cannot be a point or probability vector.

Two screens are used to select and define the correlations. The first screen **Select Correlated Variables** (Figure 5-22) is used to choose the variables of interest. After choosing the variables, clicking on the Continue screen takes the user to **Specify Variable Correlations** (Figure 5-25) where specific pairs are assigned target correlation values.

5.7.3.1 Select Correlated Variables

The Select Correlated Variables screen (Figure 5-22) is used to choose which variables will be used to define correlated pairs in the next screen. It does not matter if variables are selected here which are not used later. Only valid variables will be displayed in the Input Variables list box.

Move variables to the Correlate These Variables list box to include them in correlated pairs on the next screen. The single arrow moves the selected variables, the double arrows move all variables. If the user has previously defined correlated pairs, the right hand list box will initially be populated only with variables in those correlated pairs.

Clicking on the Continue button will normally take the user to the Specify Variable Correlations screen. If the user selects less than two variables and clicks on Continue, an error will be displayed (Figure 5-23), correlation will be turned off, and the user will be returned to the Variability Distributions screen.

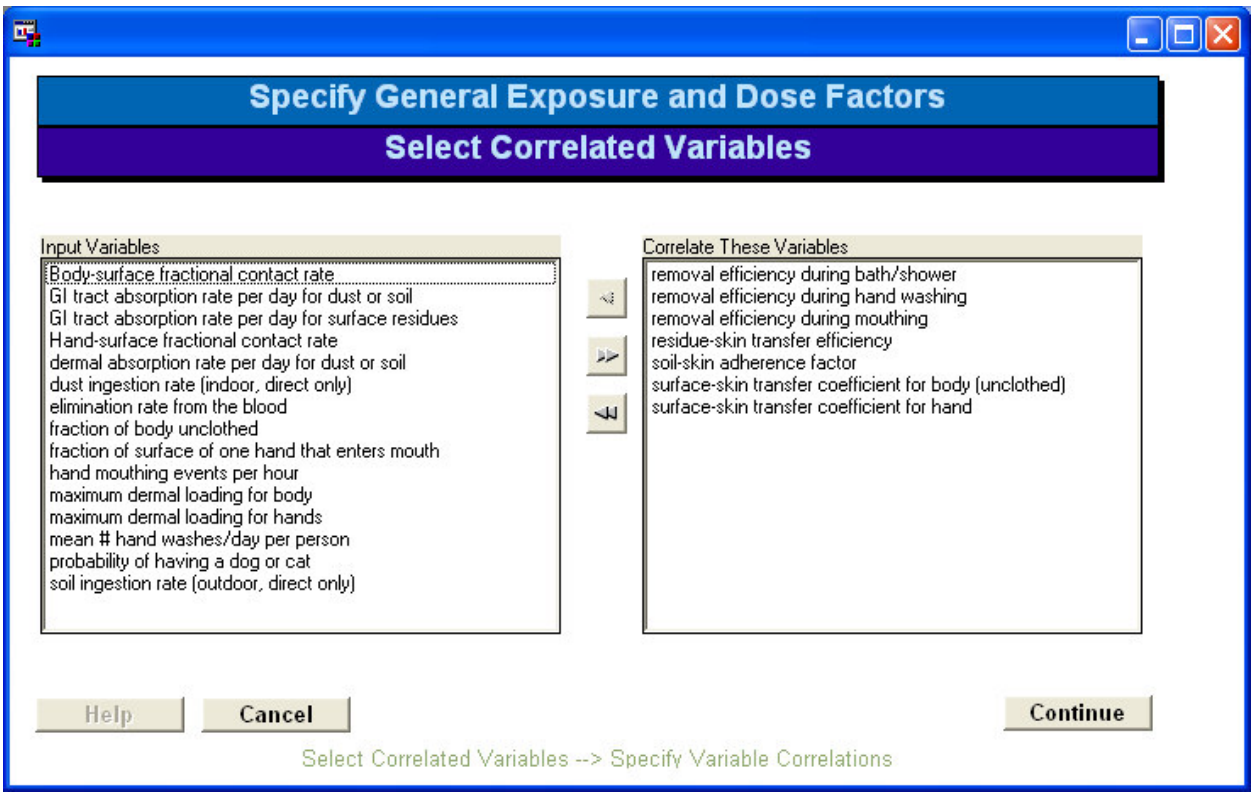


Figure 5-22. Select Correlated Variables Screen.

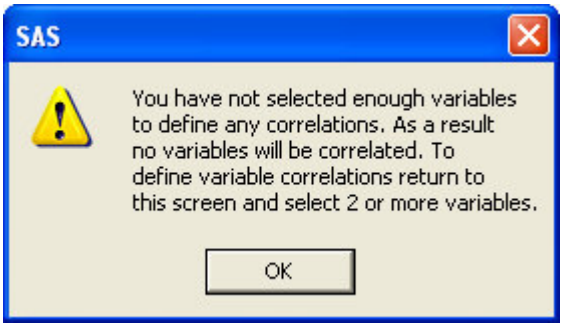


Figure 5-23. Error Displayed if Zero or One Variables are Selected for Correlation.

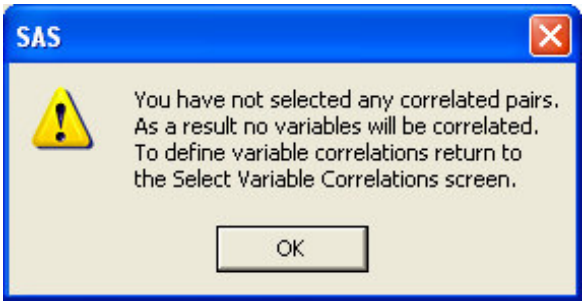


Figure 5-24. Error Displayed if No Variable Pairs are Selected for Correlation.

5.7.3.2 Specify Variable Correlations

This screen (Figure 5-25) is used to define or edit variable pairs and assign a correlation value to the pairs. A correlated pair is represented as two variable names and a correlation value from -1 to 1, inclusive. Note that the numbers in Figure 5-25 are hypothetical and for illustration purposes only; they are not intended to be recommended values.

The variables are ordered. Initially, all but the last variable are displayed in the First Variable list box. The Second Variable list box will contain all variables below the variable highlighted in the First Variable list box. The Second Variable list box will also always include the last variable.

The basic method of selecting a variable pair is to select the first variable in the First Variable list box, select the next variable from the Second Variable list box, specify the correlation value in the spin box to the right, and click on the Add Pair Button. Once added the variable pair will be displayed in the Selected Pairs Specified box on the lower portion of the screen.

If a variable pair selected in the upper list boxes was previously specified and is already listed below, then the Add Pair button will not be enabled. Instead the Replace Pair button is enabled and will replace the correlation value currently specified with the one previously specified for the pair.

The user may find it necessary to resize the columns in the Correlated Pairs Specified area. This area is capable of displaying both variables in the pair and the correlation value. Sometimes the columns are not initialized such that all three are visible.

To delete a pair, highlight the pair in the Correlated Pairs Specified area. This will enable the Delete Pair button. Click on this button and the pair will be removed from the list.

Clicking on Continue saves the values defined and returns the user to the Variability Distributions screen. Once uncertainty is implemented, the user will be returned to the Uncertainty Distributions screen if doing an uncertainty run.

If no correlated pairs are chosen, then an error screen will be displayed (Figure 5-24), and correlation will be turned off in the simulation. Begin from the Variability Distributions screen to turn correlated inputs on once again.

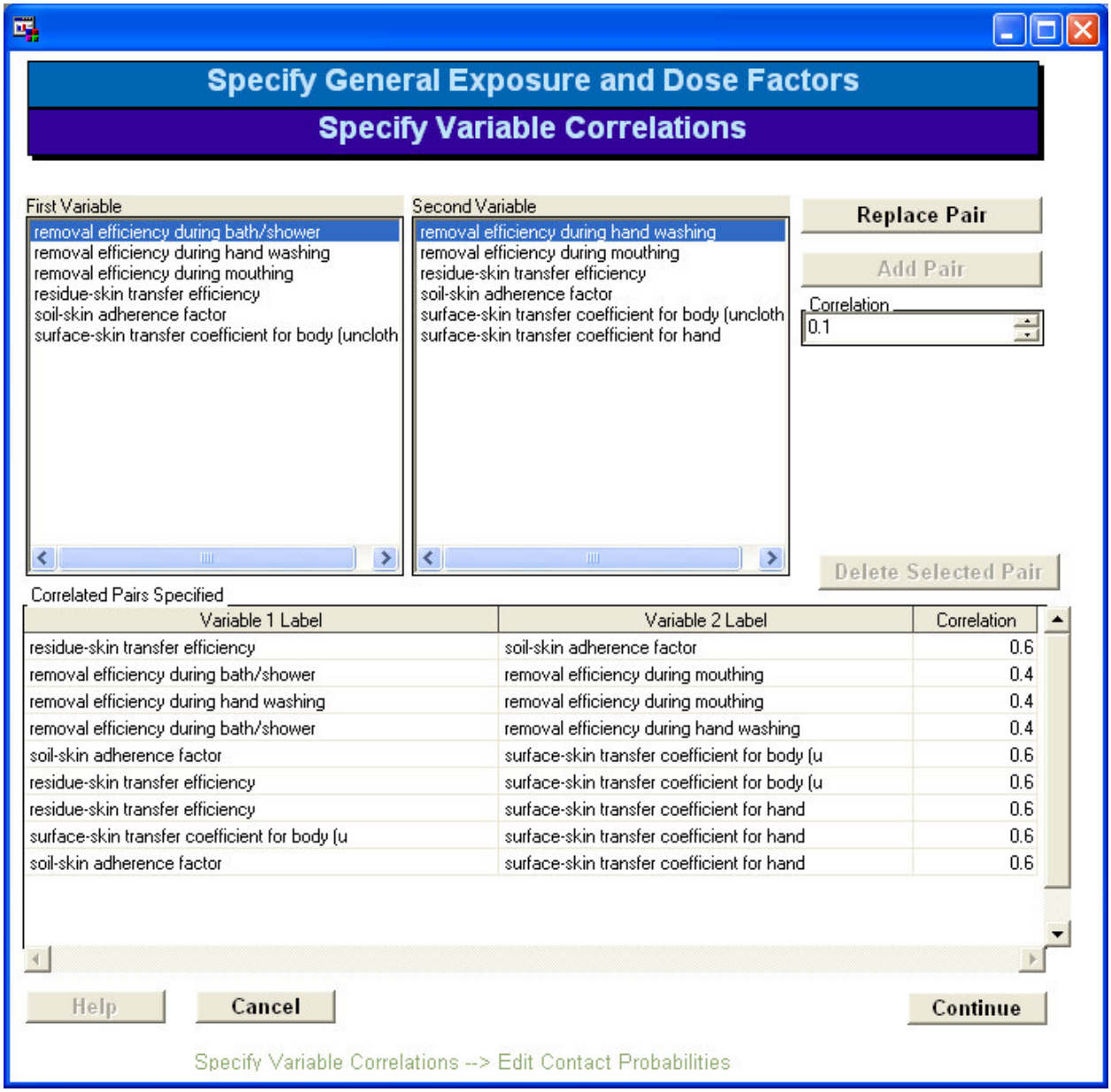


Figure 5-25. Specify Variable Correlations Screen.

5.7.3.3 Contact Probabilities

During each event in the simulation the model must decide where the individual is and what that person is touching. This is done in three stages: the first is deterministic; the second and third are probabilistic.

First, the location, or microenvironment, is decided deterministically based on the person's diary. For a specific diary-day and event this will always resolve to the same value: inside a residence,

outside a residence, inside other (stores, schools, etc.), or inside a vehicle. The SHEDS-Multimedia version 3 GUI includes only allows data entry for the first two of these microenvironments.

Second, the events determined to be inside a residence are stochastically assigned to one of three "sub-microenvironments": treated, untreated, or far away (i.e., neither). A "treated room" in this context refers to a part of the house that has been or will be treated (have chemical applied) during the simulation. An "untreated room" is one which is never directly treated, but may receive chemical contamination from a nearby treated room. The "neither" category refers to rooms which are sufficiently remote from a treatment location that they will always have zero chemical concentration. One common interpretation of "neither" is time spent in houses other than one's own. However, it could also include time in detached buildings at one's home, or even in parts of one's house that are far enough from a treatment location to never acquire any chemical. This will depend on many factors, and judgment may have to be used. A conservative assumption is that all "inside residence" events are either in treated or untreated rooms, in which case the probability of "neither" should be set to a point value of zero.

