The Stochastic Human Exposure and Dose Simulation Model for Multimedia, Multipathway Chemicals (SHEDS-Multimedia): Residential Module

SHEDS-Residential version 4

Quick Start Guide

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1 Purpose of this Quick Start Guide

SHEDS-Residential is the residential exposure module of the SHEDS-Multimedia exposure model. It provides a flexible framework for stochastic simulation of population exposures to single or multiple chemicals applied in residential homes, yards, and gardens. This Quick Start guide is intended for persons familiar with chemical exposure and risk assessment who would like to quickly learn how to use SHEDS-Residential via a hands-on approach. This guide presents a quick introduction to the SHEDS model's capabilities and the basic steps required to initialize and run a SHEDS exposure simulation, as demonstrated through an example tutorial case study.

This guide assumes the user is familiar with the general features of the SAS software program. More detailed instructions, scientific explanations, file formats, and relevant references are available in the SHEDS-Residential User Guide and Technical Manual. In this Quick Start Guide, readers will be directed to the relevant sections of these additional manuals for more information. This manual assumes that the user has already downloaded and installed the SHEDS-Residential model (**see Section 3** of the SHEDS-Residential User Guide).

In order to use this Quick Start Guide effectively, it is recommended that the user have at least:

- A basic understanding of the SAS software package, including the ability to locate and view SAS datasets created by the program.

- A basic understanding of the concepts behind Monte Carlo modeling, including a general understanding of continuous and discrete probability distributions.

- A basic knowledge of the chemical and exposure factors that influence residential exposures, including (but not limited to) chemical application rates, application patterns, application types, and human behaviors (hand-to-mouth and object-to-mouth factors, bathing, handwashing).

2 Introduction to the SHEDS-Residential Module

SHEDS-Residential is a sophisticated but user-friendly cumulative human exposure model for chemicals contacted in a residential setting.

SHEDS- Residential Version 1 is a stand-alone module that can be used in conjunction with the SHEDS-Multimedia Version 4 dietary module to estimate cumulative exposures to both residential and dietary sources.

Residential exposure simulations performed using the stand-alone SHEDS- Residential interface. The interface provides a user-friendly environment for:

- Creating the required SHEDS-Residential input files, including creation of concentration data for the residential media (air, surfaces, pets, etc.), specification of chemical application scenarios (crack-crevice, fogger, etc.), and specification of probability distributions for the wide variety of general home and behavior factors that influence exposures

- Running the SHEDS-Residential model and monitoring the run progress

- Viewing the model output in chart, graph, and tabular form

The main features of the SHEDS-Residential algorithms include:

- Estimation of population exposures for cohorts of interest incurred via inhaling contaminated air, touching contaminated surface residues, and ingesting residues from hand- or object- to-mouth activities

- Ability to model single (aggregate) or multiple (cumulative) chemical exposures

- Flexibility in defining chemical application dates for simulated individuals (user-specified dates or dates randomly selected by the model according to user-specified daily and hourly probabilities)

- Cross-sectional and longitudinal analysis capabilities

- Merging of chemical usage, human activity data, concentrations data and exposure factors to generate time series of exposure for simulated individuals

- Ability to perform a number of sensitivity analyses as well as two-stage Monte Carlo uncertainty simulations

- Ability to optionally model dose estimates based on a simple built-in PBPK model

3 Steps in Creating and Running a SHEDS-Residential Simulation

The following are the main steps the user will take in setting up and running a SHEDS-Residential exposure simulation (i.e. "model run"). These steps can be accomplished via the SHEDS user interface:

1) **Define the Run**. The user will give the simulation a name and tell SHEDS where to store all input files and results associated with the simulation.

2) **Define the Population and Sampling Settings.** The user will specify the general type of run (variability, sensitivity, or uncertainty), and the population to be modeled (ex. all persons, children).

3) **Specify Simulation Information:** The user will define the length of simulations, the source-to-concentration method (user-defined concentration time-series or distributions or a decay-dispersion approach), and a number of other global simulation variables.

4) **Specify Chemicals**: The user will specify the chemicals to be included in the run and their general properties.

5) **Specify Application Scenarios:** The user will specify the application scenarios to be used in the run. The dates and times of applications, reentry times, and relationships between application dates are defined.

