SHEDS-Wood

Stochastic Human Exposure and Dose Simulation Model

Wood Preservative Exposure Scenario

USER'S MANUAL
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FINAL DRAFT

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Preface

Conventions

This section describes some of the conventions used in discussing the user interfaces.

User Actions

These are the terms that will be used to describe user actions.

Mouse

Point	Move cursor over a specific object.
Click	A standard single left click with the mouse or equivalent hardware.
Right Click	A single click or the right mouse button.
Double Click	Two rapid clicks with the left mouse button.
Drag	Hold down the left mouse key, and move the mouse, thus moving some object on the screen.

Keyboard

Press	Press a key on the keyboard.
Enter	Key in some information and press the Return key.
Tab	Press the Tab key.

GUI Interaction

Enter	Type text or numbers in a text box, text entry, or combo box.
Highlight	Select text or other elements, usually by dragging with the mouse.
Activate	Make a screen or dialog active and ready to receive input, usually by clicking on its title bar.
Select	Select a menu or sub-menu choice, or a listbox or combo box item.

Some selections require the user to navigate through several menus, submenus, or other GUI controls. These sequences will be shown with the name of each control in bold, separated with ">" signs. For instance, to run SAS from the **Start** button in MS Windows, you would need to click on the **Start** button, then the **Program** menu item, then the **SAS** sub-menu, where you would finally choose the item labeled **The SAS System for Windows V8**. This would be represented as follows:

Start > Programs > SAS > The SAS System for Windows V8

GUI Elements

The name of visual GUI elements (except for screens and dialogs) will be placed in bold face type. Typically the name is given by a label on the GUI element or widget. When this is not the case additional explanation will be given.

GUI Element States

The widgets, whether screens, list boxes, or buttons, have several states. Not all widgets can take all states. The states are described here along with their opposite states.

Activated	The widget or screen is currently active and expecting input. Typically, the widget or screen would also be highlighted at this time. Only one window can be active at any given time. Its title bar is typically painted using a different color than the non-activated windows.
Highlighted	Either the background color is different than normal or a line or other graphic convention shows when a widget is highlighted.
Enabled	This indicates that a widget is usable currently. It is not necessarily currently active, but could be made active. Often widgets will get disabled or 'greyed out' when they are not appropriate to use under the current situation.

Other Typographical Conventions

File Names

File names and path names are set in bold font. For example when discussing a specific file extension (**.msi**), file name (**setup.exe**) or directory path (**d:\program files**) the text will be formatted as shown.

Code and ASCII Output

Examples of programming code, text for the user to enter, and text output from the programs are set in `Courier New` typeface.

Installation

Requirements

To install and use SHEDS, you will need a computer running SAS version 8.1 or higher. The newer versions of the model have not been tested under SAS version 8.0, they may or may not work on that version. On a computer running Windows 98, NT, or 2000, it is necessary to have

a 300 MHz processor,
64 MB of RAM, and
100 MB of free disk space.

However, it is recommended that you have

a 600 MHz processor,
128 MB or more RAM, and
more than 200 MB of free disk space.

The software should run on other systems where SAS version 8.1 is implemented, but this has not been tested.

If run under Windows 98 SE, SAS 8.1 or higher is strongly recommended due to memory leaks in SAS version 8.0 under these operating systems.

The model should run under other operating systems (non-Windows) as is or with minor modifications. It has not, however, been tested under other systems.

Installation Under MS Windows

The installation software used to build the install wizard for SHEDS is Wise for Windows. As the name implies this software only works under MS Windows in its many variations. To install under other operating systems one will need to request an alternate install package.

If you do not have Administrative privileges on your computer, you must either have the administrator install the software or request a special distribution that can be installed without administrative privileges.

Starting the Installation Process

The standard distribution for SHEDS-Wood is by email or CD.

Starting with a CD

If you received 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.
3. Double click on the **setup.exe** file to initiate the installation.

Starting with an Email Distribution

You may receive the installation file via an email attachment. If so, follow these instructions to start the install process.

1. Save the attachment to a local or network hard drive. The method you use to do this will vary depending on the email program used. Make sure the saved file has an extension of ".msi". A typical name might be ShedsWoodv401.msi.
2. Use the Windows explorer to navigate to the saved file.
3. Double click on the saved file to start the installation.

The Standard Installation Process

Once the installation wizard is initiated, simply follow the instructions. This will install the necessary program and data files, define an environmental variable called WOOD_MODEL_ROOT, and place a desktop icon used to execute SAS and start the model.

If the user has an earlier version of SHEDS-Wood installed, the user will initially see the screen in Figure 1. Select Remove, follow the instructions, and start the installation process again to install the new version.

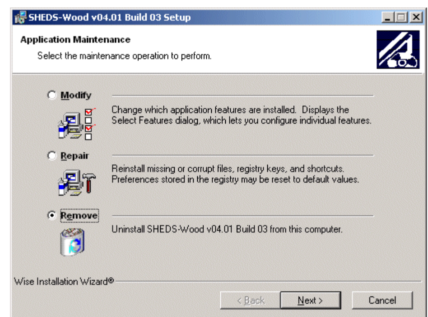


Figure 1. The initial "Install" screen if you have an old version of SHEDS-Wood installed.

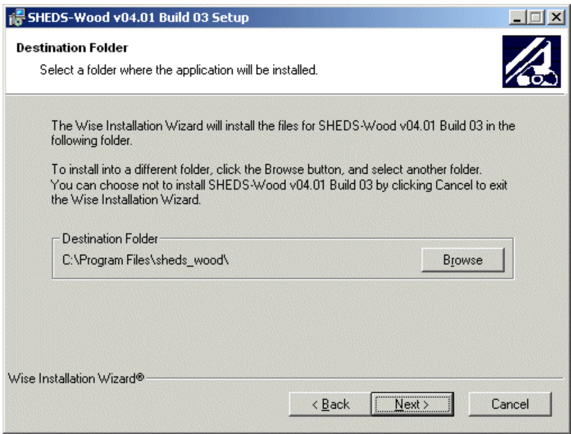
The typical screens and an explanation of each are shown in the following figures.

Figure 2. The initial welcome screen displayed while the installer prepares its files and searches for the installed SAS software.

The first installation screen appears for a short time while the installer searches the user's computer for SAS. If SAS version 8 is found the installation will continue with the next screen.

Figure 3. The welcome screen for the SHEDS-Wood installation.

This screen simply specifies which version will be installed. Exit any unnecessary programs before the install. Click the **Next** button to continue.

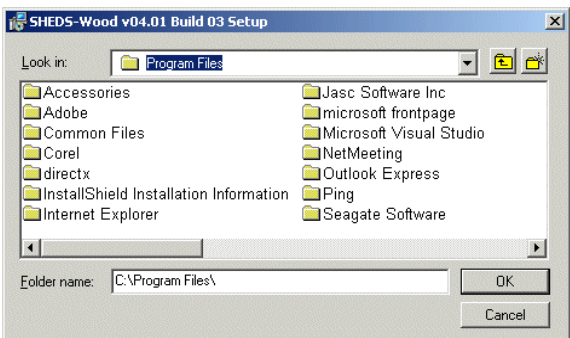


This screen gives the user a chance to install the files somewhere besides the default location,

C:\Program Files\sheds_wood\.

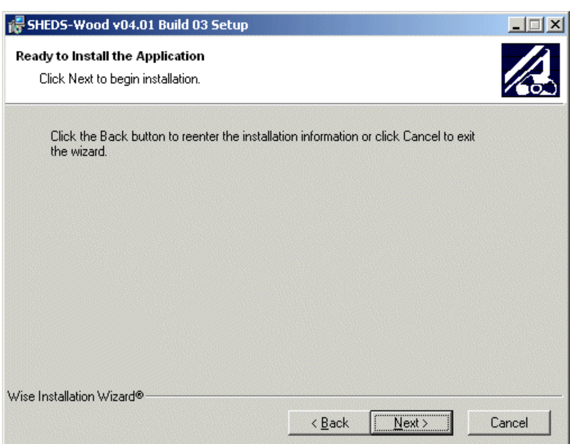
If the user desires, the **Browse** button can be clicked and a dialog allowing him to choose an alternate location will come up. See the next screen.

Figure 4. Installation location window.



If the **Browse** button is clicked on the previous dialog, this dialog appears. It is used to navigate the disk drives and directories to specify the location for the top level installation directory.

Figure 5. File navigation window.



This is the final window before install begins. It allows the user to go back and change any values entered.

Figure 6. Confirmation window.

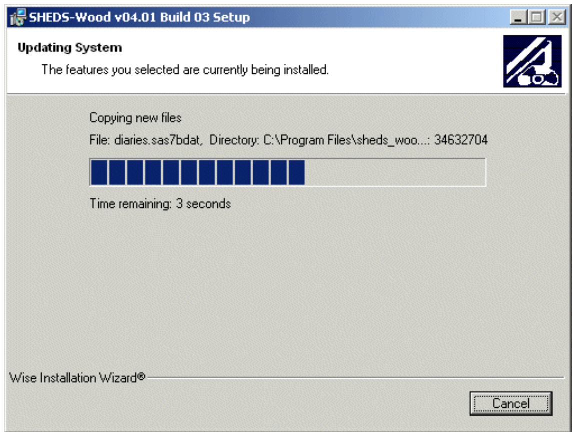


Figure 7. Installation progress dialog.

While the installer is copying files to the installation directory, a blue progress bar will be displayed. This step should take less than one minute.

Figure 8. The final installation screen.

After the files have been extracted and placed in the sheds directory, and the desktop icon has been placed, this dialog will indicate that the installation is complete.

Be sure to wait at least 20 seconds before attempting to start the SHEDS-Wood interface.

On some Windows systems (95, 98SE) the user may need to reboot the computer before SHEDS will launch without error.

Installation Details

The installation basically carries out three operations.

1. Uncompress and copy files to desired location.
2. Create a desktop icon to start SAS and the model interface.
3. Define a User Environmental Variable, WOOD_MODEL_ROOT, that points to the top level of the installation directory.

Starting the Model Interface

The installation will place an icon on the user's desktop (Figure 9). Double click on the icon to start SAS and the main screen of the SHEDS Interface. See the section on "Navigating in SAS" for additional information on opening Log or Output windows and viewing results.

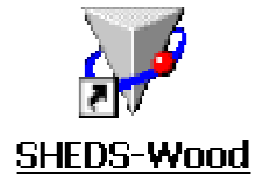
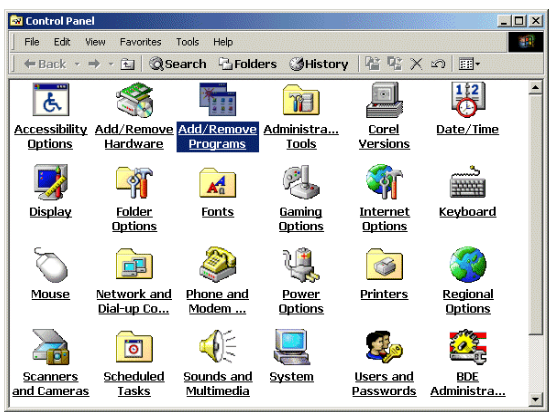


Figure 9. Desktop icon.

Removing SHEDS-Wood

If SHEDS was installed using the installation wizard, then the user can uninstall it as one would most any windows program. This process will not remove the user's simulation output files. They will need to be removed by hand.

To start the removal process, click the Windows **Start** button. Go to **Settings**, then **Control Panel** (**Start>Settings>Control Panel)**. The following figures and text describe the remainder of the process.



Typical appearance of the Control Panel.

Figure 10. The control panel.

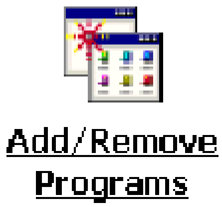


Figure 11. The Add/Remove Programs icon in the Control Panel.

Double click on the **Add/Remove Programs** icon

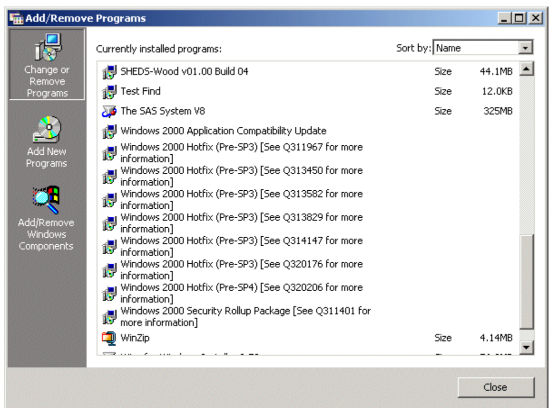


Figure 12. List of programs that can be uninstalled using Add/Remove Programs.