Third, the surface being contacted is determined probabilistically. If the microenvironment is inside a residence, the possibilities are smooth (e.g., vinyl, hard furniture), textured (e.g., carpet, cloth upholstery), pet, dust, and nothing; if outside, the possibilities are garden, lawn, pet, soil, and nothing. Only one surface is contacted during a single event. It is assumed that one is always in contact with the air. To increase the number of contacts, decrease the maximum event time on the Simulation Information screen (see Figure 5-7).

Figure 5-26 shows the screen used for choosing groups of contact probabilities and editing them. It functions the same as the Variability Distribution Screen (page 46). The user chooses a variable group by selecting one in the Probability Variable Groups list box. This will cause the variables in that group to be displayed in the Variable Descriptions list box. The first group is used to determine the probabilities used in step two above. The other three determine the probabilities for step 3 above. The variable groups are:

1. Inside Residence: probability vector assigning an inside individual to a sub-microenvironment of treated, untreated, or far away (neither).
2. Within Treated Rooms: for an individual that has been determined to be inside and in a treated room, this probability vector is used to assign the contact surface: smooth, textured, pet, no surface.
3. Within Untreated Rooms: as previously for people determined to be in untreated rooms. Possible contact surfaces include: smooth, textured, pet, no surface.
4. Outside Residence: for an individual determined to be outside in the first step, this probability vector assigns the contact surface: lawn, garden, pet, or no surface.

To edit the distributions for the contact probabilities, the user clicks on Specify Inputs. This will display the Edit Contact Probabilities screen (Figure 5-26) with the proper variables available for editing. Once those values are edited and the user returns to this screen, the variable group just edited will be added to the Groups Completed list box. Once all groups have been completed, the Continue button will be enabled. Clicking on the continue button will complete the entry of all of the general exposure and dose variables. The user will be returned to the main screen and be permitted to begin a simulation run.

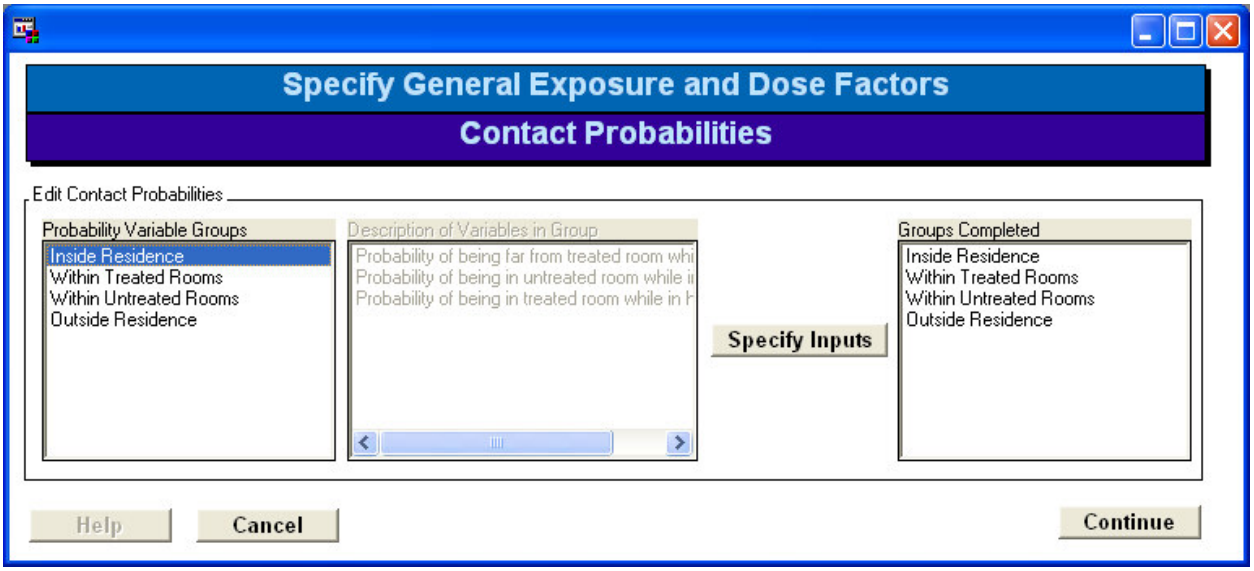


Figure 5-26. Contact Probabilities Screen.

5.7.3.4 Edit Contact Probabilities

This screen (almost identical to Figure 5-20) is used to edit the individual contact probability distributions. The user comes here when the Specify Inputs button is clicked from the Contact Probabilities Screen. It functions exactly like the Edit Variability Distributions screen (Figure 5-20).

The set of probabilities being edited at one time will form a probability vector of mutually exclusive possibilities. For Inside Residence three variables can be assigned distributions. Each variable is a probability, and together they form the probability vector representing the likelihood of that an individual assigned “Inside Residence” will be assigned to one of the three “sub-microenvironments”: treated, untreated, or far away. During the run a value will be selected from each of the probability distributions and the three values will be normalized to equal one. For the remainder of the run this probability vector will represent likelihood of that individual being assigned to the three “sub-microenvironments”.

The other probability vectors work the same way with one exception. An individual without a pet, (or lawn, or garden) cannot contact that surface. In this case those probabilities are set to zero before the vector is normalized.

The screen will always have the same basic layout, but the specific variables that can be edited will change based on the variable group highlighted when the Specify Inputs button was clicked. The third title, in blue, will always indicate the variable group being edited. Below the Help, Cancel, and Save buttons are a series of container boxes for editing individual variables. The variable description is given on the container box. The distribution for a variable is defined by first selecting the desired distribution type and then filling in the individual parameter values.

To accept the current values click on the Save button. If any of the parameter values are in error, they will be highlighted in yellow and the Save button will be disabled. Clicking on the Cancel button returns the user to the Contact Probabilities screen without saving any changes.

More detailed information on editing distributions is given in "Individual Distribution Widgets" in Section 2.3.5.

5.8 Run Simulation

Only when all information has been specified will the Run Simulation button on the main menu (see Figure 5-1) be enabled. Clicking on it brings the user to the Run Simulation screen (Figure 5-27). The screen displays the current run name and estimated run time. If 20 or fewer people are being simulated, then the user will have the option of turning on the diagnostic mode.

"Write Inputs to Excel" generates a file containing all of the user editable model inputs. The file is an XML file, but can be read by MS Excel 2003 or later. The file is placed in the install directory and is named using the run name and the standard Excel file extension (.xls).

"Check Input for Errors" forces two routines to run and check inputs. Comments and errors will be displayed to the log which will be made visible if is not already. These same checks are also carried out when the simulation is run.

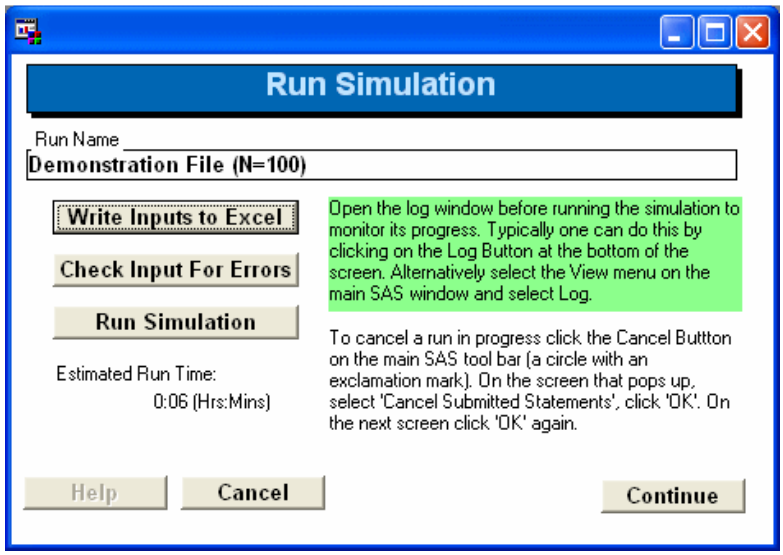


Figure 5-27. Run Simulation Screen.

Clicking on “Run Simulation” will begin the simulation. Informational messages will be displayed in the log (Figure 5-28). Among other items, the number of people completed and the number total are indicated as the run progresses. When the simulation is completed, the final timing information will be displayed in the log. Clicking the Continue button after run completion will return one to the main menu where View Results can be selected.

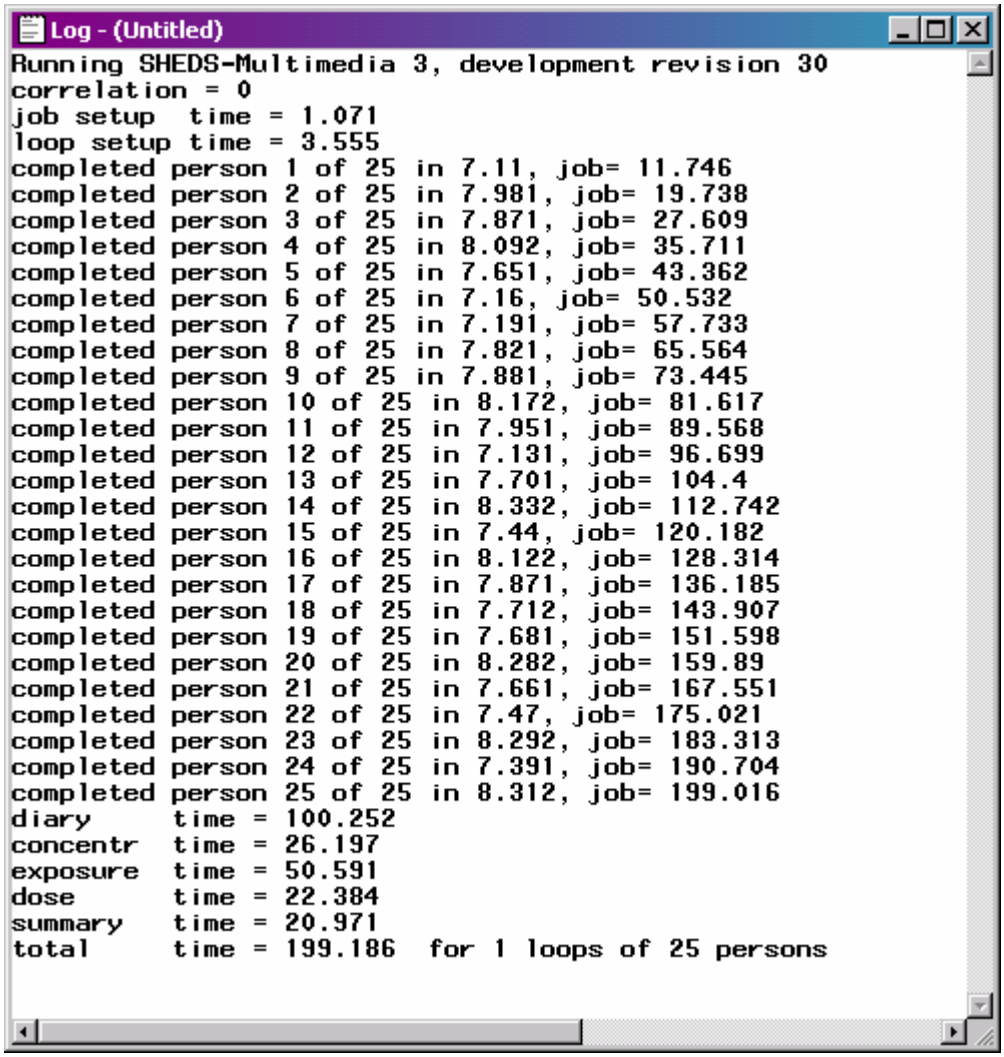
Typically you will want to open the log window before running a simulation. If the log window has been minimized, clicking the button along the bottom of the main SAS window will open it. This can be done after the run has started. If not open yet, the log window can be opened by selecting the View menu on the main SAS menu bar and then selecting Log. This must be done before the simulation has started.

The correlated pairs are checked for validity at the beginning of the run. If problems are found an error message will be printed in the log.

The diagnostic mode is only available for simulations with twenty or fewer people. The option for diagnostic mode does not show up if using the Demonstration File since that has 100 individuals. Typically, a user will not want to run in diagnostic mode. If one is very familiar with the model it may be helpful in locating errors. Three things happen when the model is run in diagnostic mode.

1. SAS prints detailed notes to the log detailing how macros were compiled and data steps completed.
2. Intermediate variables are saved on the datasets. This option is also available on the Simulation Information screen.
3. Event level datasets and variables are saved for each individual simulated.