6) **Specify Concentration-Related Inputs:** Based on the source-to-concentration method specified, the user will enter decay and dispersion inputs, or concentration distributions for different time-periods, or time-series data.

7) **Specify General Exposure and Dose Factors**: The user specifies all other inputs including exposure factors, transfer variables, input variable correlations, etc.

8) **Run Simulation**: Run the current simulation and monitor its progress via a progress screen.

9) **View the Results.** The user may employ the built-in tools provided by SHEDS to view results for the population or for individuals.

The following tutorial is designed to guide the user through these steps for a simple, single-chemical SHEDS-Residential run.
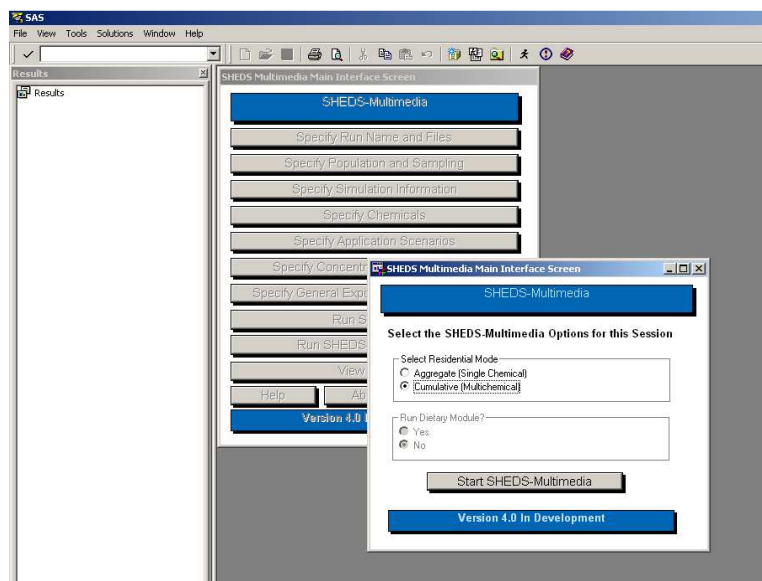
4 Example Tutorial Case Study: Exposure to Permethrin from a Residential Application Scenario

This section provides an example of creating a SHEDS-Residential run from start to finish. The run presented herein is a single-chemical variability run for Permethrin. The run considers a single application scenario (an indoor crack-crevice aerosol); the application dates are model-determined. This example run is included in the SHEDS-Residential installation; it will be available for selection when Edit an Existing Run is selected under the name Permethrin Case Study. However, the steps presented here show the user how to create the run from scratch. Each step in creating the run will be illustrated with an accompanying screenshot.

Note: Since SHEDS is in development, the results seen here may differ from that seen by the user.