In the Add/Remove Programs dialog, find the entry for SHEDS-Wood and click on it.

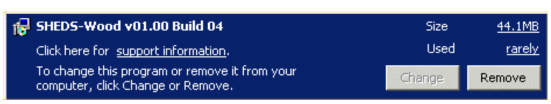


Figure 13. Expanded description of the SHEDS Program.

The entry will expand. Click on the **Remove** button and follow the instructions.

The SAS User Interface

The SAS Screen

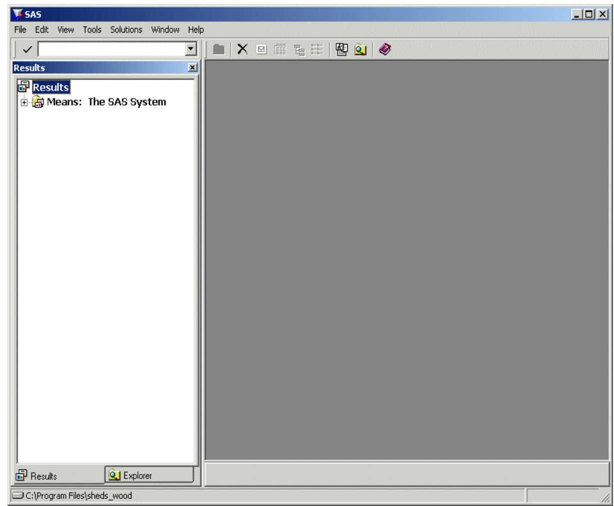


Figure 14. The SAS screen showing the narrow tabbed windows to the left and a blank work area.

The SAS screen is split into a number of distinct areas (Figures 14 and 15). At the top are the title bar, menu bar, and tool bar. SAS puts most dialogs and output in the main work area (empty in Figure 14, and containing many windows in Figure 15). At the bottom of the work area are a series of buttons each representing one window in the work area. Windows can be selected by clicking on these buttons.

To the left of the main work area there can be a narrow set of tabbed windows (Figure 14). The tabbed windows are typically the SAS Explorer and the Results Explorer, although other windows can be displayed there. When displayed, the user can switch between these windows using the tabs at the bottom.

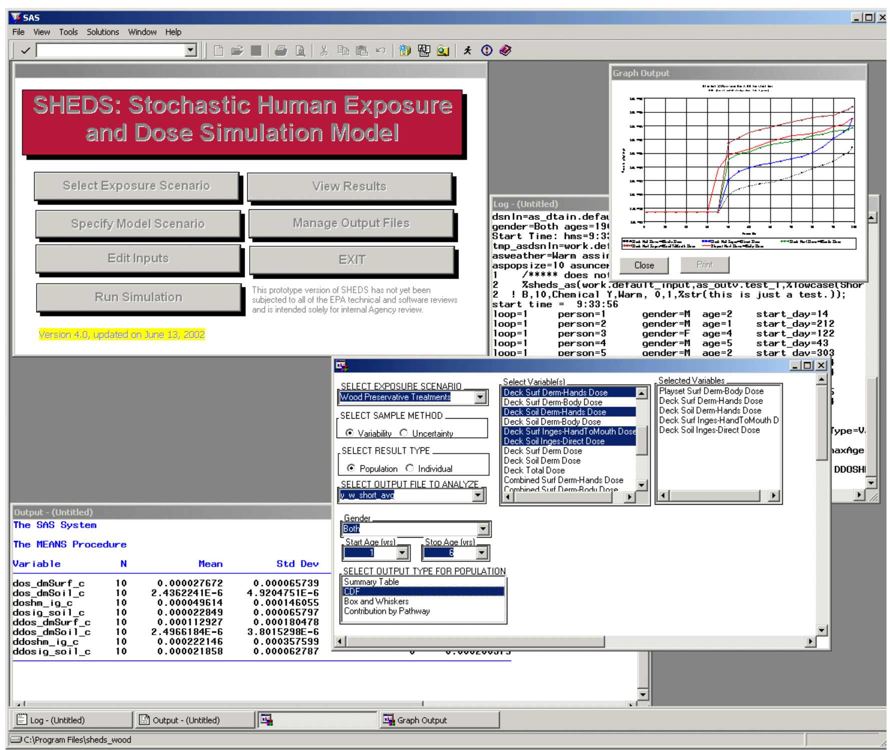


Figure 15 The main SAS screen showing the layout of the user interface and several model outputs.

Standard SAS output goes to one of three window types in the main SAS screen. All system messages, errors, and occasional program comments are put in the **Log** screen. There is one **Log** screen shared by all SAS programs. Charts and plots are output to the **Graph** window. Graphic output from all programs are put in the same window. This window often does not automatically scroll down so you must scroll it to the bottom to see your new chart. Tabular information goes to the **Output** window.

> NOTE: The SHEDS Interface does not use the standard Graph Window as described here. The interface will display graphs in individual windows. Additionally, most tabular output is accessible through the interface.

Setting Up the Work Area

SHEDS typically starts with only the main work area active. The main SHEDS dialog may be maximized, taking up the entire working area (Figure 16).

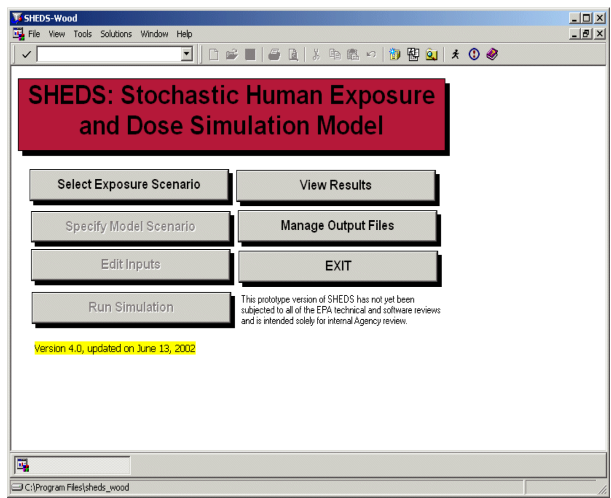


Figure 16. Main dialog of SHEDS-Wood at startup.

How To

Expose the work area

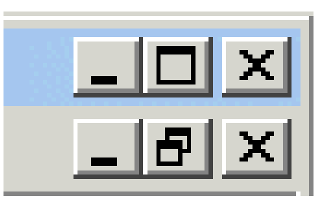


Figure 17. Icons used to minimize, maximize and close SAS windows.

If the SHEDS main menu is occupying the entire work area then click on the small middle icon at the upper left on the gray bar (Figure 17). The upper set applies to the entire SAS application window. The lower set applies to the current window in the work area.

Display the Log Window

Figure 18. The SAS View menu.

SAS sends messages and notes to its Log Window. If this window is not open in the main work area, select the **View** menu (Figure 18) and select **Log** (**View>Log**). If the Log Window is open, but not visible, click on the button for the log beneath the main work area.

Display the Output Window

The Output Window is where SAS sends tabular output from statistical procedures. After each simulation SHEDS puts some basic statistics about the calculated exposures in the Output Window. Like the Log Window it can be opened with SAS's **View** menu (**View>Output**).

Display the SAS Explorer

The SAS explorer is used to navigate SAS libraries and catalogs (Figure 19). The libraries contain the data and code used by or produced by SHEDS. Selecting **Contents Only** from the SAS **View** menu will display the explorer window (**View>Contents Only**).

Display the SAS Results Explorer

This window is used to navigate results in the Output Window (Figure 20). It uses an expandable node format allowing one to progressively delve into the output for each run. It can be displayed by selecting **Results** from the SAS **View** menu (**View>Results**).

Figure 19 The Explorer window in SAS.

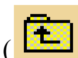
NOTE: SHEDS' results are typically viewed using the output menus in the model interface. These will be discussed shortly. The discussion here addresses use of SAS independent of SHEDS.

Navigate Procedure Output in Results

Each time new tabular output is created from a SAS procedure, another entry is added to the SAS **Results** window (Figure 20). Clicking on one of the plus signs opens up one output set. Clicking on a particular entry in the output set opens the corresponding window and brings it in front of the other windows for viewing. You can scroll through that window using the sliders to the right of the window.

Navigate Data Sets in SAS Explorer

The SHEDS model uses and creates many data sets; in SAS, a data set is essentially a table of data. The Explorer window is used to navigate the data sets. Initially, the Explorer window will have two icons. Double click on the filing cabinet to get a list of the directories (folders) that contain data sets, shown with file drawer icons. Double clicking on these will show the data sets or additional folders. Double clicking on one of the data set icons, a square table with a red dot, will bring the data set into a visible table showing column names at the top and values below.

To move up the directories (i.e., into the parent directory or folder) make the Explorer Window active (clicking on the title bar or tab will activate it). Then click on the Move to Parent tool () just above and to the right on the SAS tool bar.

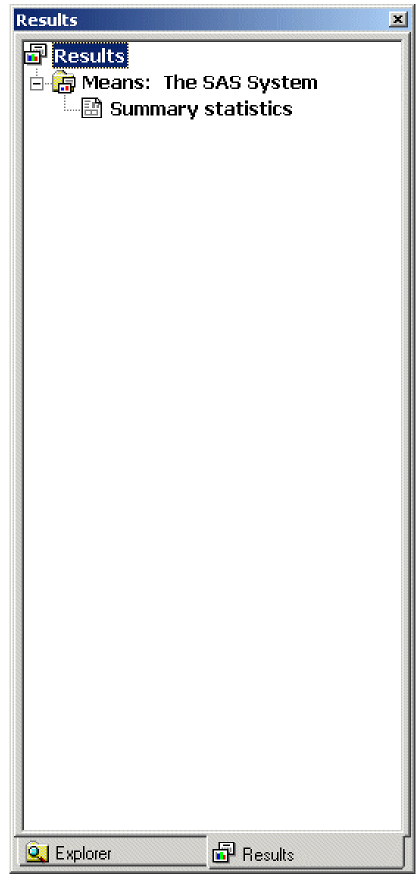


Figure 20 The Results window in SAS.

SHEDS-Wood Graphical User Interface

Main Window

SHEDS' main dialog (Figure 21) includes seven buttons:

1. **Select Exposure Scenario**,
2. **Specify Model Scenario**,
3. **Edit Inputs**,
4. **Run Simulation**,
5. **View Results**,
6. **Manage Output Files**, and
7. **Exit**.

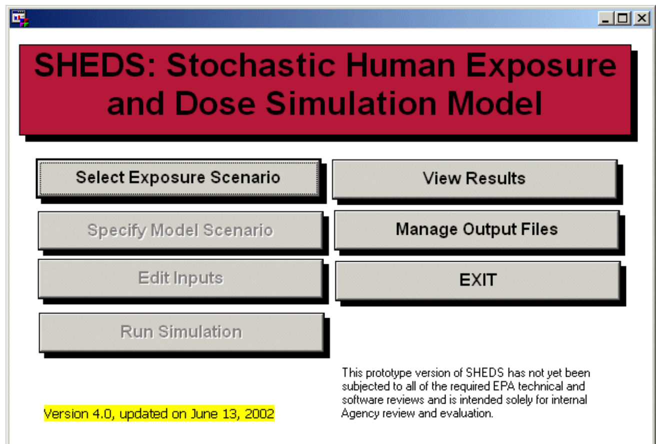


Figure 21. The main dialog for the SHEDS user interface.

Initially, the only enabled buttons are **Select Exposure Scenario**, **View Results**, **Manage Output Files**, and **Exit**. These buttons allow the user to view results and manage files from previous SHEDS simulations, or to move through the proper sequence of steps to conduct a new model run. After the exposure scenario is specified with the **Select Exposure Scenario** button, the **Specify Model Scenario** button becomes enabled. After the user specifies the model scenario, the **Edit Inputs** and **Run Simulation** buttons are enabled. Both of these buttons are enabled since the user is not required to edit inputs prior to running a simulation.

Indicated on the bottom of the Main screen are the SHEDS model version number and date of last changes.

The following sections detail the results of selecting each of the main window buttons.

Select Exposure Scenario

This dialog (Figure 22) allows the user to select which SHEDS exposure scenario(s) will be included with a new SHEDS simulation. For the purposes of peer review, the only available option in this version of SHEDS is **Wood Preservatives**. Other exposure scenarios that have currently been implemented in SHEDS (lawn, garden, indoor crack and crevice treatment) or are planned for inclusion in the near future (e.g., pets, broadcast, fogger) are listed with an "NA" to indicate "Not Activated" in this version.

If the user clicks on the **Select Exposure Scenario** button, and does not select "Wood Preservatives," an error message appears: "Only the Wood Preservatives scenario is supported by the interface at this time."