Once started, the run can be cancelled by following the instructions on the Run Dialog.



```
Log - (Untitled)
Running SHEDS-Multimedia 3, development revision 30
correlation = 0
job setup  time = 1.071
loop setup time = 3.555
completed person 1 of 25 in 7.11, job= 11.746
completed person 2 of 25 in 7.981, job= 19.738
completed person 3 of 25 in 7.871, job= 27.609
completed person 4 of 25 in 8.092, job= 35.711
completed person 5 of 25 in 7.651, job= 43.362
completed person 6 of 25 in 7.16, job= 50.532
completed person 7 of 25 in 7.191, job= 57.733
completed person 8 of 25 in 7.821, job= 65.564
completed person 9 of 25 in 7.881, job= 73.445
completed person 10 of 25 in 8.172, job= 81.617
completed person 11 of 25 in 7.951, job= 89.568
completed person 12 of 25 in 7.131, job= 96.699
completed person 13 of 25 in 7.701, job= 104.4
completed person 14 of 25 in 8.332, job= 112.742
completed person 15 of 25 in 7.44, job= 120.182
completed person 16 of 25 in 8.122, job= 128.314
completed person 17 of 25 in 7.871, job= 136.185
completed person 18 of 25 in 7.712, job= 143.907
completed person 19 of 25 in 7.681, job= 151.598
completed person 20 of 25 in 8.282, job= 159.89
completed person 21 of 25 in 7.661, job= 167.551
completed person 22 of 25 in 7.47, job= 175.021
completed person 23 of 25 in 8.292, job= 183.313
completed person 24 of 25 in 7.391, job= 190.704
completed person 25 of 25 in 8.312, job= 199.016
diary      time = 100.252
concentr   time = 26.197
exposure   time = 50.591
dose       time = 22.384
summary    time = 20.971
total      time = 199.186  for 1 loops of 25 persons
```

Figure 5-28. Log Screen after Running a Small Simulation.

5.9 View Results

Model results from previous or current SHEDS simulations can be viewed by selecting the View Results button on the main window. This button will become active once a simulation run has been made or after a previously run simulation is specified in the Run Name dialog. Pressing this button opens a dialog (Figure 5-29) allowing the user to select one of the following:

- View Results for the Population,
- View Results for an Individual,

Each of these buttons opens a new dialog.

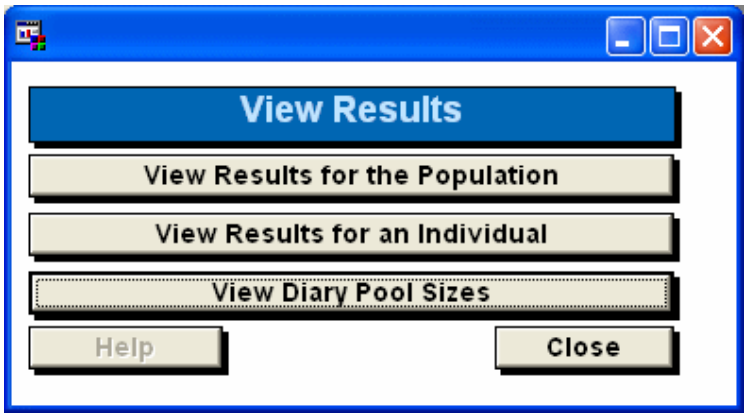


Figure 5-29. View Results Screen.

5.9.1 Additional Outputs and Files

A number of outputs cannot be viewed through the interface. For information on the log files, export files, and exporting files from SAS for analysis in other software see Appendix A for more information.

5.9.2 View Results for the Population

The View Results for the Population window is used to generate graphical or tabular results for output variables for the population as a whole, or for subgroups of the population. The outputs will utilize the average daily values for the simulation just run or that specified most recently in the Run Names dialog. When considering the population, the output variables of utilized are the daily values (of exposure, dose, etc.) for each person, averaged over the simulation period. The outputs generated examine the variability of these personal mean daily values over the population.

In general the user will want to work from the top down, selecting the output units and thus the output dataset of interest, then the sub-population of interest, output type, and specific variables desired.

The Run Name box shows the name of the current run, while the Output Data Set supplies the name of the corresponding SAS dataset that will be used to generate the results.

The Output Units menu is used to indicate the units for the output data, either Milligrams per Kilogram body weight or Micrograms. The appropriate output dataset will be displayed in the Output Data Set box.

The menus in the Select Population box (Gender, Start Age, Stop Age, Min Rank, and Max Rank) can be used to select a subgroup of the run population for analysis. Subsetting is based on

the fact that each simulated individual is assigned a specific age, gender and bin rank. The entire simulated population is divided into 100 bins labeled 0 to 99; as nearly as possible, the bins contain the same number of people. (If the simulated population is less than 100, some of the bins will be empty and will not appear in the pull down menu.) The bins are ranked based on the total chemical absorption over the entire simulation period. The user may subset the population by restricting the age range, gender, bin rank, or any combination of these. For example, the user may choose to examine only the women or only the children. The pull down menus only display genders, ages, and ranks that exist in the output dataset. The final selections and count of individuals will appear on any resulting tables and graphics generated. The Selected Count field updates after each user selection to display the final number of people in the sub-group.

The Output Type list box includes the analyses that may be performed. The user selects one option from this list at a time. The options for results analyses in SHEDS-Multimedia version 3 are the following:

- Summary Table
- CDF (Cumulative Distribution Function)
- Box and Whiskers
- Contribution by Pathway

Pressing the Display button then performs the analysis and displays the results in a new window. That window must be closed to return to this dialog to define new outputs.

The Variable Groups and Select Variables menus are used to select the model output variables to analyze. The Variable Groups menu is used to pick a general category of model variables (such as dose, exposure, or loading variables). Selecting this variable group will update the Select Variables menu to include all corresponding model variables. For example, in Figure 5-30 the Variable Group selected is Absorption: New, so the Select Variables menu has been updated to include all the corresponding absorption variables. The user then selects one or more variables from this list to analyze. Clicking on display generates the output. Specific details of each of the Output Types are covered next.

The dose/exposure terminology varies slightly between the figures generated, the dialog menu, this manual, and the Technical Manual; the differences are summarized in Table 5-1.

Table 5-1. Output Variable Group and Dose/Exposure Terminology Differences

Short Description	Pull Down Menu Text	Technical Manual Term
Absorption	Absorption: New	Absorption or absorbed dose
Exposure	Exposure: New	New exposure
Dose	Dose (chemical mass in blood)	Blood dose
Elimination	Eliminated Dose (urine)	Elimination
Loading	Loading (chemical mass on body part)	Running Exposure

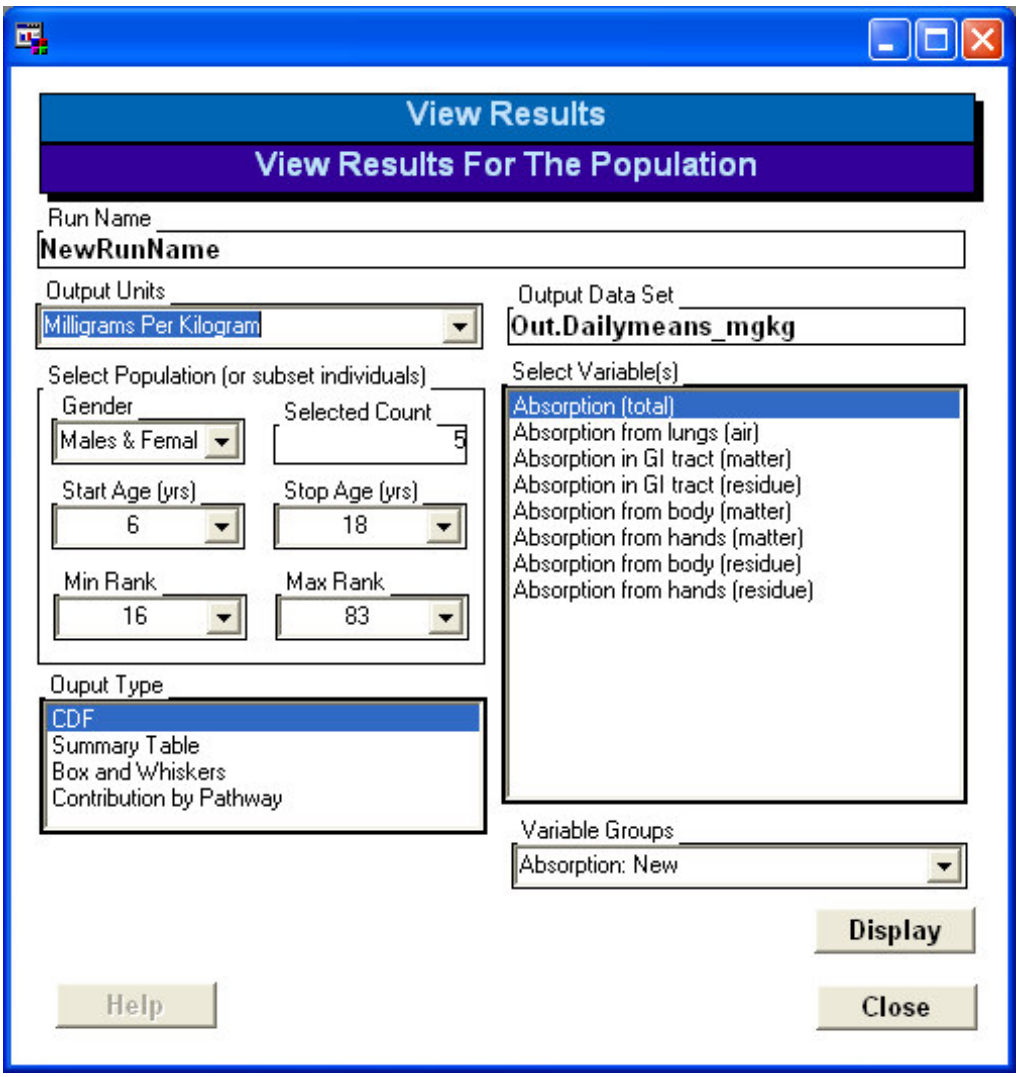
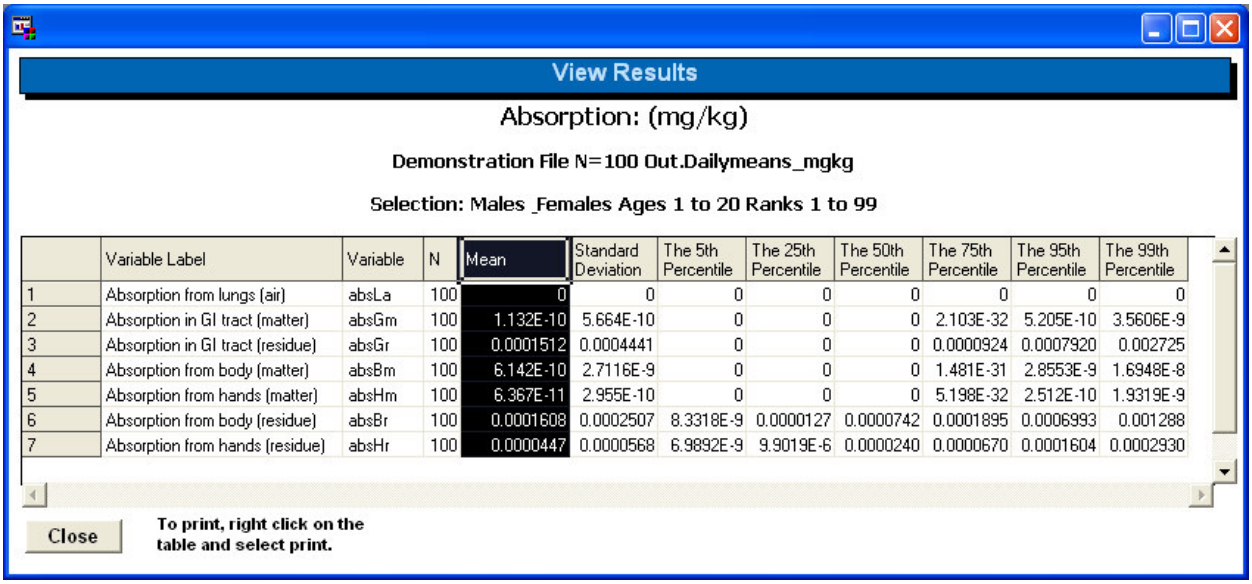


Figure 5-30. View Results for the Population Screen.