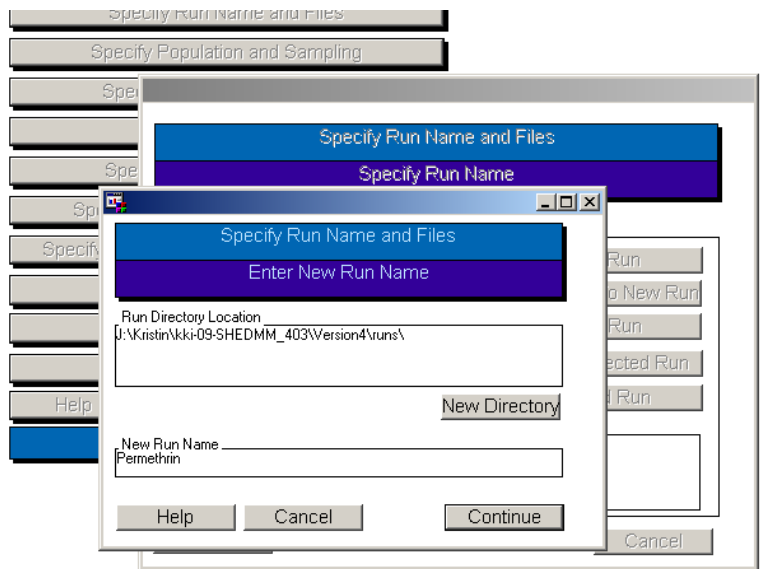|	
Start the SHEDS-Residential interface. Select Cumulative Mode. Although this is a single-chemical run, this example will step through the Cumulative Model screens so the user can see the steps they would need to complete for a multichemical run. Click <Start \SHEDS-Residential>.	
Start the process of creating a new SHEDS Run by clicking <Specify Run Name and Files>. Detailed instructions for creating a new run are given in **Section 5.3 of the SHEDS-Residential User Guide**.	
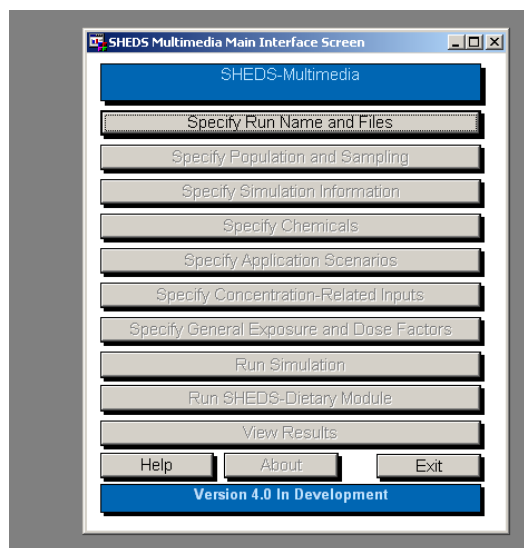
Click <Create a New Run >. Enter a name for the run, in this case, "Permethrin." Click <Continue>. The location of the information for the run (input and output) can be changed on this screen, if desired.	
Enter a description for the run, if desired (this is optional). Click <Save>.	
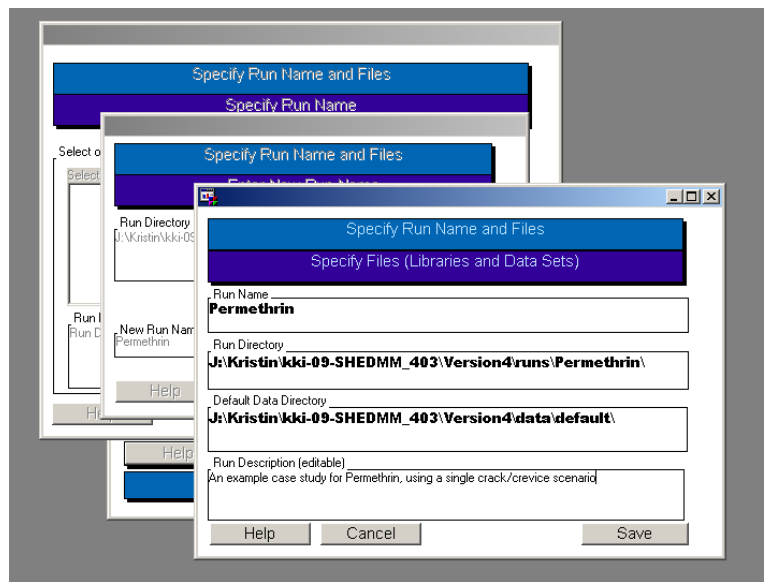
Click <Specify Population and Sampling>. The run type "Variability" will be selected by default.

Select "Optional Group Definitions," and choose to run males and females 3-5 years of age by highlighting the age groups.

Enter a population size of 500 profiles, which are simulated persons (this can be directly typed in, or the arrows can be used to select common population sizes). The number of total iterations is automatically updated. Since this is a variability run, the number of iterations is the same as the number of profiles. If this were a sensitivity or uncertainty run, the number of iterations would be the number of profiles times the number of times the entire population is run (i.e. the number of model runs).

Click <Save>.

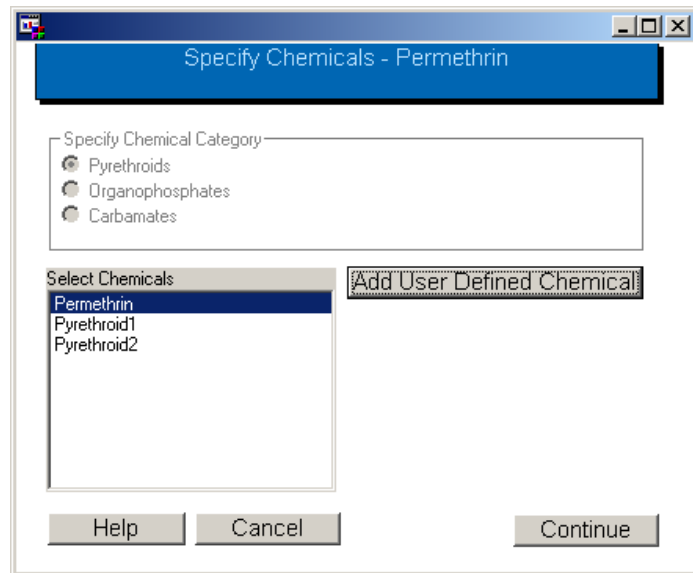Detailed instructions for specifying these options are given in **Section 5.4 of the SHEDS-Residential User Guide**.