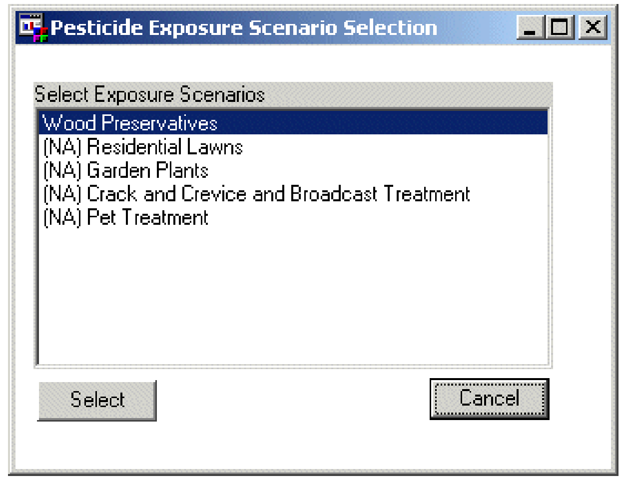


Figure 22. Scenario exposure selection dialog.

Specify Model Scenario

Clicking on this button pops up a dialog (Figure 23) that allows the user to set various options for a new simulation. The dialog is separated into three sections using container boxes: **SPECIFY SIMULATION**, **SPECIFY POPULATION**, AND **SPECIFY INPUT AND OUTPUT DATASETS**.

NOTE: Depending on the size of your screen, it may be necessary to scroll down on this and other dialogs to see the bottom portion of a list box or of the dialog itself.

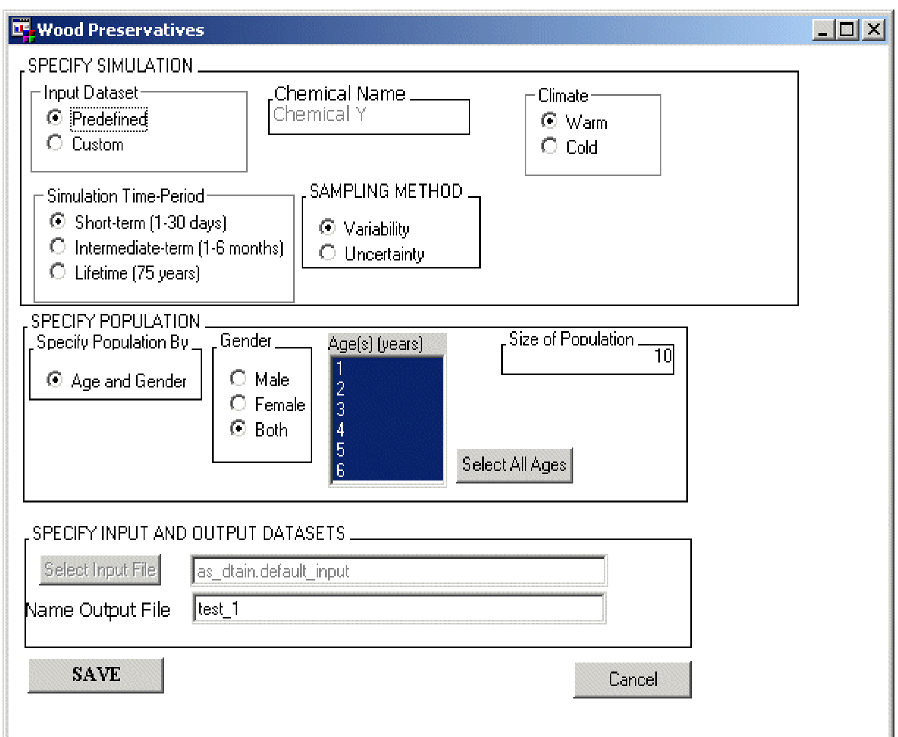


Figure 23. The scenario specification dialog.

Specify Simulation

The **Input Dataset** box in the upper left corner of the screen allows the user to select whether SHEDS should use a predefined default dataset or a custom dataset. If the "Predefined" option is selected, then the input dataset is determined by the choice of the chemical name, climate, and simulation time-period. The user cannot select an input dataset in the **SPECIFY INPUT AND OUTPUT DATASETS** box (*i.e.*, the **Select Input File** button is not available).

If the "Custom" option is selected, the user must select an input dataset by clicking on the **Select Input File** button. In this case the chemical name and climate entered serve only as labels in the output; they do not affect the simulation.

The **Climate** allows the user to specify whether a warm or cold climate is being simulated to assess children's exposure to a wood preservative from playsets and home decks. The predefined files contain parameters specific to warm or cold seasons.

The **Simulation Time-Period** allows the user to specify the simulation length and averaging time.

1. Short-term (1-30 days)		The model uses a 15-day averaging time.
2. Intermediate-term (1-6 months)		The model uses a 90-day averaging time.
3. Lifetime (75 years)		The model simulates individuals over their lifetimes.

The Short-term and Intermediate-term simulations use 15-day, and 90-day time periods, respectively. Each simulation for an individual is started at a randomly selected day and runs for the time period indicated. In these cases the average daily absorbed dose that SHEDS computes is calculated based on these time periods.

For the lifetime simulations, an individual is simulated for six full years. The method for calculating the lifetime average absorbed dose is described in the SHEDS-Wood Preservatives Technical Manual.

The **SAMPLING METHOD** box allows the user to specify "Variability" or "Uncertainty", which will determine whether a 1-stage or 2-stage Monte-Carlo analysis will be used. This choice will affect the form of the parameter inputs required by SHEDS, as well as the types of available outputs. For additional discussion of Monte-Carlo simulation see the "Background Topics" chapter.

Specify Population

In the **SPECIFY POPULATION** box the user selects Ages(s) and Gender of interest in the simulation. All ages from 1-6 years, or any subset of those ages are available for selection. The **Size of Population** combobox allows the user to specify the sample size for the 1-stage simulation. If "Uncertainty" has been selected as the sampling method, then an additional combobox (**Number of Populations**) appears for the user to specify the number of populations of input distributions to be simulated in the 2-stage Monte Carlo simulation.

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. Examples of simulation times are given in Table 2 on page 19.

Specify Input and Output Datasets

The **SPECIFY INPUT AND OUTPUT DATASETS** box allows the user specify the input dataset and name the output file containing simulation results. The button to change the input dataset will only be enabled if a custom file was specified in the **Input Dataset** box. To change the input file click the **Select Input File** button. To name the output dataset, simply edit the text in the text box. The name entered will be prefixed to all output dataset names. The suffixes on the names indicate the type of dataset.

> NOTE: All simulation output is placed in predetermined libraries. These libraries are:
>
> as_outv: Variability outputs
>
> as_outu: Uncertainty outputs
>
> Metadata are stored in as_idv and as_idu, but the user will probably not have much need for these outputs.

> NOTE: The input datasets are initially read from the as_dtain library.

Edit Inputs

The Main Editing Dialog

Selecting the **Edit Inputs** button allows the user to edit the parameters in the user-specified input file. Initially, a screen appears (Figure 24) displaying the categories of input parameters in the file. The default file contains the following categories:

- Activity factors
- Dose Factors
- Exposure Factors
- Soil concentrations and residue levels around/on decks, and
- Soil concentrations and residue levels around/on playsets.

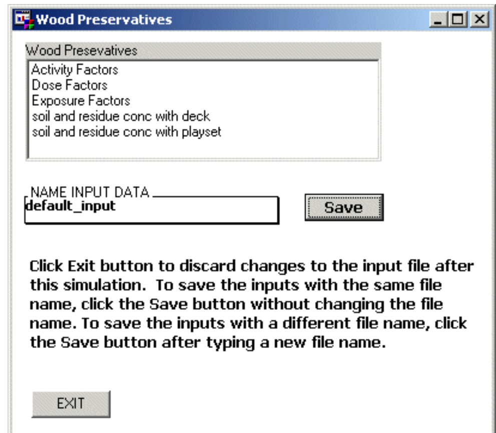


Figure 24. The main editing dialog.

Double clicking on a category in the list box chooses that category, displaying a dialog used to edit the variability or uncertainty distributions of its input parameters. The dialogs for each category are nearly identical in most respects. However, those used to edit variability parameters are different from those used to edit uncertainty parameters. The type of run specified in the **Sampling Method** box of the Scenario Specification dialog determines whether variability or uncertainty parameters are shown here. The details of actually editing individual parameters will be covered shortly.

The other box that appears in the Edit Inputs dialog is **NAME INPUT DATA**. As indicated on the screen, the user can discard changes made to the input file after the simulation by hitting the **Exit** button after making changes. Alternatively, the user can save the changes made to the inputs with either the same name or a different one typed in this box, by clicking the **Save** button.

Editing Variability Parameters

An example dialog for variability parameters is shown in Figure 25. A title at the top indicates the category being edited. The length of the dialogs vary depending on the number of parameters in the category. For

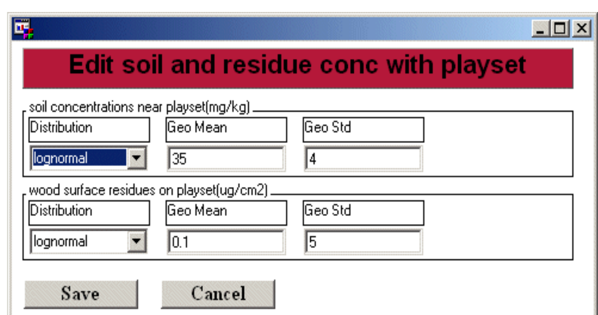


Figure 25. An example variability distribution editing dialog.

some categories it is necessary to scroll down the dialog to see the bottom where the **Save** and **Cancel** buttons are.

There is one container box for each parameter. A description of the parameter is given across top of the box. Within the box, in the first column, the type of variability distribution is specified with a pull down list. (See the "Background Topics" chapter for information on distributions.) One to three text entry boxes appear below labels in the second through fourth columns. An appropriate number appear to specify values for the chosen distribution. The labels above the boxes indicate the distribution parameter to be edited. See Table 1 for distributions supported and their parameters.

Table 1. Distributions supported in SHEDS.

Distribution	**Number of Parameters**	**Parameter Names**
Point	1	Value
Uniform	2	Minimum, Maximum
Normal	2	Mean, Standard Deviation
Log Normal	2	Geo Mean, Geo Standard Deviation
Triangle	3	Minimum, Mode, Maximum

The number of text boxes will change as the distribution is changed (Figure 26). Invalid numbers are highlighted in yellow (Figure 27). These will typically occur when the user changes the distribution to one with a greater number of parameters. Boxes which contain invalid values will be colored in red (Figure 28). An invalid value might be one that contains a negative standard deviation or a minimum that is greater than the maximum.

The **Save** button saves the currently displayed parameter values back to the parameter dataset. The **Save** button is disabled while any invalid values are on the form. The **Cancel** button exits this screen without saving any values.

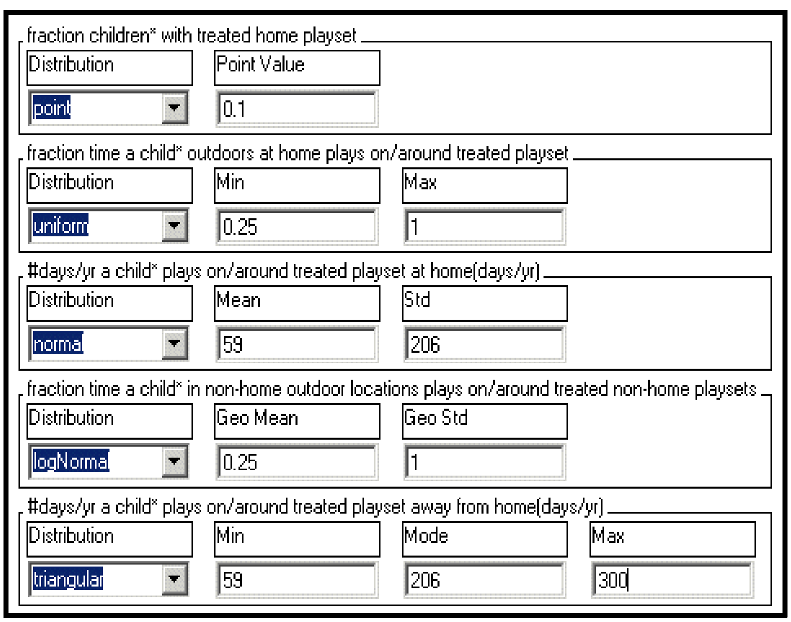


Figure 26. Examples of all supported distributions in the variability distribution editing dialog.