5.9.2.1 Summary Table

Selecting this option yields a summary statistics table for the selected variable(s) and specified model simulation, including sample size, mean, standard deviation, median, 5th,25tt, 75th, 95th, and 99th percentiles. An example is shown in Figure 5-31. If multiple variables are analyzed, the results are displayed on individual rows of the table; the variable name and description (label) are included on each row. Again, note that the subpopulation that is being examined is printed in the table window – in this hypothetical example the user is examining males and females between the ages of 4 and 19.



View Results

Absorption: (mg/kg)

Demonstration File N=100 Out.Dailymeans_mgkg

Selection: Males _Females Ages 1 to 20 Ranks 1 to 99

	Variable Label	Variable	N	Mean	Standard Deviation	The 5th Percentile	The 25th Percentile	The 50th Percentile	The 75th Percentile	The 95th Percentile	The 99th Percentile
1	Absorption from lungs (air)	absLa	100	0	0	0	0	0	0	0	0
2	Absorption in GI tract (matter)	absGm	100	1.132E-10	5.664E-10	0	0	0	2.103E-32	5.205E-10	3.5606E-9
3	Absorption in GI tract (residue)	absGr	100	0.0001512	0.0004441	0	0	0	0.0000924	0.0007920	0.002725
4	Absorption from body (matter)	absBm	100	6.142E-10	2.7116E-9	0	0	0	1.481E-31	2.8553E-9	1.6948E-8
5	Absorption from hands (matter)	absHm	100	6.367E-11	2.955E-10	0	0	0	5.198E-32	2.512E-10	1.9319E-9
6	Absorption from body (residue)	absBr	100	0.0001608	0.0002507	8.3318E-9	0.0000127	0.0000742	0.0001895	0.0006993	0.001288
7	Absorption from hands (residue)	absHr	100	0.0000447	0.0000568	6.9892E-9	9.9019E-6	0.0000240	0.0000670	0.0001604	0.0002930

Close

To print, right click on the table and select print.

Figure 5-31. Example Summary Table for a Population.

5.9.2.2 CDF

This option yields a cumulative distribution function (CDF) plot for the selected variable(s) and specified model simulation. The plot illustrates how the percentiles of the selected variable(s) behave as a function of the variable value. Each selected variable will appear as a separate line on the plot; a legend appears at the bottom of the plot to identify each variable. An example is shown in Figure 5-32. In the example, the CDFs for seven absorption variables are plotted (only three can be seen in this particular case, since all the percentiles for the others were zero in this simulation.) The plot can be printed by clicking on the Print button. The default printer will be used and the plot will be formatted for default SAS printer.

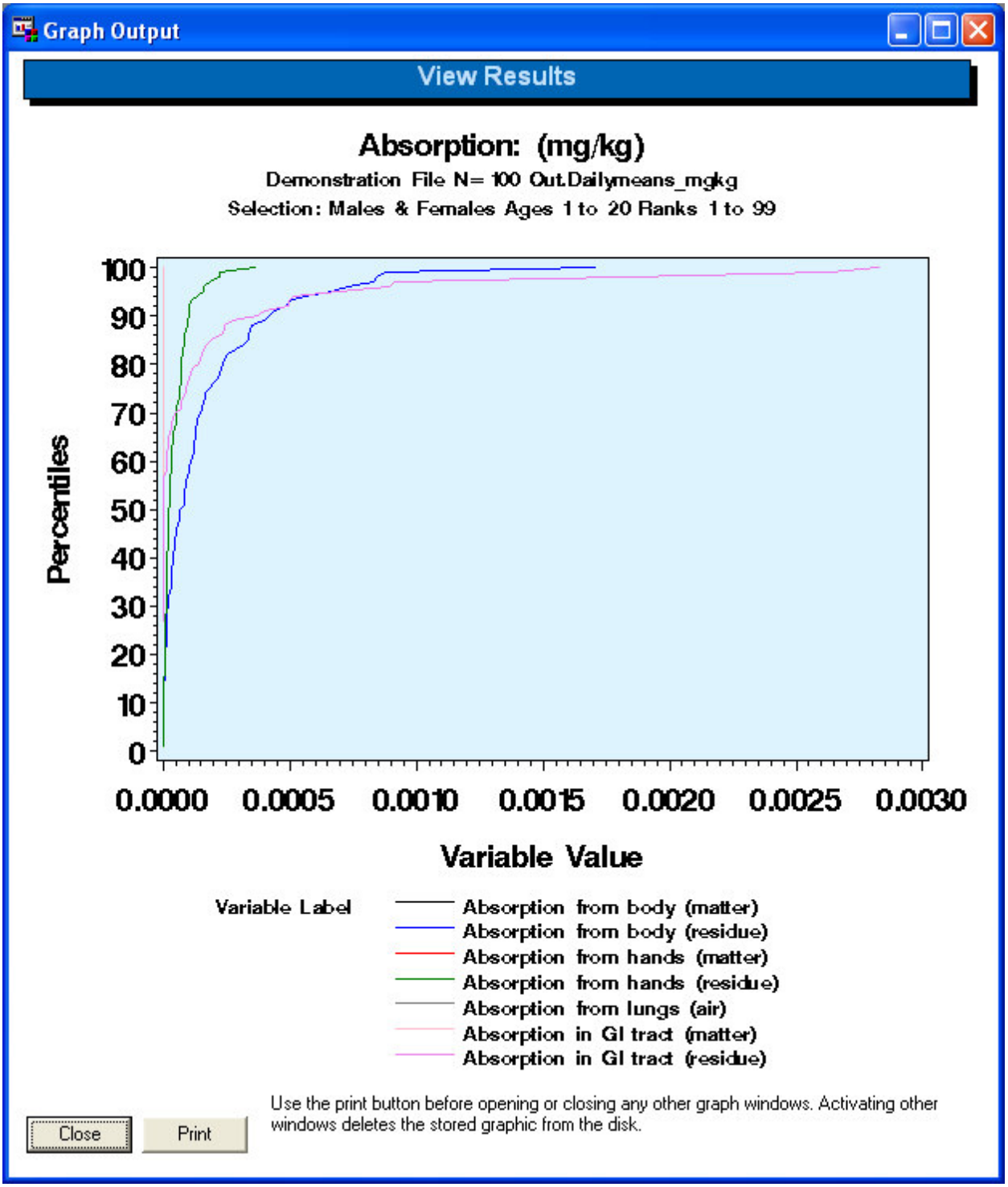


Figure 5-32. Example CDF for a Population.

5.9.2.3 Box and Whiskers

Selecting the Box and Whiskers option yields a box and whiskers plot for the selected variable(s) for the current simulation for the defined population subgroup. Multiple variables are shown on a single plot. An example for seven absorption variables is given in Figure 5-33. Unlike other plots, the Box and Whiskers plots use the variable names rather than the variable labels. The longer labels will overwrite one another or be suppressed by SAS. The boxes, whiskers, and other symbols on the plot are interpreted as follows:

- The midlines of the boxes are equal to the median
- The plus (+) symbol inside the boxes is equal to the mean
- The upper edge of the box is the 75th percentile of the population, while the lower edge is the 25th percentile. Thus, these edges define the width of the interquartile range (IQR).
- The whiskers define the maximum or minimum observations that fall within 1.5 times the IQR, measured from the quartile value (i.e., the 75th or 25th percentile).
- The square symbols indicate data points outside of the range defined by 1.5 times the IQR.

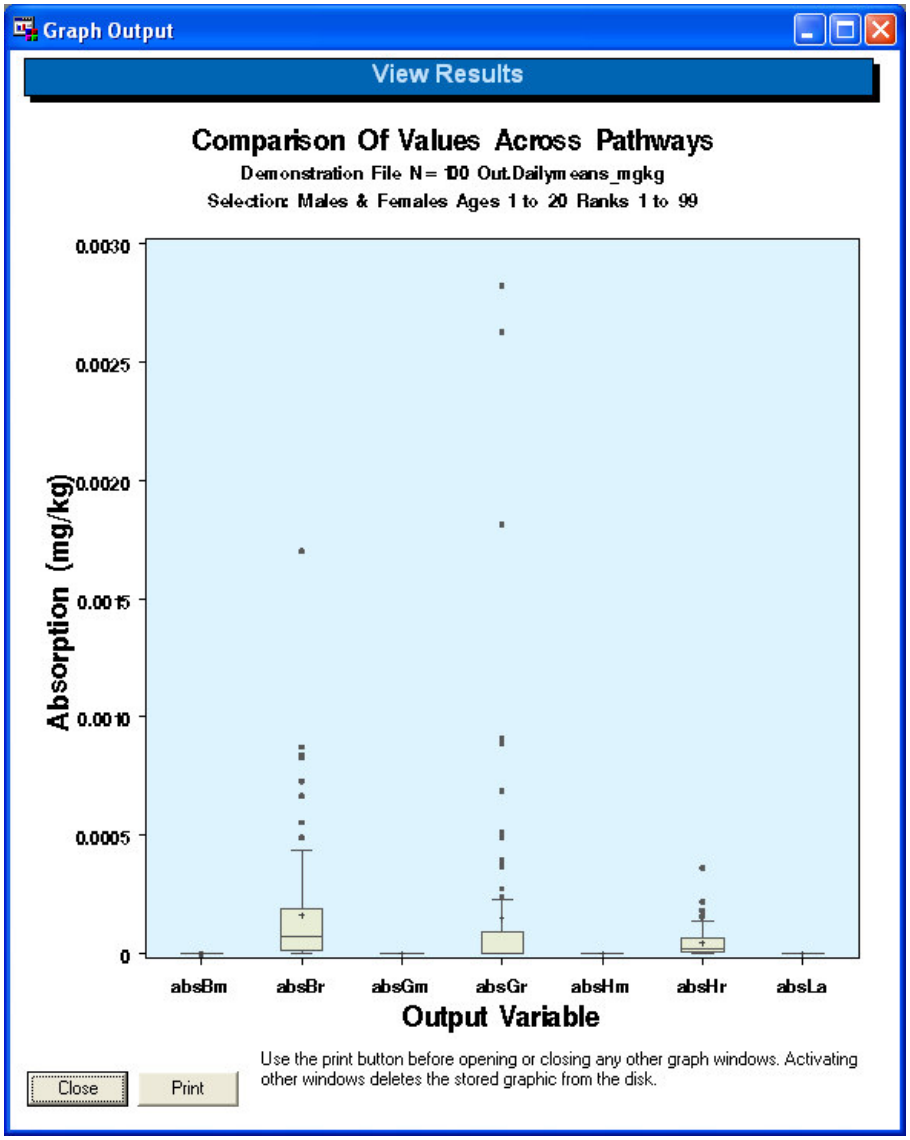


Figure 5-33. Example Population Box and Whiskers Plot.

5.9.2.4 Contribution by Pathway

The Contribution by Pathway option is different from the other options in the Output Type menu. It does not require (or allow) selection of individual model variables. Only a selection from the Variable Group menu is required: Dose, Exposure, Absorption, or Loading. Clicking on Display yields a pie chart showing percent contribution to one of these summary variables (based on population or population subgroup means) for the following pathways:

- **Body Residue:** The chemical mass contained in residues transferred from surfaces to the skin (excluding the hands). Possible surfaces include smooth surfaces, textured surfaces, the lawn, the vegetable garden, and pets.
- **Body Soil/Dust:** The chemical present in soil (outdoors) or dust (indoors) that is transferred onto the skin (excluding the hands).
- **GI Tract Residue:** The chemical mass contained in residues transferred from surfaces to the gastrointestinal (GI) tract. Some of the GI tract residues may have first transferred to the hands before being ingested.
- **GI Tract Soil/Dust:** The chemical present in soil (always found outdoors) or dust (always found indoors) that is transferred into the GI tract.
- **Hands Residue**: The chemical mass contained in residues transferred from surfaces to the skin on the hands. This is tabulated separately from the body since the model allows chemical on the hands to subsequently be transferred to the GI tract by hand mouthing, while chemical on the rest of the body is not transferred in this manner.
- **Hands Soil/Dust:** The chemical present in soil or dust that is transferred to the skin on the hands. If indirect soil/dust ingestion is chosen, then this can subsequently be transferred to the GI tract. If direct ingestion were chosen instead, then the amount of soil and dust entering the GI tract is determined without reference to the amount on the hands.
- **Inhalation:** The amount of chemical mass in air that enters the lungs. The mass is determined by multiplying the chemical concentration in air by the volume of air inhaled. Since the latter quantity is time dependent, the inhalation exposure becomes larger for the longer-duration diary events.