Click on <Specify Simulation Information> on the Main screen.

Select January, 1, 2010 as the start date. By default, 365 as the number of days in the year, since 2010 is not a leap year. If the year selected was a leap year, by default SHEDS would set 366 days as the default simulation length. Note, however that the user is free to choose any simulation length if they wish.

Select "Model-Determined Dates" as the Application Dates method.

Select "Transfer Efficiency" as the dermal exposure method.

For the Diary Assembly method, highlight "Longitudinal Diary." This will enable the key variable, diversity, and autocorrelation widgets.

Select "Time Spent at Home While Awake" as the key variable, 0.2 as the diversity statistic, and 0 for mean day-to-day autocorrelation. See the Discussion of the meaning of these variables in **Section 5.5.5** of the User Guide.

By default, the Source-to-Concentration approach is Decay/Dispersion model. Leave this selection as is. This means SHEDS will prompt the user later for variables (ex. initial concentrations, decay rates) that will describe the concentrations in the residential environmental media according to a decay/dispersion model. However, note that SHEDS

provides other concentration options; see **Section 5.5.2** of the User Guide and the Technical Manual for more information. Leave other variables at defaults (Specifically, we will not specifically be modeling people who handle the chemical directly, saving intermediate variables to SHEDS output files, or writing the SHEDS run log to a file in this example). Click <Save>. Detailed instructions for specifying these options are given in **Section 5.5 of the SHEDS-Residential User Guide**.	
Click <Specify Chemicals> on the main screen. Choose to model Permethrin by highlighting it (and only it) in the Select Chemicals list box. Chemicals can be toggled between selected/unselected by clicking on them in the list box. Click <Continue>. Detailed instructions for specifying these options are given in **Section 5.6 of the SHEDS-Residential User Guide**.	

Accept the default values for Permethrin on the Specify Chemical Information screen by clicking <Continue>. This will return the user to the main screen. Detailed instructions for specifying these options are given in **Section 5.6.2 of the SHEDS-Residential User Guide**.	
Click <Specify Application Scenarios> on the Main Screen. This will open the Select Scenarios screen. Select "Indoor Crack and Crevice (aerosol)" from the Scenario Library. This defines a run with a single application scenario that the use will define on subsequent screens. The user can define his/her own scenarios using the Create User-Defined Scenario button, but this option is not used in this example **(see Section 5.7.1.1 of the User Guide).** (Note: the "Alter Selection Priority" buttons are used to identify the order of dependence of the scenarios when multiple scenarios are present and co-occurrence of chemical application exists; see **Sections 5.7.1 and 5.7.6 of the User Guide** for more information on these options.) When the scenario appears in the Selected Scenarios box, click <Continue> to move to the Specify Scenario Details screen. Detailed instructions for specifying	