NOTE: In this version of the model the minimum or maximum of a triangle distribution cannot be the same as the mode.

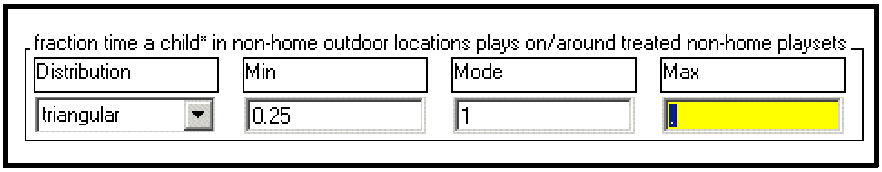


Figure 27. Non-numbers highlighted in yellow.

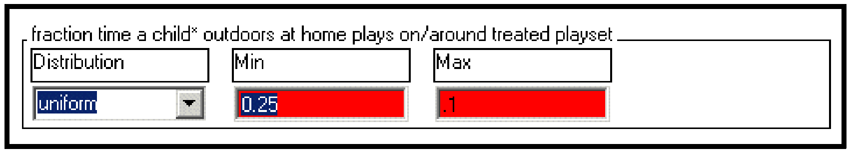


Figure 28. Invalid values highlighted in red.

Editing Uncertainty Parameters

Editing uncertainty parameters works in essentially the same manner as variability parameters. The big difference is that there is one uncertainty distribution for each variability parameter. Figure 29 shows an example uncertainty editing screen for two parameters. The top row contains the variability distribution. There will be from one to three distributions below that, one for each parameter. Each individual uncertainty distribution works essentially like the variability parameters. The number of text boxes to enter values will change based on the distribution.

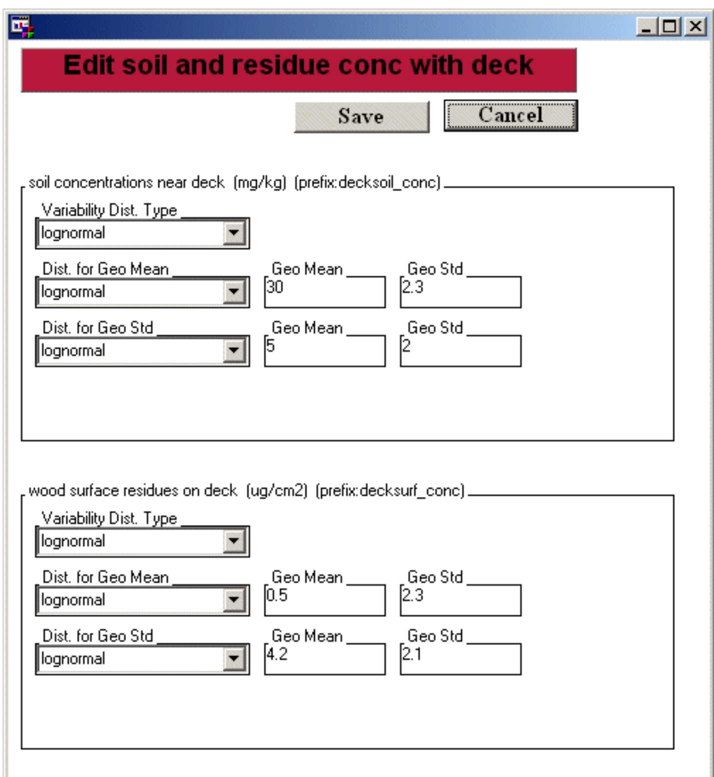


Figure 29. Uncertainty parameter editing dialog.

NOTE: If you are defining an uncertainty run and do not want to include uncertainty in one or more parameters, then define each distribution for the variability parameters as a point distribution. For example if you wanted define the parameter value as a point in all uncertainty runs, change the variability distribution to 'Point'. One uncertainty distribution will be displayed. Change this distribution to 'Point' and define the value desired.

NOTE: Although values are checked within each uncertainty distribution, there is no check on the validity of the relationships among the uncertainty distributions

Run Simulation

After specifying the scenario and model inputs, the user can press the **Run Simulation** button to start the model run. When the simulation is completed, a pop-up message appears. To track the iteration while the model is running, the user can click on the **Log** menu bar at the bottom of the interface. After viewing the Log, the user should click back on the menu bar with "SHEDS" at the bottom of the interface screen.

Duration of Simulations

The time it takes to run a simulation depends on: the speed of your computer, the size of population, the number of uncertainty populations (if any), and whether the simulation is short-term, medium-term, or lifetime. It is difficult to say how long a simulation will take on a specific machine. Table 2 indicates some typical simulation times on a 900 MHz PC.

Table 2. Minutes to execute 1000 individuals (iterations) for short, intermediate, and lifetime simulations using either variability or uncertainty sampling.

Simulation Time Period	Variability	Uncertainty	
Short	7.6	11.7	For uncertainty runs, the number of individual iterations is equal to the size of the population multiplied by the number of samples. A user running 100 individuals and 10 uncertainty samples, results in 1000 individual iterations.
Intermediate	8.8	12.6	
Lifetime	93	108	

Logging of Simulation Progress

During the simulation, the individuals being simulated and progress on the entire run will be printed to the Log Window. During variability runs, the person ID, gender, age, simulation start day (i.e., between 1 and 351), and percent completion are printed to the log (Table 3). One line is printed for each individual. The time is printed at the beginning and end of the simulation.

Table 3. Logging during variability simulations.

```
Time = 11:23:36
 Person=1    gender=M  age=5   start day=149  Percent Done=33.33
 Person=2    gender=M  age=2   start day=59   Percent Done=66.67
 Person=3    gender=F  age=3   start day=330  Percent Done=100.00
Stop Time = 11:23:38
```

During uncertainty simulations this same information is logged. Additionally, the uncertainty iteration is printed with the output for each individual and the time is printed at the beginning of each uncertainty iteration (Table 4).

Table 4. Logging during uncertainty runs.

```
Time = 11:22:58
Uncert Iter=1    Person=1    gender=F  age=2   start day=203  Percent Done=16.67
Uncert Iter=1    Person=2    gender=F  age=5   start day=212  Percent Done=33.33
Uncert Iter=1    Person=3    gender=M  age=6   start day=200  Percent Done=50.00
Time = 11:23:01
Uncert Iter=2    Person=1    gender=F  age=3   start day=94   Percent Done=66.67
Uncert Iter=2    Person=2    gender=F  age=5   start day=103  Percent Done=83.33
Uncert Iter=2    Person=3    gender=M  age=1   start day=59   Percent Done=100.00
Stop Time = 11:23:03
```

View Results

Model results from current or previous SHEDS simulations can be viewed by pressing the **View Results** button. This opens a dialog (Figure 30) to specify desired outputs. There are a variety of graphical and tabular outputs available. The specifications and output options change based on the sampling method used and result type of interest.

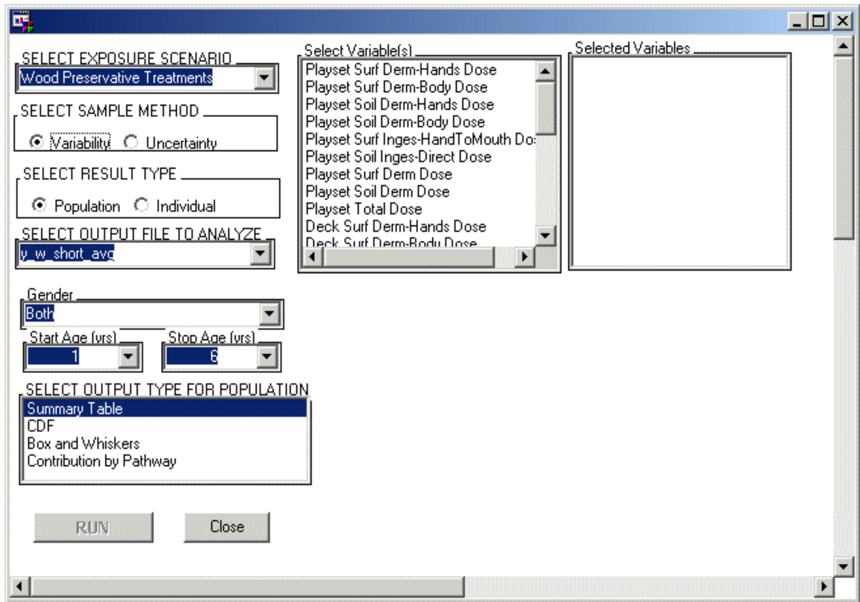


Figure 30. Dialog to specify analysis of simulation results.

Select the Wood Preservative scenario in the top left combo box; this is the only scenario available in this version of SHEDS. Then select the sampling method (uncertainty or variability) and the population type (population or individual) currently of interest in the two radio boxes below. A list of the available output datasets will be put in the **Select Output File To Analyze** combobox. Select the file to analyze and continue.

Manual Sensitivity Analysis

Automated procedures for conducting sensitivity analyses are not implemented in this version of SHEDS. To determine which input variables contribute the most to variability in model outputs, the user can fix each input value as a point estimate, then vary one at a time (e.g., increase then decrease by a factor of 2) keeping the rest fixed, and comparing output results for variability simulations.

Variability Results for a Population

If the user selects “Variability” as the sample method and “Population” as the “Result Type,” options will appear for the user to specify the Gender(s) (Male, Female, or Both), Start Age (yrs), and Stop Age (yrs) corresponding to the model simulation results/output file selected. The “Gender” and “Age” selected on this screen will appear on the output tables and graphics selected by the user.

NOTE: IT IS THE USER'S RESPONSIBILITY TO SELECT THE CORRECT GENDER AND AGE CORRESPONDING TO THE SELECTED OUTPUT FILE TO ANALYZE.

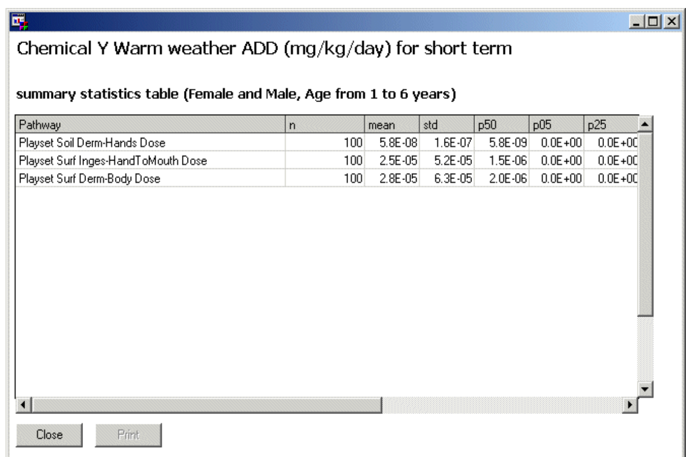
The output options for viewing variability results for a population are listed in the **SELECT OUTPUT TYPE FOR POPULATION** box:

- Summary Table,
- CDF,
- Box and Whiskers, and
- Contribution by Pathway.

For each of these output types, the user must select (by clicking) variable(s) of interest from the **Select Variable(s)** listbox. The selected variables will appear in the **Selected Variables** listbox. The available output variables are described in Table 5. To unselect a variable, click on it again in the **Select Variable(s)** listbox.

Summary Table

This yields a summary statistics table (Figure 31) for the selected dose variable(s) and specified model simulation, describing the basic distribution of the variable: sample size, mean, standard deviation, median (p50), 5th percentile (p05), 25th percentile (p25), 75th percentile (p75), 95th percentile (p95), and maximum.


Chemical Y Warm weather ADD (mg/kg/day) for short term

summary statistics table (Female and Male, Age from 1 to 6 years)

Pathway	n	mean	std	p50	p05	p25
Playset Soil Derm-Hands Dose	100	5.8E-08	1.6E-07	5.8E-09	0.0E+00	0.0E+0
Playset Surf Inges-HandToMouth Dose	100	2.5E-05	5.2E-05	1.5E-06	0.0E+00	0.0E+0
Playset Surf Derm-Body Dose	100	2.8E-05	6.3E-05	2.0E-06	0.0E+00	0.0E+0

Figure 31. Example summary table for a population.

Cumulative Density Function

This yields a cumulative density function (CDF) plot (Figure 32) for the selected dose variable(s) and specified model simulation. The CDF shows the percent of the population that had less than a specific value for a simulation run. The whole population is represented in one curve. The entire population has values of less than or equal to the maximum which occurs at the 100th percentile.

The percentile is given on the X-Axis. The value for the output variable is given on the Y-Axis. The median value for a variable will occur at the 50th percentile.