A hypothetical example is given in Figure 5-34. In this example, the largest single contributor to the variable under consideration (Exposure) is body residue.

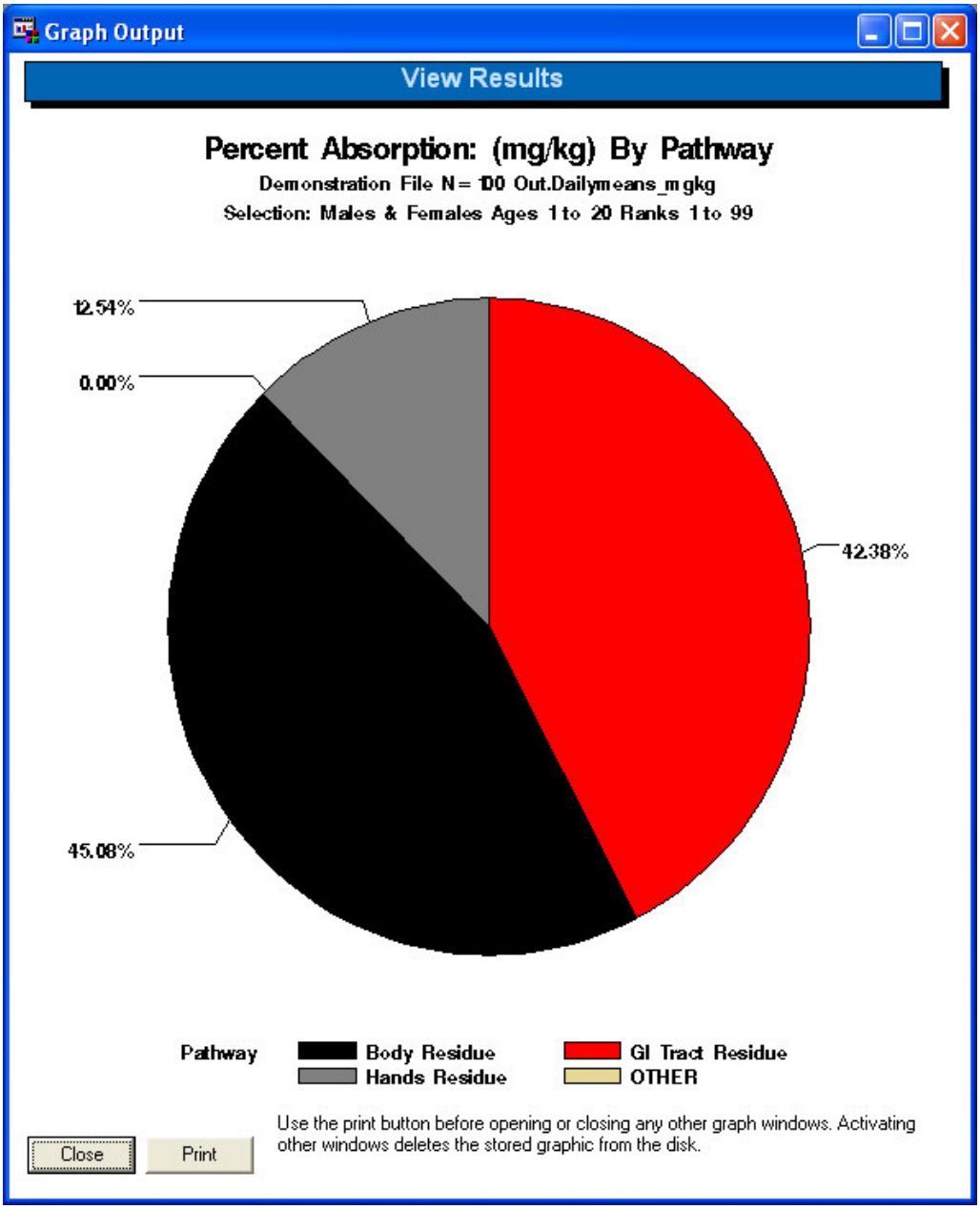


Figure 5-34. Example Pie Chart Showing the Contribution by Pathway for a Population.

5.9.3 View Results for an Individual

The second results window accessible from View Results is the View Results for Individual. Selecting this button brings up the window for performing analysis of the results for a single individual within a simulation run. Many of these options are similar to those for View Results for Population. When considering an individual, the output variables of interest are the daily values for the selected individual. Obviously, a specific simulated individual must be selected. Additionally, the analysis may be limited to a specific time period. As on the population results screen, it is best to work from the top down on the left side of the screen, and then choose the Variable Group and specific variables of interest. All resulting outputs will contain a second title giving the basic individual statistics and dates considered in the analysis.

The View Results for an Individual dialog is shown in Figure 5-35. The Run Name box shows the name of the current run, while the Output Data Set supplies the name of the corresponding SAS dataset that will be used as the basis of the results. The output dataset is dependent on the units chosen. As in the Results for Population window, one can select genders, an age range, and a rank range in the Select Population box. In this case, the Select Individuals list box is populated only with individuals meeting these criteria. The individual list box provides minimal information on each individual: the identifier used in the simulation, the gender (shown as 'M' or 'F'), age, and the individual's rank or percentile of total absorption. The user clicks on an individual to select and then analyze data from that individual.

In addition to selecting an individual, the user may also select a particular range of dates to analyze from the Dates of Interest menu. The Start Date and Stop Date may be selected the corresponding menus, which are populated with all the dates covered by the current simulation.

The output options for viewing variability results for an individual are listed in the Output Type list box. These include:

- Time-Series;
- CDF (Cumulative Distribution Function);
- Box and Whiskers;
- Contribution by Pathway;
- Summary Table; and
- Detailed Table.

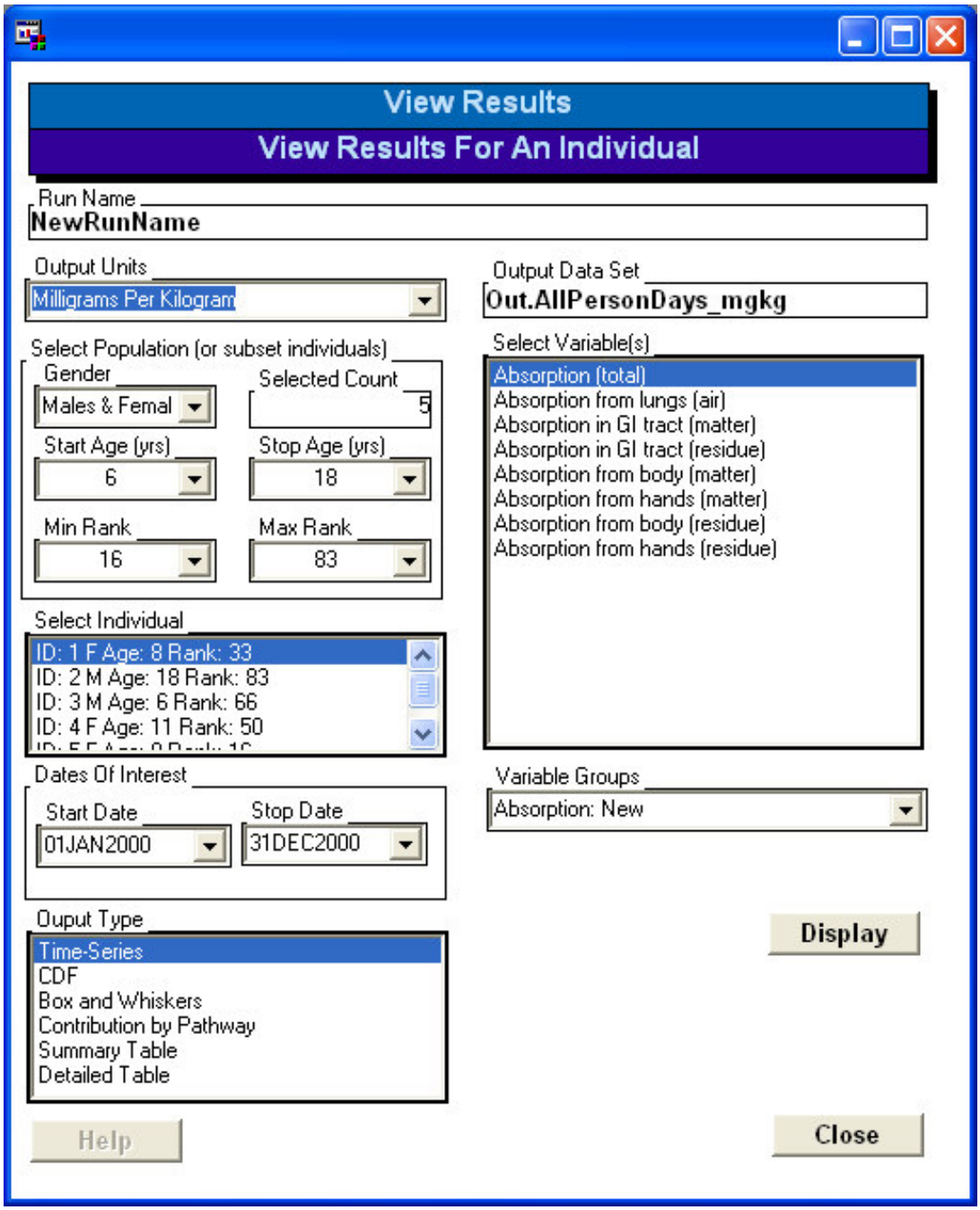


Figure 5-35. View Results for an Individual Screen.

As in the View Results by Population dialog, the output units may be selected as either Microgram or Milligrams per Kilogram from the Output Units menu, and the Variable Groups and Select Variables menus are used to select the model output variables to analyze. As before, multiple variables may be selected for analysis. The appropriate analysis variables will automatically be chosen for Contribution By Pathway. All variables will automatically be used for the detailed table. Each of the output types are described next.

5.9.3.1 Time-Series

Selecting the Time-Series button produces a time-dependent plot of the selected variable(s). Each data value on the plot is the value for a single day in the simulation. Multiple variables will be plotted as multiple curves on the same time-series plot; the legend that appears at the bottom of the plot identifies which variable is associated with each plotted curve. Time-Series simulations are useful for observing the behavior of dose, exposure, loadings, or absorption in the days following a pesticide application. An example showing seven absorption variables (some of them essentially equal to 0) is given in Figure 5-36.

5.9.3.2 CDF

The CDF option for an individual is similar to that for the population (See Figure 5-32). The option yields a cumulative distribution function plot for the daily values of the selected variable(s) for the specified individual. Each selected variable will appear as a separate line on the plot; a legend appears at the bottom of the plot to identify each variable.

5.9.3.3 Box and Whiskers

The Box and Whiskers option for an individual is similar to that for the population (see Figure 5-33 on page 66 and the previous discussion), with the exception that the plot is generated by examining the daily variable values for a single person rather than the mean daily values for the population. Selecting Box and Whiskers and clicking on Display will yield a plot for the selected variable(s) for the current simulation, selected person,

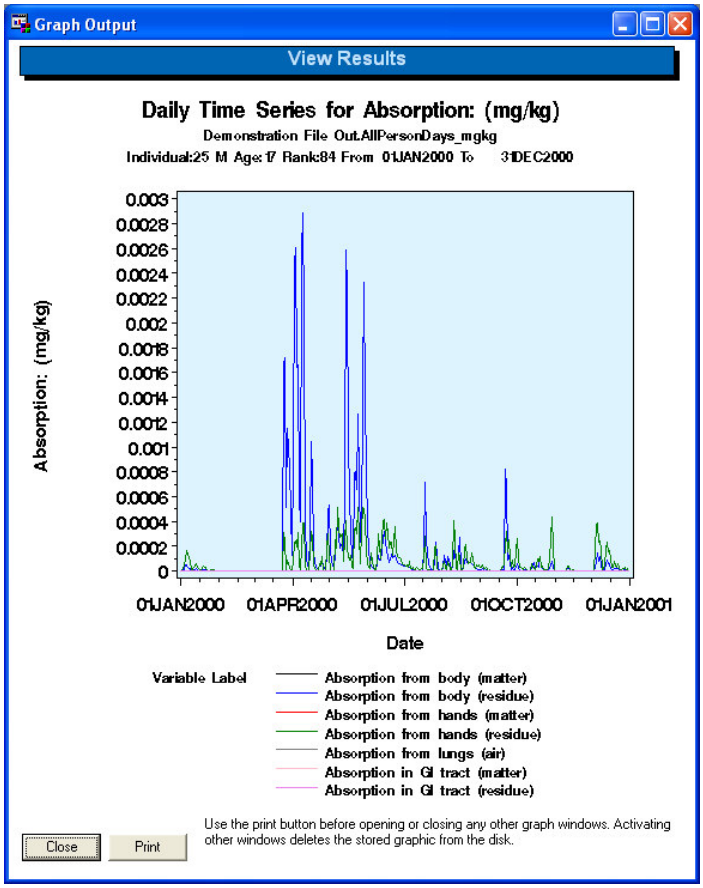


Figure 5-36. Example Time-Series for an Individual.

and selected dates. Multiple variables are shown on a single plot.