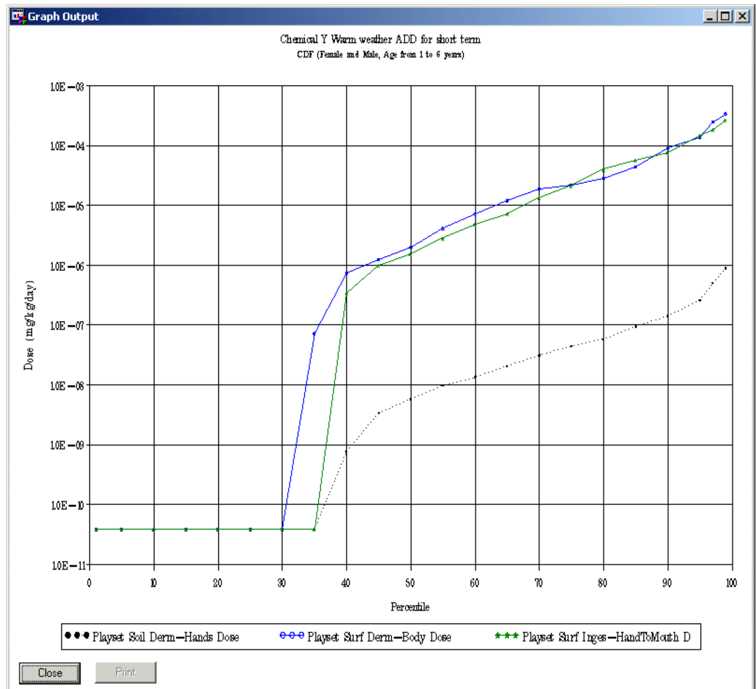


Figure 32. Example CDF for a population.

Box and Whiskers

This yields a box and whiskers plot (Figure 33) for the selected dose variable(s) and specified model simulation. The box and whiskers plot shows the distribution of a variable for the entire population graphically. Each column, three in the example, represents one variable described in the legend. The absolute variable values are given on the Y-Axis. The rectangle represents the median and one quartile above and below the median. The tails extend to the 5th and 95th percentiles.

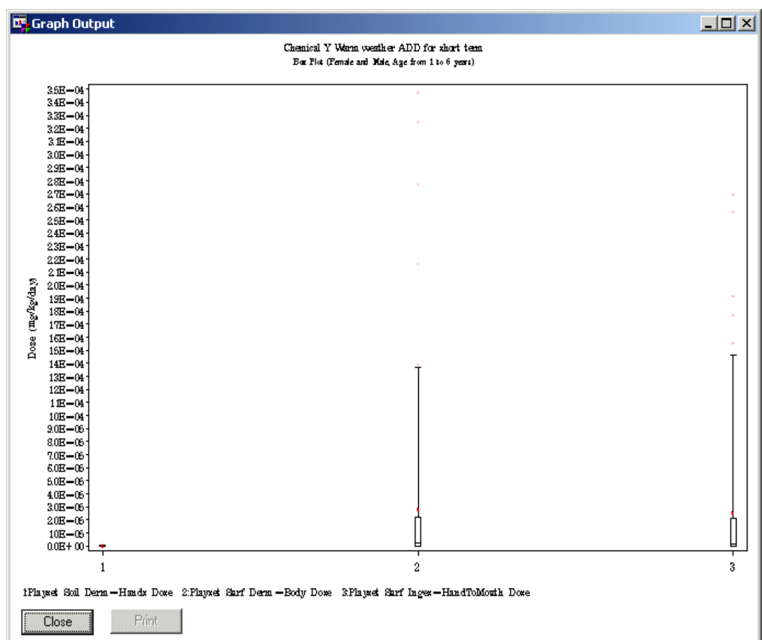


Figure 33. Example of Box and Whiskers plot for a population.

Contribution by Pathway

This yields a pie chart (Figure 34) showing percent contribution of each pathway to the total dose (based on population means) for the following pathways (See Table 5):

- Combined Surf Derm Dose,
- Combined Soil Derm Dose,
- Combined Surf Inges-HandToMouth Dose, and
- Combined Soil Inges – Direct Dose.

The user does not have the option to select variables for this output (*i.e.*, the **Select Variable(s)** and **Selected Variables** listboxes do not appear).

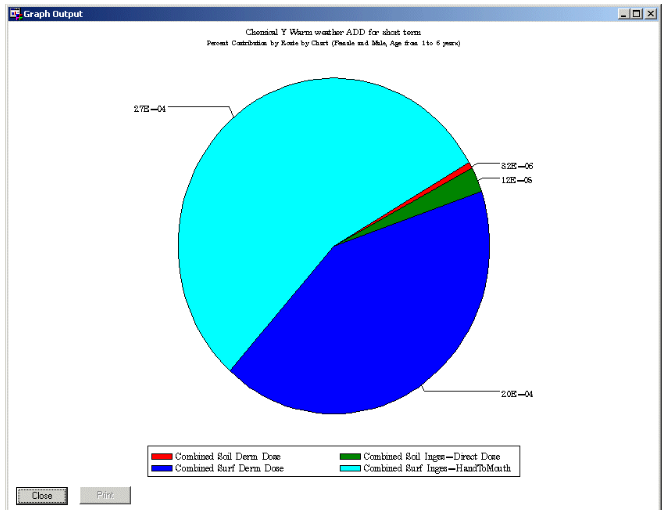


Figure 34. Example of the contribution by pathway chart.

Variability Results for an Individual

If the user selects "Variability" as the sample method and "Individual" as the "Result Type," options will appear for the user to "Select Individual", "Start Date" and "Stop Date" of the calendar year for that individual in the model simulation results/output file selected. The output options for viewing variability results for an individual are listed in the "SELECT OUTPUT TYPE FOR INDIVIDUAL" box:

- Detailed Data,
- Absorbed Dose Time Profile, and
- Contribution by Pathway.

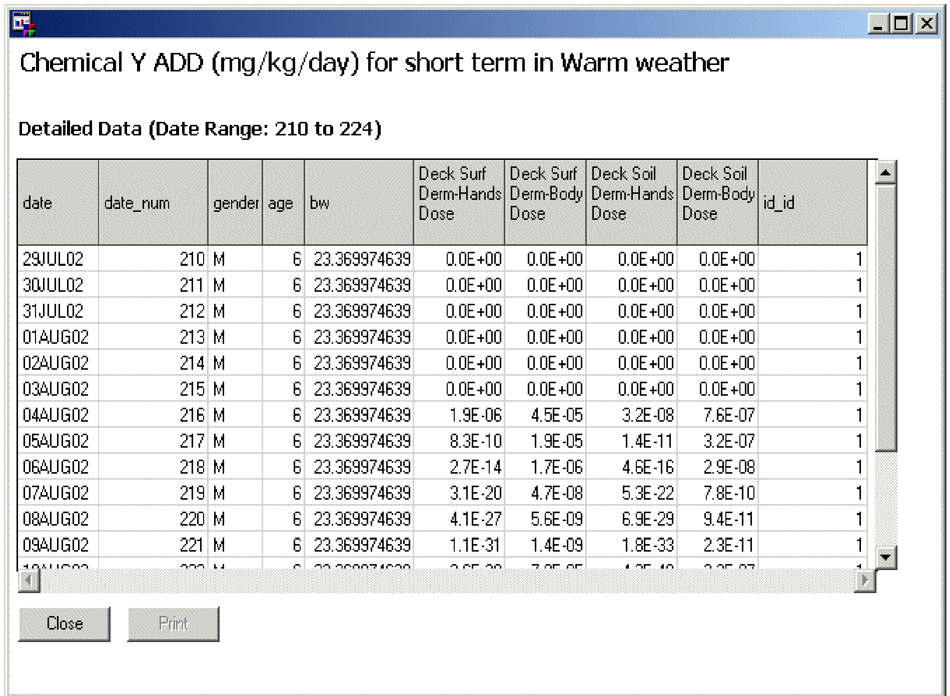
For each of these output types, the user must select (by clicking) variable(s) of interest from the "Select Variable(s)" box. The selected variables will appear in the "Selected Variables" box. Options for output variables are the same as the previous section (Table 5).

Table 5. Output variable descriptions.

Playset Surf Derm-Hands Dose (absorbed dose from dermal hand contact with playset surfaces)
Playset Surf Derm-Body Dose (absorbed dose from dermal body contact with playset surfaces)
Playset Soil Derm – Hands Dose (absorbed dose from dermal hand contact with soil around playsets)
Playset Soil Derm-Body Dose (absorbed dose from dermal body contact with soil around playsets)
Playset Surf Inges-HandToMouth Dose (absorbed dose from ingested playset surface residues from hand-in-mouth events)
Playset Soil Inges – Direct Dose (absorbed dose from ingested soil around playsets)
Playset Surf Derm Dose (absorbed dose from hand and body dermal contact with playset surfaces)
Playset Soil Derm Dose (absorbed dose from hand and body dermal contact with soil around playsets)
Playset Total Dose (total absorbed dose from playsets)
Deck Surf Derm-Hands Dose (absorbed dose from dermal hand contact with deck surfaces)
Deck Surf Derm-Body Dose (absorbed dose from dermal body contact with deck surfaces)
Deck Soil Derm – Hands Dose (absorbed dose from dermal hand contact with soil around decks)
Deck Soil Derm-Body Dose (absorbed dose from dermal body contact with soil around decks)
Deck Surf Inges-HandToMouth Dose (absorbed dose from ingested deck surface residues from hand-in-mouth events)
Deck Soil Inges – Direct Dose (absorbed dose from ingested soil around decks)
Deck Surf Derm Dose (absorbed dose from hand and body dermal contact with deck surfaces)
Deck Soil Derm Dose (absorbed dose from hand and body dermal contact with soil around decks)
Deck Total Dose (total absorbed dose from decks)
Combined Surf Derm-Hands Dose (absorbed dose from dermal hand contact with playset and deck surfaces)
Combined Surf Derm-Body Dose (absorbed dose from dermal body contact with playset and deck surfaces)
Combined Soil Derm – Hands Dose (absorbed dose from dermal hand contact with soil around playsets and decks)
Combined Soil Derm-Body Dose (absorbed dose from dermal body contact with soil around playsets and decks)
Combined Surf Inges-HandToMouth Dose (absorbed dose from ingested playset and deck surface residues from hand-in-mouth events)
Combined Soil Inges – Direct Dose (absorbed dose from ingested soil around playsets and decks)
Combined Surf Derm Dose (absorbed dose from hand and body dermal contact with playset and deck surfaces)
Combined Soil Derm Dose (absorbed dose from hand and body dermal contact with soil around playsets and decks)
Total Dose (total absorbed dose from playsets and decks)

Detailed Data

This displays information for the selected individual and simulated days (Figure 35). Variables shown include date, day number (1 to 366), gender, age, body weight (kg), child ID, and the daily dose averages for the selected variables.



Chemical Y ADD (mg/kg/day) for short term in Warm weather

Detailed Data (Date Range: 210 to 224)

date	date_num	gender	age	bw	Deck Surf Derm-Hands Dose	Deck Surf Derm-Body Dose	Deck Soil Derm-Hands Dose	Deck Soil Derm-Body Dose	id_id
29JUL02	210	M	6	23.369974639	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1
30JUL02	211	M	6	23.369974639	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1
31JUL02	212	M	6	23.369974639	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1
01AUG02	213	M	6	23.369974639	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1
02AUG02	214	M	6	23.369974639	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1
03AUG02	215	M	6	23.369974639	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1
04AUG02	216	M	6	23.369974639	1.9E-06	4.5E-05	3.2E-08	7.6E-07	1
05AUG02	217	M	6	23.369974639	8.3E-10	1.9E-05	1.4E-11	3.2E-07	1
06AUG02	218	M	6	23.369974639	2.7E-14	1.7E-06	4.6E-16	2.9E-08	1
07AUG02	219	M	6	23.369974639	3.1E-20	4.7E-08	5.3E-22	7.8E-10	1
08AUG02	220	M	6	23.369974639	4.1E-27	5.6E-09	6.9E-29	9.4E-11	1
09AUG02	221	M	6	23.369974639	1.1E-31	1.4E-09	1.8E-33	2.3E-11	1

Close Print

Figure 35. Example detailed data table for an individual.

Absorbed Dose Time Profile

A dose profile (Figure 36) is plotted with absorbed dose on the y-axis and day on the x-axis, for the selected variables. The x-axis defaults to the days an individual was simulated, but can be changed in the output specification dialog.