5.9.3.4 Contribution by Pathway

The interpretation of the Contribution by Pathway option for an individual is identical to that for the population. As before, this option does not require or permit selection of individual model variables; only the Variable Group needs to be specified--Dose, Exposure, Absorption, or Loading. (The Select Variables menu will be inactive if Contribution by Pathway is selected). Selecting Display then yields a pie chart showing percent contribution to one of these summary variables by pathway. See the earlier discussion on page 66 for additional details.

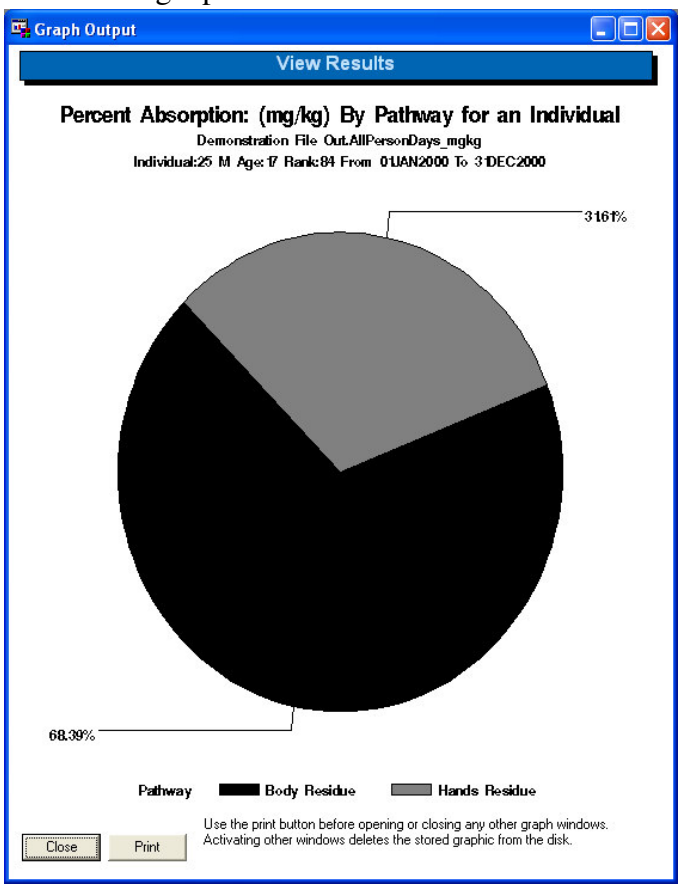


Figure 5-37. Example Pie Chart Showing the contribution by pathway for an individual.

5.9.3.5 Summary Table

If Summary Table is selected, clicking on Display will open a new window containing the percentiles of the selected variable(s), with each variable appearing on its own row in the table. Specifically, the table contains the sample size, mean, standard deviation, median (p50), 5th percentile (p05), 25th percentile (p25), 75th percentile (p75), 95th percentile (p95), and 99th percentile. The age and gender of the individual being examined appears in the descriptive heading. The resulting table looks very similar to the summary table for the population (see Figure 5-31), with the exception that the statistics represent the variation in the variables across days for a single person (rather than the variation in the averaged daily values across persons).

5.9.3.6 Detailed Table

Selecting the Detailed Table option opens a new window and displays a table that contains detailed information for all daily average variables generated by the model (Figure 5-38). It is not required or permitted to select a variable group or specific variables. The detailed table contains one row for each of the days being analyzed. The table contains the year, month, and day, the number of diary events for the day, and the values for each model variable related to the Variable Group. All variables will not fit on the screen at once. The scroll bar at the bottom of the window can be used to view the variables that appear to the right.

View Results

Absorption: (mg/kg)

Demonstration File Out.AllPersonDays_mgkg

Individual:25 M Age:17 Rank:84 From 01JAN2000 To 31DEC2000

	year	month	day	numevents	New exposure on hands (residue)	New exposure on hands (matter)	New exposure on body (residue)	New exposure on body (matter)	New GI tract exposure (residue)	New GI tract exposure (matter)	New exposure in lungs (air)	Hand-to-mouth transfer (residue)	Hand-to-mouth transfer (matter)
1	2000	1	1	45	0.0005423788	0	0.0000649554	0	0	0	0	0	0
2	2000	1	2	45	0.0013086779	0	0.0002119785	0	0	0	0	0	0
3	2000	1	3	35	0.0077826981	0	0.0021549869	0	0	0	0	0	0
4	2000	1	4	35	0.0090457132	0	0.0025256305	0	0	0	0	0	0
5	2000	1	5	35	0.0043012457	0	0.0008109217	0	0	0	0	0	0
6	2000	1	6	35	0.0053764162	0	0.0010057031	0	0	0	0	0	0
7	2000	1	7	35	0.0057079914	0	0.0018959812	0	0	0	0	0	0
8	2000	1	8	45	0.001948092	0	0.0006239717	0	0	0	0	0	0
9	2000	1	9	45	0.0005491866	0	0.000408084	0	0	0	0	0	0
10	2000	1	10	35	0.0011498622	0	0.0004871039	0	0	0	0	0	0

Close

To print, right click on the table and select print.

Figure 5-38. Example Detailed Table for an Individual.

5.9.4 View Diary Pool Sizes

Activity diaries are selected at random from pools that are characterized by different personal and temporal characteristics. Figure 5-39 provides an example of counts of diaries available for each diary pool as determined by the user's inputs for the simulations. The user is reminded that larger diary pools better represent the population.

View Results

Diary Pool Sizes in Diary-Days for Current Run

Season: P-Spring, S-Summer, F-Fall, W-Winter

Weekend: 0-Weekday, 1-Weekend Day

	cohort	Label	gender	subgroup	season	weekend	diarycount
1	3	1 to < 2 years	F	1	P	0	96
2	3	1 to < 2 years	F	2	P	1	70
3	3	1 to < 2 years	F	3	S	0	52
4	3	1 to < 2 years	F	4	S	1	36
5	3	1 to < 2 years	F	5	F	0	38
6	3	1 to < 2 years	F	6	F	1	30
7	3	1 to < 2 years	F	7	W	0	16
8	3	1 to < 2 years	F	8	W	1	13
9	4	1 to < 2 years	M	1	P	0	82
10	4	1 to < 2 years	M	2	P	1	66
11	4	1 to < 2 years	M	3	S	0	34
12	4	1 to < 2 years	M	4	S	1	34
13	4	1 to < 2 years	M	5	F	0	50
14	4	1 to < 2 years	M	6	F	1	41
15	4	1 to < 2 years	M	7	W	0	22
16	4	1 to < 2 years	M	8	W	1	11
17	5	2 to < 3 years	F	1	P	0	84
18	5	2 to < 3 years	F	2	P	1	75
19	5	2 to < 3 years	F	3	S	0	50
20	5	2 to < 3 years	F	4	S	1	33

Close

To print, right click on the table and select print.

Figure 5-39. Example Diary Pool Size Table.

6 SHEDS-Multimedia: Batch Mode

The SHEDS model may also be run in batch mode. Runs in batch mode do not open any SAS windows. They are usually submitted via the Run dialog on the Start menu in Windows. Batch mode uses fewer computer resources, which may speed up long runs. This may be appropriate for overnight runs where the user has no need to view the progress of the job. Multiple batch jobs may be submitted at one time, also useful for overnight runs. Finally, the GUI does not currently support the running of SHEDS in sensitivity analysis or uncertainty analysis mode. Such runs may be conducted in batch mode, or by submitting the appropriate commands in a standard SAS session.

6.1 Installing Batch Capability

Along with the SAS program "Multimedia3.sas" and the default input files used by the interface, two additional files ("batchmultimedia.sas" and "multimedia.bat") are needed to run SHEDS-Multimedia in batch mode.

The file "batchmultimedia.sas" does not require editing. Its contents are:

```
%Let comma = %index(%quote(&sysparm),%str(,));
%Let dir = %substr(%quote(&sysparm),1,%eval(&comma-1));
%Include "&dir\prg\multimedia3.sas";
%multimedia3(&sysparm);
```

The other file is "multimedia.bat", which must have its path names altered to match the SHEDS installation directory on the user's machine. The default contents of "multimedia.bat" are shown below.

```
"C:\Program Files\SAS\SAS 9.1\sas.exe"
"C:\Multimedia\prg\batchmultimedia.sas"
-sysparm "C:\multimedia,%1 %2 %3 %4 %5"
```

In the batch file, the text should be on a single line with spaces where there are currently line breaks. The command in this file contains three pathnames which may need to be edited. The first is the location of the sas.exe file itself. The second gives the location of the "batchmultimedia.sas" program, which is usually in the \prg directory under the SHEDS Multimedia installation directory. The third (the part up to the comma) gives the location of the installation directory itself. The file can be edited in any text editor.

6.2 Defining Inputs for a Batch Run

The main difficulty in submitting a SHEDS run is ensuring that all the necessary inputs are defined. This is a primary function of the interface itself. Hence, the easiest way to prepare a batch run is to define and save all the inputs using the interface. Inputs for several runs could be

defined and saved without submitting any of these jobs. Alternatively, the user could prepare the required input files using a standard SAS editor, but this places a greater burden on the user to ensure that all inputs have been supplied in a consistent manner.

Each set of inputs and settings is saved under a user-supplied job name. For example, suppose the user chooses the name "job1". Whether defined through the interface or not, this requires the addition of a new record to the "runinfo" file found in the SHEDS installation directory, and new directories called "runs\job1\input" and "runs\job1\output" need to be created. Appropriate versions of the following SAS datasets must be placed in the \input directory:

agegroups
applications
appmedia_decay
appmedia_postapp
contactmedia
cooccurrence
correlations
diarydetails
distributions
modeldates
timeseries
userdates

These steps are automatic if the interface is used to define the job.

6.3 Submitting a Batch Run

To submit a SHEDS run in batch mode, use the Run dialog on the Windows Start menu. Enter the full path to the "multimedia.bat" file (with quotes needed if the path contains blanks or spaces), followed by a space and the name of the job to be run. For example,

```
"C:\SHEDS\multimedia.bat" job1
```

Do not quote the name of the job itself, even if it contains spaces. To submit the job "lawn and garden" (assuming that the "multimedia.bat" file is located in "C:\SHEDS"), type

```
"C:\SHEDS\multimedia.bat" lawn and garden
```

and hit the return key to submit the commands.

A black DOS window should appear, along with another SAS window indicating the location of the source code, output, and log files. The rest of the output from the run should be located in the \output directory under the job name.

6.4 Uncertainty Runs

Only two modifications to the above process are necessary to submit an uncertainty run. First, the user must ensure that the "distributions" input file contains the data for the uncertainty clouds. This occupies four variables: "n", "v1_un", "v2_un", and "v3_un". Each record except the probability vectors can be assigned uncertainty clouds (simply set "n" to zero on the probability vectors or any other variables without uncertainty clouds). The variable "n" indicates the number of points in the uncertainty cloud for the given input variable. This is also the number of items in the list for "v1_un" (and "v2_un" and "v3_un", if needed). For example if n=3, a valid list for "v1_un" would be ", 0.8, 0.9, 1.0". Each number, including the first, is preceded by a comma. Spaces can be added as needed to make the data more readable. For point distributions, only "v1_un" is needed. For triangles, all three are needed. All other shapes (indicated by the variable "form") require both "v1_un" and "v2_un", but not "v3_un".

The values at the corresponding positions in each of the lists "v1_un", "v2_un", and "v3_un" are to be used together. For example, for a uniform distribution, "v1_un" contains values for the lower bound, while "v2_un" contains corresponding values for the upper bound. A method called the "modified bootstrap approach" for generating suitable values for the uncertainty clouds is discussed in the SHEDS Technical Manual. Once suitable data for "n", "v1_un", "v2_un", and "v3_un" have been added to the "distributions" file, these data can remain there, even when using the file for standard variability-only runs.