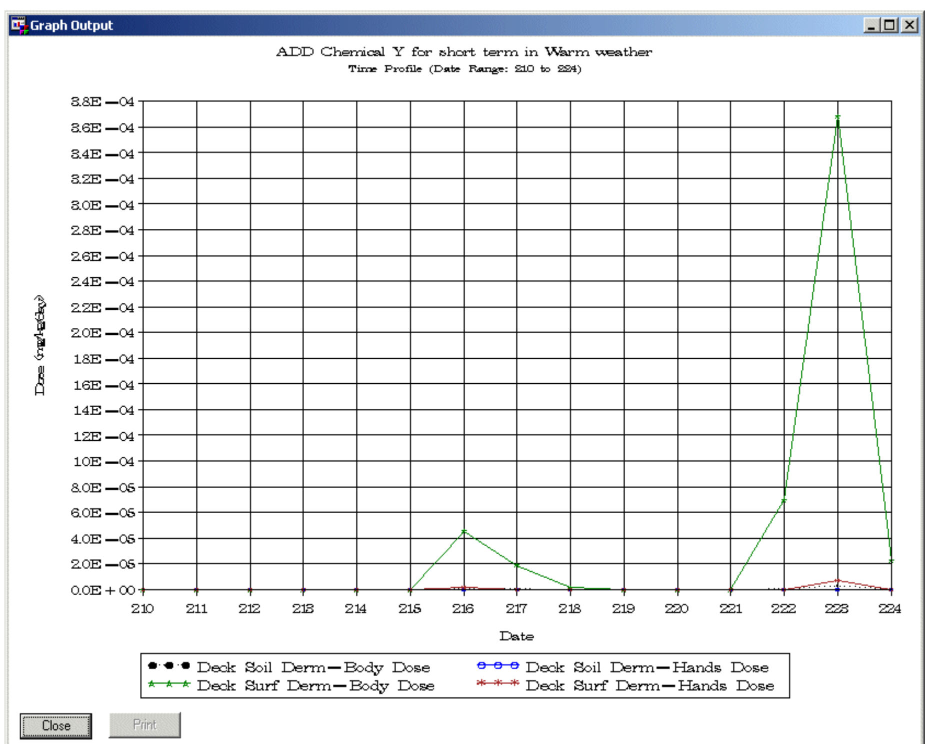


Figure 36. Example absorbed dose time profile for an individual.

Contribution by Pathway

A pie chart showing each pathway's percent contribution to total dose is displayed. The pathways represented are fixed:

1. Combined Surf Derm Dose,
2. Combined Soil Derm Dose,
3. Combined Surf Inges-HandToMouth Dose, and
4. Combined Soil Inges – Direct Dose.

The user does not have the option to select variables (i.e., the **Select Variable(s)** and **Selected Variables** list boxes do not appear).

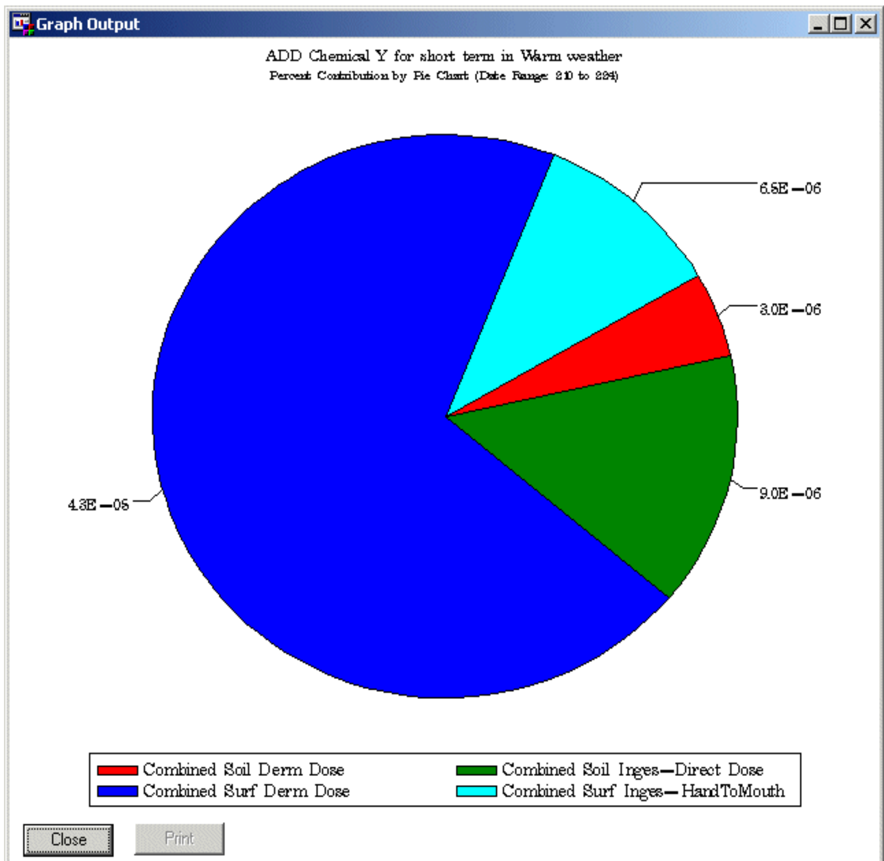


Figure 37. Example "Contribution by Pathway" pie chart for an individual.

Uncertainty Analyses

If the user selects "Uncertainty" in the **SELECT SAMPLE METHOD** box on the View Results dialog, the "Uncertainty Analyses" dialog appears.

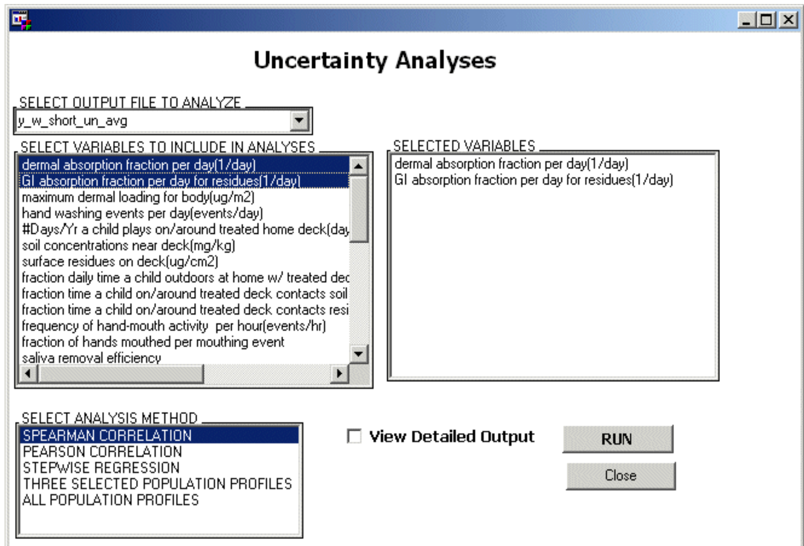


Figure 38. The uncertainty analysis specifications dialog.

In the **SELECT OUTPUT FILE TO ANALYZE**, the user can select only from outputs of uncertainty simulations.

If either the Spearman Correlation, Pearson Correlation, or Stepwise Regression analysis methods are selected by the user in the **SELECT ANALYSIS METHOD** list box at the bottom of the screen, the user can select variables to include in these uncertainty analyses using the **SELECTED VARIABLES TO INCLUDE IN ANALYSES** list box. One or more variables can be selected. The selected variables will appear in the **SELECTED VARIABLES** list box. To unselect variables, click again on those variables in the **SELECTED VARIABLES TO INCLUDE IN ANALYSES** list box.

Correlations

For "Spearman Correlation" and "Pearson Correlation" selections, the selected variables appear along with their correlation to the total dose aggregated over all pathways for both playsets and decks (Figures 39 and 40).

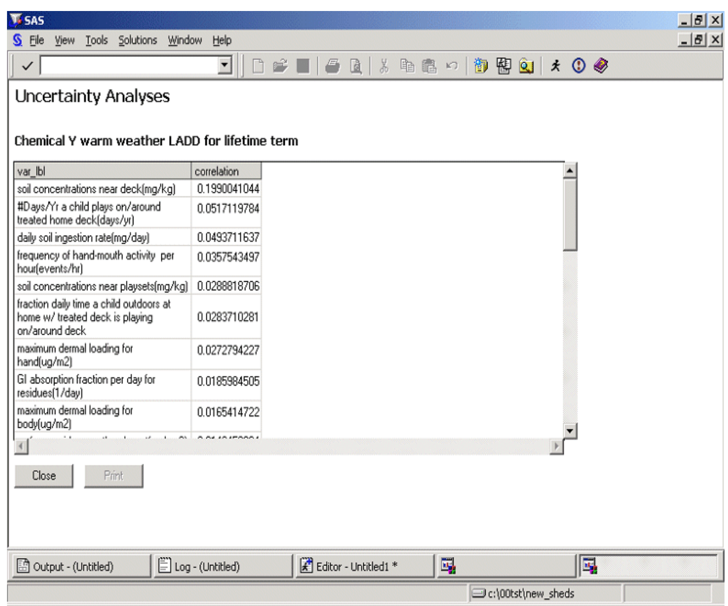


Figure 39. Pearson correlation coefficients between selected simulation output variables and the total aggregated dose over all pathways.

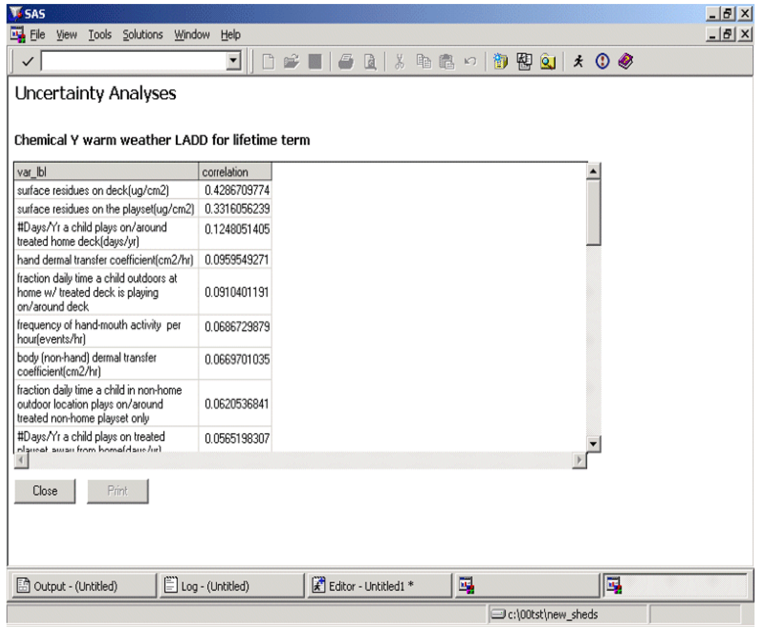


Figure 40. Spearman correlation coefficients between the selected output variables and the total dose aggregated over all pathways.

Stepwise Regression

For "Stepwise Regression", the selected variables are listed in a table along with results of the analysis. The analysis adds and/or deletes individual input variables into a regression model predicting the total aggregated dose over all pathways. The results of this analysis give a statistical relationship between the model inputs and the output dose (Figure 41). The statistics displayed include partial R^2 correlation coefficient, model R^2 correlation coefficient, and significance probability (Pr>F). If none of the selected variables have a significant relationship with the total dose then the table will be empty.

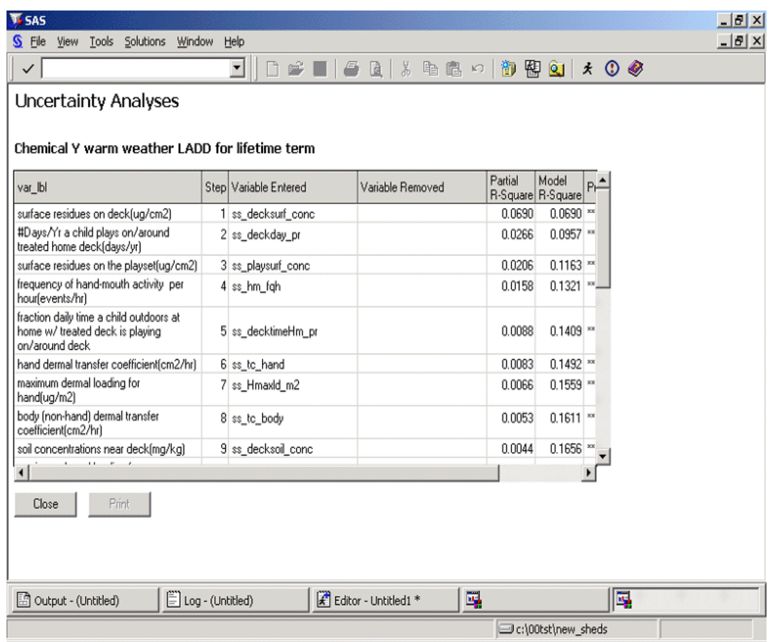


Figure 41. Sensitivity analysis of output data using stepwise regression.