The other modification needed for an uncertainty run is to select the number of populations to be run. For each population, sample values for the distribution parameters are drawn from each uncertainty cloud. Everyone in the population then draws samples from distributions using these parameters. Suppose one decides to run 200 populations of 500 persons each. Then the third variable on the RunInfo file (labeled "population size") is set to 500, while the fourth variable (labeled "uncertainty iterations") is set to 200. For variability-only runs, the number of uncertainty iterations is set to zero.

Uncertainty runs are submitted in exactly the same way as other batch runs.

Note that uncertainty runs may take a long time to complete. A run of 200 populations of 500 persons each takes the same time to complete as a variability-only run of 200x500 = 100,000 persons. This may take several days.

Once the run is complete, the user may run the macro %UncSummary that is built into the SHEDS-Multimedia code. The user must first ensure that the SAS library "out" points to the \output directory for the selected job. The %UncSummary macro takes three arguments. The first is the variable to be analyzed, for which a common choice is "abstot", the time-average of the total daily absorbed dose across all pathways. The second argument is the choice of units, either

“ug” for quantities expressed in micrograms, or “mgkg” for quantities expressed as milligrams of chemical per kilogram of body mass. The third argument is the lower bound for the output values. This macro produces two graphs with logarithmic scales, which are used since the output typically covers several orders of magnitude. However, in some cases the output values may be zero or very close to zero. To avoid trying to plot such values on a logarithmic scale, these are replaced by values at the designated lower bound.

Note that the code for producing uncertainty plots is still under development and not considered to be fully operational in version 3, so the user might have to debug or modify the code if problems are found.

6.5 Sensitivity Runs

There are various types of sensitivity analysis available in SHEDS, as discussed in the Technical Manual. The Pearson and Spearman correlation methods, along with the stepwise regression approach, can be run on any model run (either uncertainty or variability-only), as long as the “keep intermediate variables” option was selected. This appears as a check box on the “Specify Simulation Information” screen in the interface, or can be set directly in the RunInfo file by setting the variable “Save intermediate variables” to one.

The final method of sensitivity analysis currently available is the percentile scaling approach. This requires a special model run. Somewhat like uncertainty runs, a percentile scaling run requires two modifications by the user. First, the variable “pctSensitivity” (which is labeled as “Sensitivity Run”) on the RunInfo file should be set to one. Second, the user should copy the file “variables” from the \default directory to the \input directory for the job, and change the setting of the “sensitivity” column to select the variables to be analyzed. Variables for which sensitivity=1 will be analyzed, while those with sensitivity=0 will not.

Sensitivity runs are submitted exactly like any other runs. The program will perform a run for the base population, plus two additional populations for each selected variable. Hence, if 10 variables are selected, the job will take 21 times longer than a standard variability-only run.

The SHEDS-Multimedia version 3 code has two built-in macros for processing sensitivity output. The first, %SensPct, is used for percentile scaling runs. It cannot be invoked via the interface. Instead, use a standard SAS editor window and submit the macro call. Two arguments are required: the analysis variable (often “abstot”, as for uncertainty analysis) and the units (either “ug” for micrograms of chemical, or “mgkg” for milligrams of chemical per kilogram of body mass). Also, the SAS library “out” must point to the \output directory for the selected run. The %SensPct macro creates a table listing the influences of the input variables selected for analysis.

The second, %SensCorr, is used with the output from a standard variability-only run or with output from an uncertainty run. As with the other macros discussed above, the the SAS library

“out” must point to the \output directory for the selected run. The %SensCorr macro takes four arguments. The first is the output variable to be analyzed (often “abstot”), the second is for the units (either “ug” or “mgkg”, as above), the third selects the type of correlation used (“P” for Pearson, or “S” for Spearman), and the fourth is a switch (use “1” to first take logarithms of the output variable, or use “0” to use the output variable directly). Since exposure and dose distributions are often positively skewed, taking logarithms may create more symmetrical distributions. As for uncertainty runs, the macros for sensitivity runs have undergone preliminary testing only, and the user may have to identify and/or correct and problems encountered with this code.

Appendix A. Directories and Files

All of the directories that SHEDS-Multimedia uses are placed underneath the installation directory which is chosen by the user at install time. By default this is in the user's My Documents/Multimedia3.14 (or similar) directory. The install directory will be referred to as the install directory or <install> in the following discussion and diagrams.

A.1 Directories

The directories are laid out as follows on installation. The indentation of a directory name implies that it is within the directory above it.

```
<install>
    Data
        Default                 Default and constant input files
        Diet                    Currently unused
    Prg                         SAS catalogs and macros implementing model
    Runs                        All input and output related to specific runs
        Demonstration File      All input and output related to demonstration run
            Input               User edited files for run
            Output              Results for demonstration run
    Setup                       Files related to installation and un-installation
```

The interface will create a directory for each run that the user defines. These directories will always be named the same as the run name and by default are placed under the Runs directory. As initially installed the Runs directory contains only one run: Demonstration File. The user has the option to move the directory for each run to another location.

A.2 Critical Input Files

If using the interface, it is not necessary for the user to know where files are stored. For batch runs and advanced post-run analysis it becomes important. The table below shows where critical files are placed at installation or when a run is defined through the interface. All files in the Runs/<run name>/Input directory are modified by the interface (except the contactmedia.sas7bdat dataset). Additional input files (e.g., CHAD diaries) needed for runs can be found in the <install>/Data/Default/ directory.

<install>/		
	autoexec.sas	SAS start-up file. Many SAS options can be set here
	multimedia.bat	File used to run SHEDS in batch mode

	runinfo.sas7bdat	File containing run specific information generated by the interface
Runs/<run name>/Input/		
Required for Batch Runs	agegroups.sas7bdat	Defines age and genders to be used in simulation
	cooccurrence.sas7bdat	Scenario co-occurrence data, if not being used it may contain no records, but must be present
	diarydetails.sas7bdat	Contact probabilities
	distributions.sas7bdat	Variable distributions as defined for run
	contactmedia.sas7bdat	List of contact media and their short names
One of These is Required	appmedia_decay.sas7bdat	Decay and dispersion application information
	appmedia_postapp.sas7bdat	Post-application information
	timeseries.sas7bdat	User defined time series concentrations for each media
One of These is Required	modeldates.sas7bdat	Data required for model to determine stochastic application dates
	userdates.sas7bdat	Data for user defined application dates

A.3 User Specified Output Files

The major output files for a typical variability run, their structure, and variable definitions are discussed in the SHEDS-Multimedia Technical Manual. Files related to sensitivity and uncertainty runs are discussed in the section on batch runs in this manual.

If a log file is specified by the user, on the Simulation Information screen, then it is put in <install>/Runs/<run name>/Output/saslog.txt. This file can be read in the SAS editor or any other editor of the user's choosing.

If a user requests a spreadsheet of inputs, on the Run screen, it will be placed in the installation directory and named after the run name: <install>/<run name>.xls. This file can be read from MS Excel 2003 or later.

A.4 Other Output Files

A.4.1 Diary Related Output Files

The number of available one-day activity diaries for each cohort and day type is listed in the file "diarycounts" in the \output directory for the given run.

A.5 Exporting SAS Datasets

To facilitate additional analyses in the software of your choosing, you may export data in a variety of formats. The export wizard can be accessed by selecting a dataset in SAS and then selecting Export Data from the main SAS File menu. For more information on the export wizard check the SAS help file index under "exporting data/Export Wizard for". To export data programmatically, use Proc Export. Again, information on specifics can be found in the SAS help files.

A.6 Moving Run Files

It is relatively easy to move model results for analysis outside of the interface. The easiest method is simply to copy the entire output directory to another location and establish a SAS library pointing to the new directory.

If you want to use existing simulation inputs or outputs or both in the interface it is a little more difficult and requires some basic knowledge of SAS. Integrating these files on another computer with SHEDS Multimedia installed is a three step process.

1. Move the entire run directory to the Runs directory on the new computer.
2. Integrate the related records from the RunInfo file (in the <install> directory.
3. Run the %RunInfoAddDirs macro on the RunInfo file on the new machine.

A.6.1 Background on the RunInfo Dataset

The RunInfo dataset is stored in the <install> directory. When the interface is running the library is also called RunInfo, so the dataset is referred to as RunInfo.RunInfo. In the windows explorer it is named <install>/Runinfo.sas7bdat.

The RunInfo dataset stores user supplied information defining each simulation. The model reads this information during the run. On installation only one run is defined, the Demonstration File run. Each run is stored as one record with the run name being the unique identifier; records are selected based on the run name. When the interface displays the available run names it gets them from this file. Obviously having records in this file that don't have a corresponding directory in the <install>/Runs directory will cause problems. If there is no record in this file pointing to an existing directory, a user will not be able to use the interface to access the inputs or outputs associated with that run.

A.6.2 Moving the Run Directory

SHEDS-Multimedia should have a Run directory on the old and new machines. Use the windows explorer to copy the entire run directory for a specific run. That is, copy the directory containing the run name and every thing under it. If you want to move several runs copy each run directory.

Assuming that the run name was MyRun1 you would copy the directory

<machine1>/<install>/Runs/MyRun1,

to

<machine2>/<install>/Runs/MyRun1.

In this case <machine1> and <machine2> represent the full paths to the installation directories on each computer.

A.6.3 Integrating the Old and New RunInfo Records

There are two possibilities for this. The easiest is that you simply want to replace the RunInfo file on the new computer. In this case you will lose access to any previous runs on the new computer. The other possibility is that you want to integrate one or more runs from the old computer into the current runs on the new computer.

A.6.4 Replacing the RunInfo File (Dataset)

If you do not need the previous runs on the new computer then copy the SAS dataset <install>/runinfo.sas7bdat from the old computer to the new one. To keep things clean you will want to delete any records representing runs you are not moving to the new machine.

A.6.4.1 Integrating Records into the New RunInfo File

If you want to maintain access to the previous runs on the new computer then you need to integrate individual records from the old computer into the RunInfo file on the new computer. Use a SAS data step or Proc SQL to merge the desired records from the old RunInfo file into the new one. The records being integrated will need to have unique names.

A.6.5 Running the %RunInfoAddDirs Macro

The RunInfo dataset stores the full paths to several files and directories. The records for the runs that were moved to the new machine need to be altered so that these paths point to the proper location. If you were lucky enough that SHEDS Multimedia is installed on the same path on both machines, then you can skip this step. The %RunInfoAddDirs macro will update the path names. It needs to be run once for each run that was moved. You give it two arguments:

installDir	The current (new) installation directory.
runName	The run name pointing to the record that needs to be altered.

The macro is in the file <install>/prg/RunInfoMacros.sas.

A.6.6 Moving a Run: An Example

For this example assume that you used the Windows Explorer to move the run directory 'MyCopy3' to a new machine. You also copied the RunInfo file from the old machine to the installation directory on new machine and renamed it OldRunInfo. The new installation directory is named c:\Multimedia3.11\. The following code will integrate the record of interest from the RunInfo file and correct the paths in the on the MyCopy3 record in the RunInfo file.

```
* Define the runinfo library;
```

```
  libname runinfo "c:\multimedia3.11\";

* Add the record from the old runinfo file to the new one;
* This can add multiple records by adding extenting the match list;
  data runinfo.runinfo;
        set runinfo.runinfo
              runinfo.OldRunInfo (where=(runname in ("MyCopy3")));
  run;

* Including the RunInfoMacros.sas file compiles the macros;
  %include "c:\multimedia3.11\prg\RunInfoMacros.sas";

* Finally, redefine the installation directory in all the paths;
  %RunInfoAddDirs(installDir=C:\multimedia3.11\,runname=MyCopy3);
```

Appendix B. Reference Tables

B.1 Variable Names

Table B-1. Variable Names From Distributions File

Group	Variable	Label	Units
Activity-related	washprob	mean # hand washes/day per person	1/day
Activity-related	hm_freq	hand mouthing events per hour	events/hr
Activity-related	f_uncloth	fraction of body unclothed	[-]
Baths	bathdays	maximum number of days between baths	days
Chemical properties	dermaxh	maximum dermal loading for hands	ug/cm2
Chemical properties	metab_ratio	mass ratio (metabolite/pollutant)	[-]
Chemical properties	object_ratio	object-surface concentration ratio	[-]
Chemical properties	dermaxb	maximum dermal loading for body	ug/cm2
Direct-ingestion	ingestion_indoor	dust ingestion rate (indoor, direct only)	mg/hour
Direct-ingestion	ingestion_outdoor	soil ingestion rate (outdoor, direct only)	mg/hour
Dose-related	absr_gr	GI tract absorption rate per day for surface residues	1/day
Dose-related	absr_gm	GI tract absorption rate per day for dust or soil	1/day
Dose-related	bioavm	bioavailability fraction for dust/soil	[-]
Dose-related	bioavr	bioavailability fraction for surface residues	[-]
Dose-related	elimr_blood	elimination rate from the blood	1/day
Dose-related	absf_lung	absorption fraction for lungs	[-]
Dose-related	absr_dr	dermal absorption rate per day for surface residues	1/day
Dose-related	absr_dm	dermal absorption rate per day for dust or soil	1/day
Other	has_lawn_p	probability of having a lawn	[-]
Other	has_pet_p	probability of having a dog or cat	[-]
Other	has_garden_p	probability of having a vegetable garden	
ProbVector	timeofday_indoor	probability vector for hour of indoor application	[-]
ProbVector	timeofday_outdoor	probability vector for hour of outdoor application	[-]
ProbVector	re-entry_indoor	probability vector for re-entry time indoors	[-]
ProbVector	re-entry_outdoor	probability vector for re-entry time outdoors	[-]
Transfer Coefficients	tc_m	transfer coefficient for object mouthing	cm2/hr
Transfer Coefficients	tc_b	surface-skin transfer coefficient for body (unclothed)	cm2/hr
Transfer Coefficients	tc_h	surface-skin transfer coefficient for hand	cm2/hr

Transfer Efficiency	om_transfer	object-mouth transfer efficiency	[-]
Transfer Efficiency	transfer_dermal	residue-skin transfer efficiency	[-]
Transfer Efficiency	om_freq	object-mouth contact rate	events/hr
Transfer Efficiency	om_area	object-mouth contact area	cm2
Transfer-related	remv_bath	removal efficiency during bath/shower	[-]
Transfer-related	remv_dry	removal efficiency during events without water	1/hr
Transfer-related	remv_mouth	removal efficiency during mouthing	[-]
Transfer-related	remv_wash	removal efficiency during hand washing	[-]
Transfer-related	contactb	Body-surface fractional contact rate	1/hr
Transfer-related	contacth	Hand-surface fractional contact rate	1/hr
Transfer-related	adherence	soil-skin adherence factor	mg/cm2
Transfer-related	hm_fraction	fraction of surface of one hand that enters mouth	[-]

B.2 Media Descriptions

Table B-2. Media Descriptions And Symbols

Media Description	Media Symbol (medsymbol)[1]	Examples
Indoor air	ATair, AUair	
Air outside the residence	AYair	
Residue on indoor smooth surfaces	RThard, RUhard	Wood floor, laminate counter tops
Residue on indoor textured surfaces	RTsoft, RUsoft	Carpet, upholstered furniture
Indoor dust	MTdust, MUdust	
Residue on lawn	RYlawn	
Residue on vegetable garden	RYveg	
Residue on pet fur	Rpet	
The model uses these internally	Anone, Mnone, Rnone	

[1] The capital letters Y, T, and U indicate yard, treated, and untreated.

Appendix C. Probability Density Functions

The explicit probability density functions (pdf's) utilized by SHEDS are listed below. Note that some of these may have alternate parametrizations, so the user must be careful when obtaining distributions from the literature. The expressions "Exp," "Sqrt," "Log," and "Γ" refer to the exponential, square root, natural logarithm, and gamma functions, respectively.

C.1 Beta

The beta distribution in SHEDS has a lower bound of zero, an upper bound of one, and two shape parameters v1 and v2. The restrictions are v1>0 and v2>0. When v1< v2 then the mean is below ½ and the distribution is positively skewed, whereas when v1 > v2 the mean is above ½ and the distribution is negatively skewed. For v1=v2 the mean is at ½ and the shape is symmetric. The PDF is

Equation E-1

$$p(x) = x^{v1-1} (1-x)^{v2-1} \Gamma(v1+v2) / (\Gamma(v1) \Gamma(v2)), \quad \text{for } 0<x<1$$

The beta is a useful form for variables known to be bounded, due to the wide variety of shapes that it can have. For v1>1 and v2>1, the PDF of the beta has a single peak, away from the bounds. When 0<v1<=1, the PDF is large near zero, and when 0<v2<=1, it is large near one. These properties allow the beta to have the so-called 'J' or 'U' shapes. The mean of a beta distribution is at $\mu = v1 / (v1+v2)$, and the standard deviation is $\sigma = \text{Sqrt}[v1\ v2 / (v1+v2+1)] / (v1+v2)$. If one wishes to construct a beta with a given mean μ and standard deviation σ, then choose $v1 = (\mu^2-\mu^3)/\sigma^2 -\mu$, and $v2 = v1\ (1-\mu) /\mu$. This will only be possible if $0<\mu<1$ and $\sigma^2 < \mu\ (1-\mu) \leq 1/4$.

C.2 Exponential

The exponential in SHEDS has two parameters, the minimum (v1) and the mean (v2), with the restriction that v1 < v2. Some users may be more familiar with a single parameter exponential distribution, which has a minimum of zero and is characterized by a decay rate constant. The SHEDS exponential is similar, apart from a shift of v1 units to the right. The decay rate of the SHEDS exponential is given by 1/(v2-v1). The standard deviation of an exponential is (v2-v1). If the user wants an exponential with a half-life τ, then set $v2 = v1+ \tau / \text{Log}[2]$. The PDF of the SHEDS exponential is

Equation E-2

$$p(x) = \text{Exp}[-(x-v1)/(v2-v1)] / (v2-v1), \quad \text{for } x>v1$$

C.3 Gamma

The gamma distribution in SHEDS is bounded below by zero and has two parameters, the shape parameter v1 and the scale parameter v2. The restrictions are v1>0 and v2>0. The shape parameter v1 controls the appearance of the PDF. Shape parameters less than one lead to a monotonically decreasing form with the highest probability at zero. If v1=1, then the gamma is identical to an exponential that starts at zero and has a mean given by the gamma parameter v1. If v1>1, then the gamma somewhat resembles the lognormal, rising from zero to a peak probability, and then gradually declining with an overall positive

skewness. The mean of the gamma is at μ = v1 v2, and the standard deviation is σ = v2 Sqrt(v1). The PDF of the SHEDS gamma is

Equation E-3

$$p(x) = v2^{-v1}\, x^{v1-1}\, \mathrm{Exp}(-x/v2) / \Gamma(v1), \quad \text{for } x>0$$

C.4 Lognormal

The lognormal in SHEDS is bounded below by zero and has two parameters, the geometric mean GM (v1) and the geometric standard deviation GSD (v2). The restrictions are v1>0 and v2>1. Many variables in exposure science are approximately lognormally distributed, so its use is fairly common. If a variable 'x' has a lognormal distribution, then log(x) has a normal distribution.

The geometric mean (GM) of a lognormal distribution is also its median. Log(GM) is the mean of the distribution of log(x). Log(GSD) is the standard deviation of log(x). Since standard deviations must be positive, then Log(GSD)>0, which implies GSD>1. The PDF of the SHEDS lognormal is

Equation E-4

$$p(x) = \mathrm{Exp}[(-1/2)\,(\mathrm{Log}[x/v1] / \mathrm{Log}[v2])^2\,] / (x\ \mathrm{Sqrt}[2\,\pi\,]\ \mathrm{Log}[v2]\,), \quad \text{for } x>0$$

If GM and GSD are given, then the lognormal has arithmetic mean and standard deviation

Equation E-5

$$\mu = \mathrm{GM}\ \mathrm{Exp}[(1/2)\,(\mathrm{Log}(\mathrm{GSD}))^2\,],$$
$$\sigma = \mathrm{GM}\ \mathrm{Sqrt}[\mathrm{Exp}(\,[\mathrm{Log}(\mathrm{GSD})]^2)\ (\mathrm{Exp}(\,[\mathrm{Log}(\mathrm{GSD})]^2)-1)].$$

If the user knows the arithmetic mean μ and arithmetic standard deviation σ of the lognormal instead of the GM and GSD, then these can be converted as follows:

Equation E-6

$$\mathrm{GM} = \mu / \mathrm{Sqrt}(1 + \sigma^2/\mu^2),$$
$$\mathrm{GSD} = \mathrm{Exp}(\mathrm{Sqrt}(\mathrm{Log}(1 + \sigma^2/\mu^2))).$$

If instead, one has the mean μ_{log} and standard deviation σ_{log} of log(x), then use

Equation E-7

$$\mathrm{GM} = \mathrm{Exp}(\mu_{log}),$$
$$\mathrm{GSD} = \mathrm{Exp}(\sigma_{log}).$$

C.5 Normal

This is the normal or Gaussian distribution commonly used in statistics. The normal has two parameters: the mean (v1) and the standard deviation (v2), with v2>0. Note that the normal is unbounded, so it is a good idea to provide lower and upper truncation points to prevent physically impossible values from being returned. The PDF of the normal is

Equation E-8

$p(x) = \text{Exp}[-(x-v1)^2/(2\ v2^2)] / (\text{Sqrt}[2\ \pi]\ v2)$

C.6 Point

A point value means that the same value is always returned. This is sometimes called a *fixed* or *constant* form. The point has one numeric argument (v1) which is the value that is to be returned. The mean is v1 and the standard deviation is zero. The sampling frequency does not matter for points. While points are technically discrete, here they are classified with the continuous distributions since they are applied to variables that are expected to reside on a continuous scale, but happen to be assigned no variability.

C.7 Triangular

The triangular distribution has a probability density function (PDF) that is shaped like a triangle. The three parameters locate the vertices, with v1=minimum, v2=peak, v3=maximum. The restrictions are $v1 <= v2 <= v3$, with $v1<v3$. The mean value of this distribution is located at $\mu = (v1+v2+v3)/3$, which coincides with the peak only when v2 is midway between v1 and v3. The standard deviation is $\sigma = \text{Sqrt}[(v1^2+v2^2+v3^2-v1v2-v1v3-v2v3)/18]$. It is possible for the peak to be located at either extreme, forming a right triangle. The PDF of the triangular is

Equation E-9

$$p(x) = 2\ (x-v1) / [(v2-v1)\ (v3-v1)], \quad \text{for } v1 \leq x \leq v2$$
$$= 2\ (v3-x) / [(v3-v2)\ (v3-v1)], \quad \text{for } v2 \leq x \leq v3$$

C.8 Uniform

The uniform is characterized by two parameters, the minimum (v1) and the maximum (v2), with $v1<v2$. All values between v1 and v2 are equally likely to be returned. The mean is $\mu = (v1+v2)/2$ and the standard deviation is $\sigma = (v2-v1) / \text{Sqrt}(12)$. The PDF of the uniform is

Equation E-10

$$p(x) = 1 / (v2-v1), \quad \text{for } v1 < x < v2.$$

C.9 Weibull

The Weibull distribution in SHEDS is bounded below by zero and has two parameters, the shape parameter v1 and the scale parameter v2. The restrictions are $v1>0$ and $v2>0$. The Weibull has slightly different properties from a gamma, but there is a strong overall resemblance. When the shape parameter $v1 \leq 1$, the Weibull is monotonically decreasing. For $v1=1$, it reduces to an exponential. For $v1>1$, it rises to a peak and then declines gradually in a long tail. The mean is $\mu = v2\ \Gamma(1+1/v1)$, and the standard deviation is $\sigma = v2\ \text{Sqrt}[\Gamma(1+2/v1) - (\Gamma(1+1/v1))^2]$. Here 'Γ' is the mathematical gamma function, not the gamma distribution. The gamma function is a generalization of the factorial function to non-integer arguments; for integers, $\Gamma(1+n) = n!$. The PDF of the Weibull distribution is

Equation E-11

$$p(x) = v1\ v2^{-v1}\ x^{v1-1}\ \mathrm{Exp}\ [-(x/v2)^{v1}], \quad \text{for } x>0.$$

C.10 Discrete Probability Density Functions

Bernoulli variables have only two possible outcomes, for example, the outcome of yes/no tests. The usual statistical notation would be (p_1, p_2), where p_1 and p_2 are between 0 and 1 and sum to 1. However, the SHEDS code implements Bernoulli variables by having the user specify only the probability of a "yes". The probability of "no" is implied by 1 - "yes".

Multinomial variables allow more than two possible outcomes. The usual statistical notation would be (p_1, p_2, …, p_n), where each p_i is between 0 and 1 and the p_i's sum to 1. In SHEDS, multinomial variables are called probability vectors. Unlike Bernoulli variables, the user must supply the entire set of probabilities.

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