Population Uncertainty Cumulative Density Functions

These show representative cumulative density functions (CDFs) for the entire population in uncertainty runs. Only the total absorbed dose from playsets and decks is plotted. The user has no options to choose specific input or output variables.

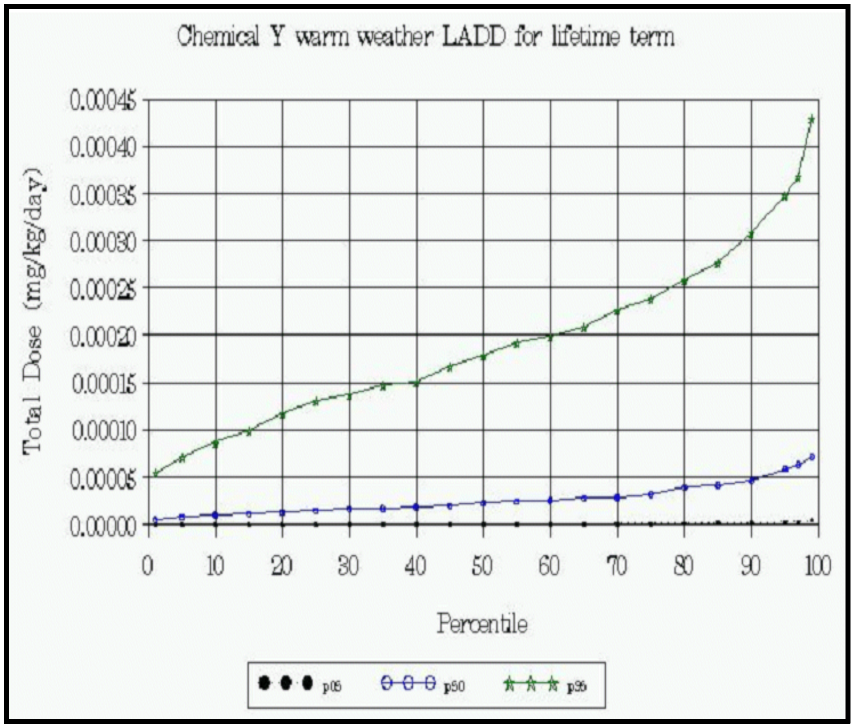


Figure 42. Variability between three representative uncertainty iterations. Each line shows the total dose of all individuals in a single uncertainty iteration.

Let us assume that the user has made an uncertainty run with a population of 1000 and a sample size of 100. This means that 1000 individuals will be simulated 100 times each. These CDFs look at the results in two ways. The first shows typical uncertainty for high dose, medium dose, and low dose individuals (Figure 42). The second shows uncertainty for the entire population (Figure 43).

Uncertainty for Representative Individuals

Choosing “Three Selected Population Profiles” allows the user to look at three representative populations (Figure 42). Using the example started previously, there are 1000 individuals which have been simulated. The uncertainty iterations can be ranked from 1 to 100 based on the median total dose calculated for each of the 1000 individuals in that iteration. The iterations that are ranked 5th, 50th, and 95th of the 100 iterations (the 5th, 50th, and 95th percentiles) are selected for this analysis. The CDFs represent the the total dose (mg/kg/day) of all individuals in these iterations. Thus, each line contains 1000 numbers for the given example.

Population Uncertainty

Choosing “All Population Profiles” allows the user to look at uncertainty for the entire population (Figure 43), which can be useful in regulatory decision making. For each of the 1000 numbers in the 100 runs, a 5th, 50th, and 95th percentile is obtained. The three CDFs in Figure 43 each represent 100 values. These show the uncertainty associated with each of these percentiles for the entire population.

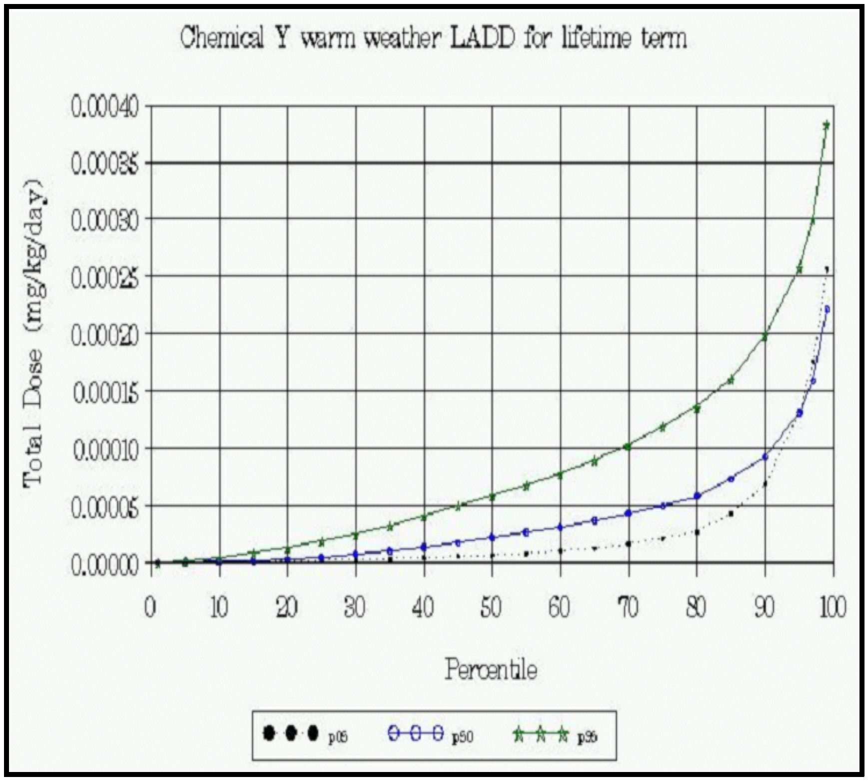


Figure 43. Uncertainty of entire population.

Manage Output Files

The dialog that appears upon clicking the **Manage Output Files** button in the main dialog is shown in Figure 44. A number of files are associated with each model run. This dialog allows the user to delete unneeded files from previous simulations. The user selects the SHEDS output files from the top list box. The selected files appear in the lower dialog. The files are deleted when the user selects the **Delete V** (for variability files) or **Delete U** for (uncertainty files) buttons.

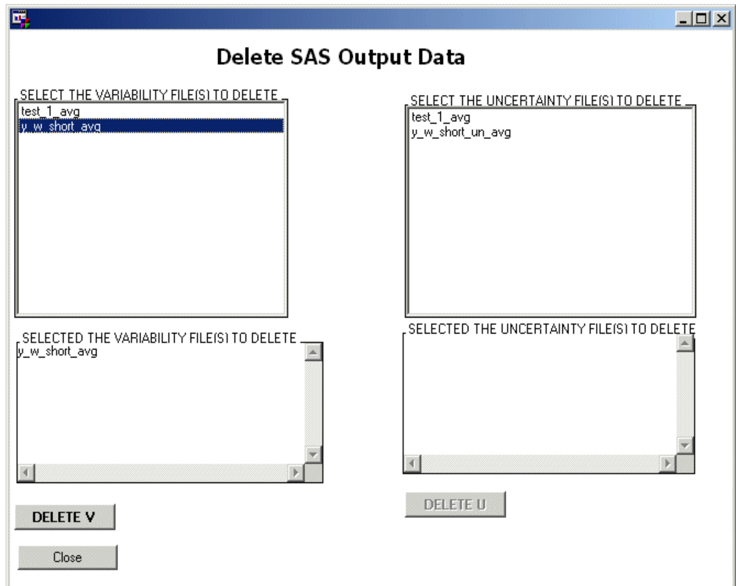


Figure 44. The dialog for user management of simulation datasets.

Exit

Clicking on the **Exit** button on the main dialog removes the SHEDS interface screen, but typically leaves the user in SAS. Output, log, editor, and graphics screens from the session will still appear unless closed by the user. The easiest method of starting a new SHEDS session is to exit SAS and restart using the the desktop icon. To exit SAS completely, select the **File**, menu then **Exit** (**File>Exit**).

Future Modifications

Some changes that may be incorporated into subsequent versions of the SHEDS-wood interface include the following: selection of different cohorts besides ages 1 to 6 years; inclusion of a "cancel run" option and an indicator for "estimated time remaining" in a model simulation; and ability to print results and export them to other software formats (e.g., Excel)

Background Topics

Distributions and Sampling

The SHEDS-Pesticide model supports five distributions as previously listed in Table 2. A diagram showing these distributions is given in Figure 45. The distributions and their parameters (as shown) are:

1. **Point:** value of 17.
2. **Uniform:** minimum 5, maximum 15.
3. **Normal:** mean 10, standard deviation 2.
4. **Lognormal:** geometric mean 3 and geometric standard deviation 1.35. or exp(0.3).
5. **Triangular:** minimum 2, mode 10, maximum 18.

Each parameter must be specified to fully define the distributions.

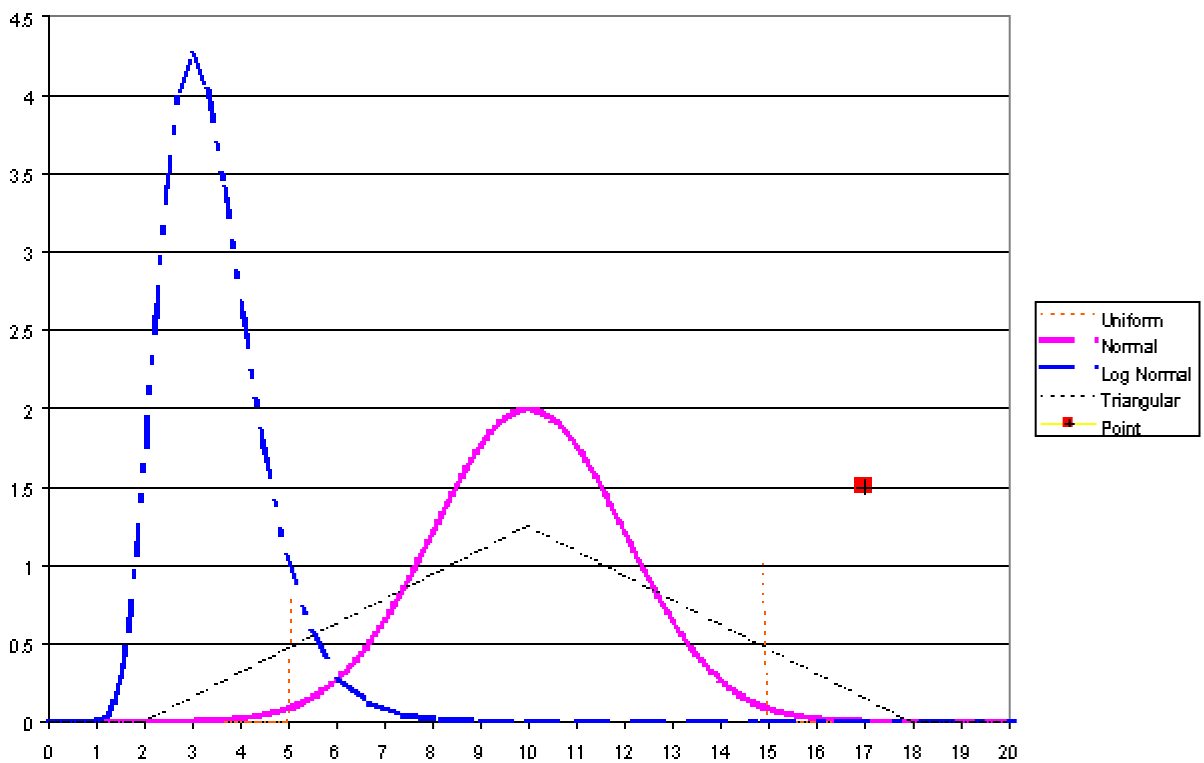


Figure 45 Distributions supported in SHEDS: point, uniform, normal, log-normal, and triangular. Each curve is normalized so that its area is approximately 10 units.

During the model run, a specific parameter may be sampled many times. There is no guarantee that the parameter will be a specific value unless the point distribution is used. If the uniform or triangular distributions are used, the value will not be greater than the maximum or less than the minimum. If the normal distribution is used, one can only be assured that the value will be within two standard deviations of the mean about 96% of the time. However, in all cases, if enough samples are tallied, the population of values will resemble the distribution used. That is, the tallied samples should have the same central tendency, spread, and skewness as the population from which they are drawn. However, the current implementation of the model sets upper and lower bounds in certain cases to prevent physically impossible values from being chosen. If the distribution returns a value outside the bounds, then the distribution is resampled.

Assume for a moment that one specifies an absorption rate for the gastrointestinal tract (GI) as a normal distribution with a mean of 0.00025 and standard deviation of 0.0001. It cannot be determined *a priori* what a specific sample value will be. We know that about 67% of the time the value will be between 0.00015 and 0.00035 within 1 standard deviation of the mean, and about 96% of the time the value will be between 0.00005 and 0.00045, or within 2 standard deviations.

Lognormal Distributions

Lognormal distributions are used for many of the SHEDS parameters. A population that is lognormal will become normal after the application of a log transform to the values. In SHEDS, these distributions are specified using the geometric mean and geometric standard deviation. These are the mean and standard deviation of the normal population that have been converted back (exponentiated) to the scale of the original data.

Single-Stage Monte-Carlo Simulation

Below is a simple equation (1) to demonstrate how the variability distributions work in the model using single-stage Monte-Carlo sampling. Single-stage sampling will account for real variation in the parameter values in the population. Equation 1 has two parameters: Variable 1 (V_1) and Variable 2 (V_2).

Equation (1) Example equation for use in explaining Monte-Carlo modeling.

$$\text{Result} = V_1 * V_2$$

Assume for the moment that this equation is part of the exposure model. Before calculating the result for any time period, the model will pick specific parameter values for V_1 and V_2 based on the input distributions. These values will remain constant for the simulation of the individual.

- **V1:** This variable will be defined as coming from a normal distribution with a mean of 20 and a standard deviation of 2.

- **V2**: This variable will be sampled from a uniform distribution with a minimum of 4 and a maximum of 6.

Having chosen the parameter values, they will be applied to the calculations for a specific time period, usually either one event, one time-step, or the simulation for one individual. Over the course of the entire simulation the value of the result will take on a variety of values. Visually this can be represented as in Figure 46 where specific values chosen during one iteration are used to calculate the final result. Additionally, the figure shows the frequency histogram of 1000 such samples.

NOTE: The example values were chosen so that the result will typically be around 100.

In the figures, defined distributions are represented by smooth curves; distributions resulting from repetitive sampling are shown as bar charts with several bars. Uncertainty distributions are shown in red, variability in blue.

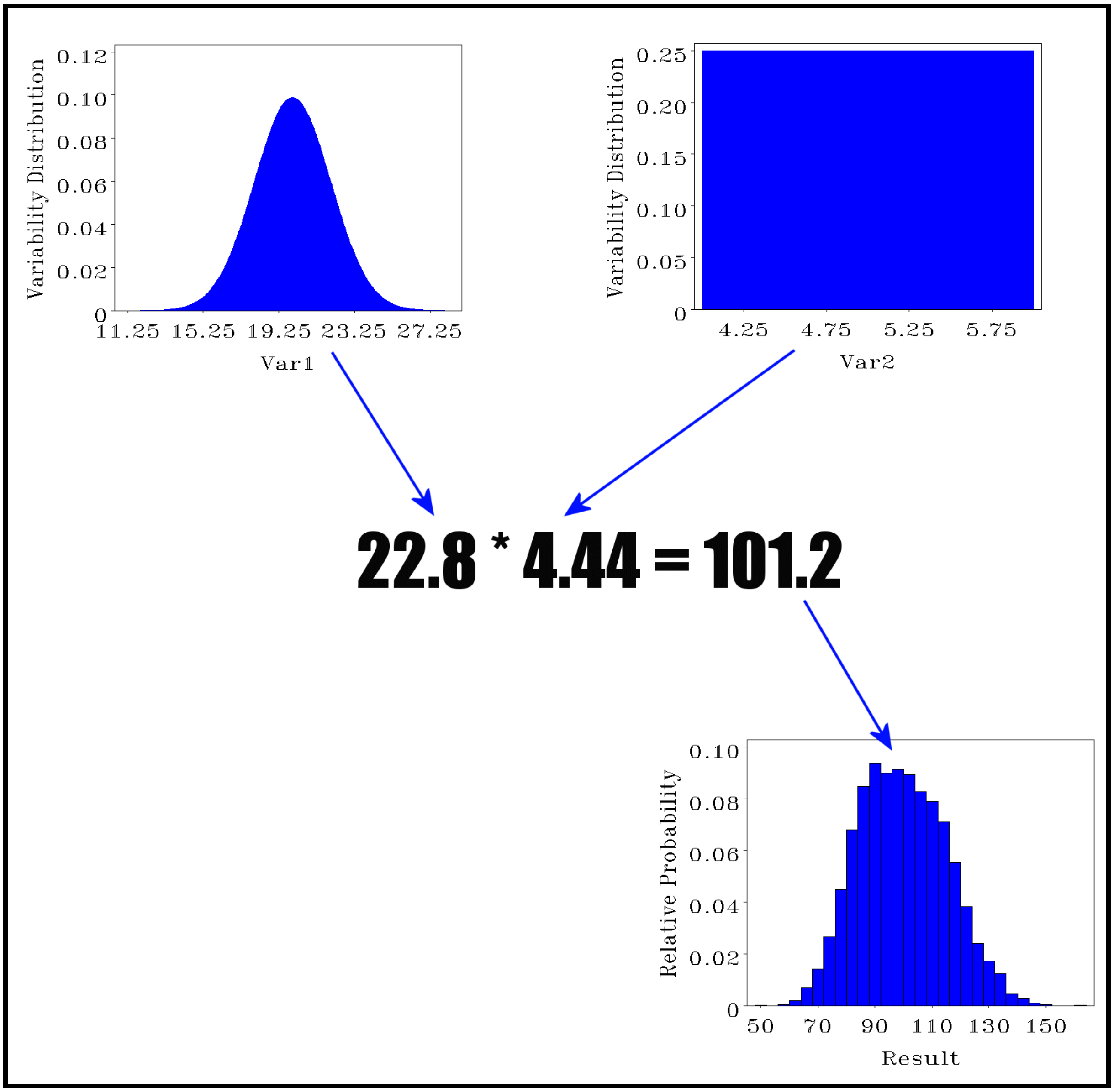


Figure 46 Visual representation of single stage Monte-Carlo sampling. One calculation for the example equation (V1=22.8, V2= 4.44, and Result = 101.2) and its relative location among 1000 such calculations.

Two-Stage Monte-Carlo Simulation

Single-stage Monte-Carlo simulation accounts for real *variability* in the population (e.g., the actual differences in metabolic rate from person to person). In contrast, two-stage Monte-Carlo simulation is used to assess *uncertainty* in the model due to our lack of knowledge about parameter values.

For two-stage simulations, it is necessary to choose a distribution for each parameter of each variability distribution. For instance, in the previous example, $\mathbf{V_1}$ was assumed to have a normal variability distribution with a mean of 20 and a standard deviation of 2 (Figure 46). The normal distribution requires two parameters, the mean and standard deviation. In two-stage sampling, we need to define a distribution for the mean, and another for the standard deviation. We might decide that the mean is "typically" between 18 and 22. This could be modeled using a normal distribution with a mean of 20 and standard deviation of 2 (Figure 47, **Mean1**, top row, left). Likewise the standard deviation of $\mathbf{V_1}$, **StdDev1**, could be modeled as a uniform value between one and three (Figure 47, top row middle).

The second variable, $\mathbf{V_2}$, has a uniform variability distribution. This also requires two parameters, the minimum and maximum. Its variability distribution uses a minimum of 4 and a maximum of 6 (Figure 46). We could model these with two distributions (Figure 47, second row), for **Min2** and **Max2**. **Min2** is modeled as uniform with a minimum of 3 and a maximum of 5. **Max2** is given by a uniform with a minimum of 5 and a maximum of 7.

The user will specify the number of uncertainty iterations and individuals to be simulated before the run. During the simulation run, at the beginning of the first uncertainty iteration, 4 values will be chosen to define **Mean1**, **StdDev1**, **Min2**, and **Max2** during the iteration. These four values will be derived from the uncertainty distributions (red distributions at the top of Figure 47). The values describe the variability distributions of $\mathbf{V_1}$ and $\mathbf{V_2}$ (third row, left and middle, Figure 47) for this uncertainty iteration. These two distributions will be used to draw samples for each individual during this uncertainty iteration (Figure 47, third row, right).

At the beginning of the next uncertainty iteration, the four distributions will be sampled again to define **Mean1**, **StdDev1**, **Min2**, and **Max2**, and thus the new variability distributions for $\mathbf{V_1}$ and $\mathbf{V_2}$ (fourth row, left and middle, Figure 47). For this uncertainty iteration these new variability distributions will be sampled each time a new value is needed for the result (fourth row, right, Figure 47). This process will be repeated for each uncertainty iteration (Figure 47, fifth row).

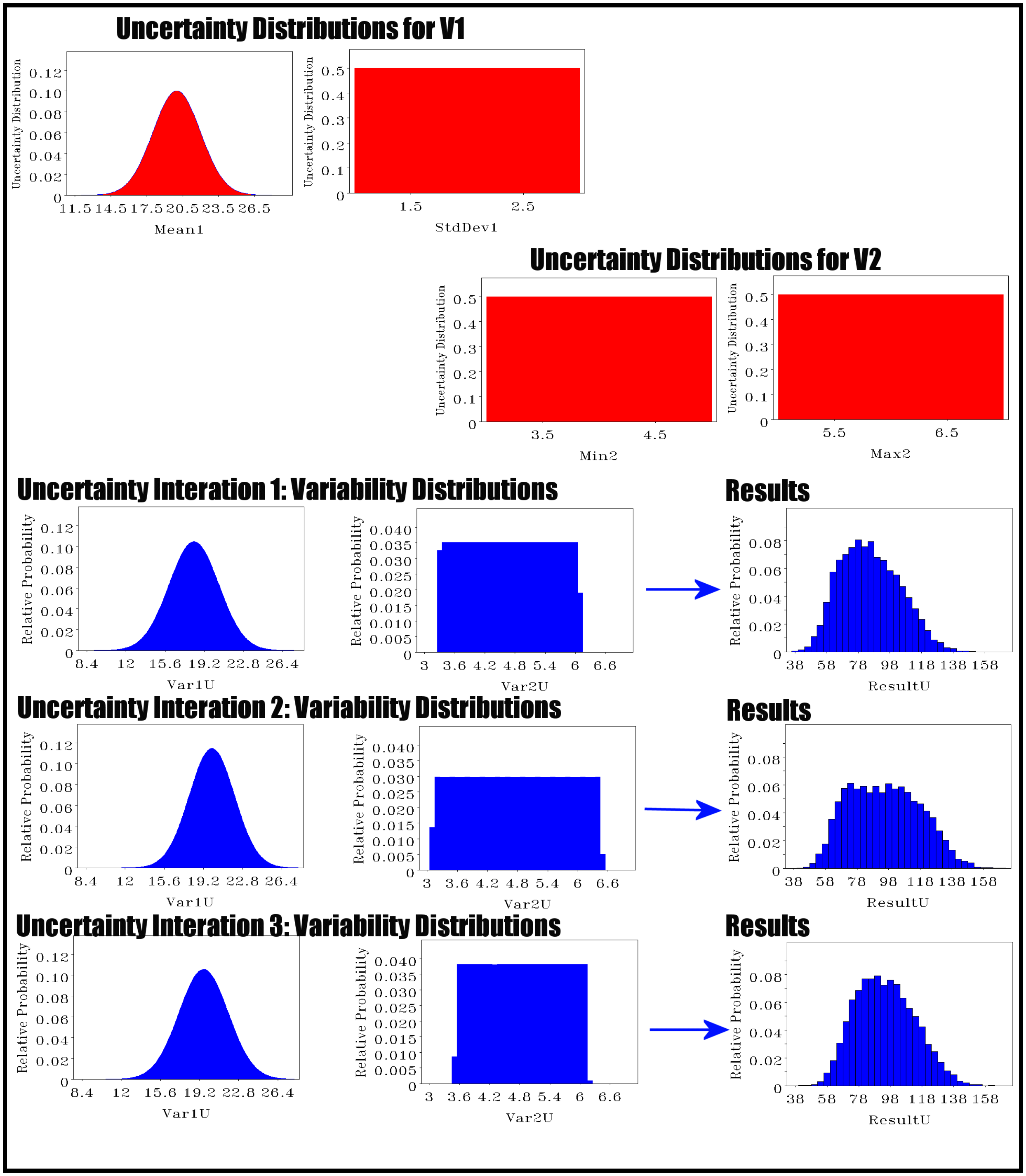


Figure 47. Visual example of two-stage Monte-Carlo sampling.