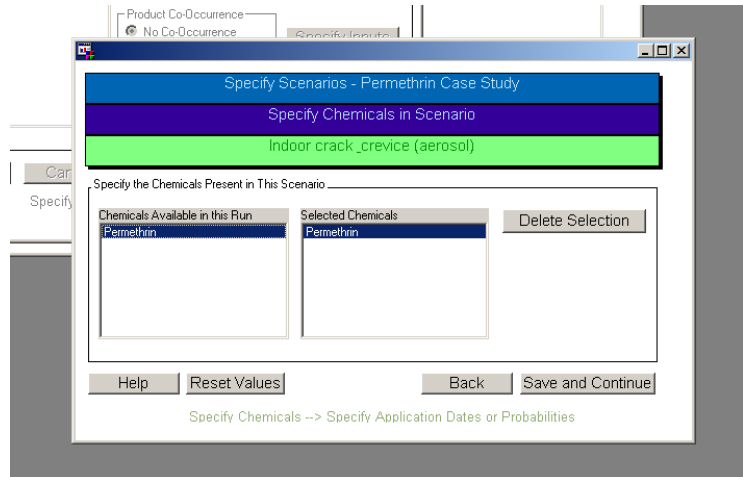|	
these options are given in **Section 5.7.1 of the SHEDS-Residential User Guide**.	
Click <Specify Inputs> to enter information for the crack/crevice scenario. Detailed instructions for specifying these options are given in **Section 5.7.2 of the SHEDS-Residential User Guide**.	
The first scenario screen is the Specify Chemicals in Scenario screen. Click on "Permethrin" to add the chemical to the scenario. In Aggregate mode, this screen is skipped because the model assumes the single chemical will be present in the scenario. If more than one chemical were available, the user could assign a subset of the chemicals to each scenario. Click <Save and Continue> to proceed. Detailed instructions for specifying these options are given in **Section 5.7.3 of the SHEDS-Residential User Guide**.	
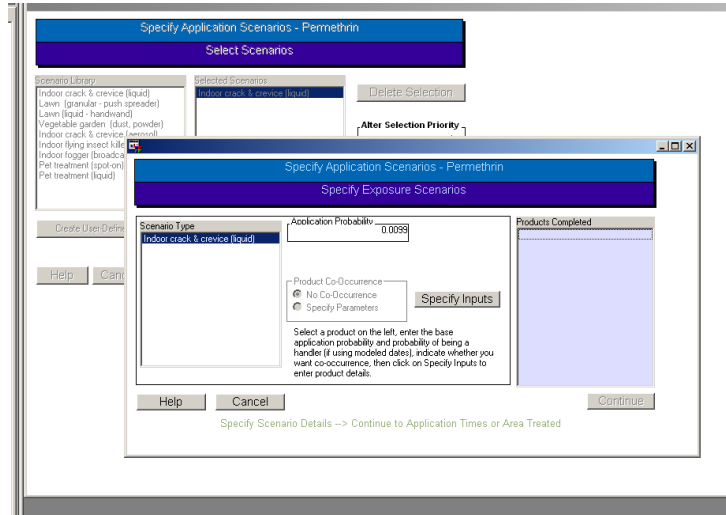
The next screen in the scenario cascade is the Application Probabilities screen. Probabilities defining day and month of application and total number of applications. The probabilities for number of applications refer to the **annual** number of applications, even if the defined simulation period is shorter or longer than 1 year.

Accept the defaults by clicking <Save and Continue>.

This returns the user to the Specify Scenarios Screen.

Click <Continue> again to proceed.

Detailed instructions for specifying these options are given in **Section 5.7.4 of the SHEDS-Residential User Guide**.

The next screen is the Application Times screen, where the user specifies a probability vector for the time of application of the chemical for any indoor scenarios. If the run includes outdoor or pet scenarios, this screen would also request probabilities for those as well.

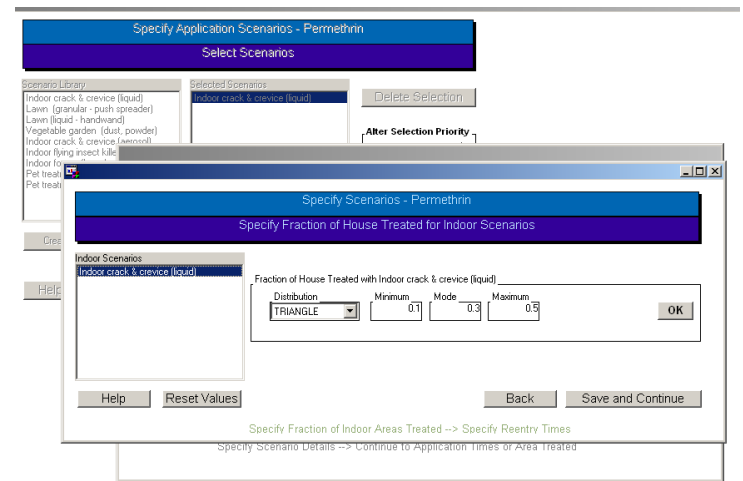Accept the defaults by clicking <Save and Continue>.

Detailed instructions for specifying these options are given in **Section 5.7.7 of the SHEDS-Residential User Guide**.
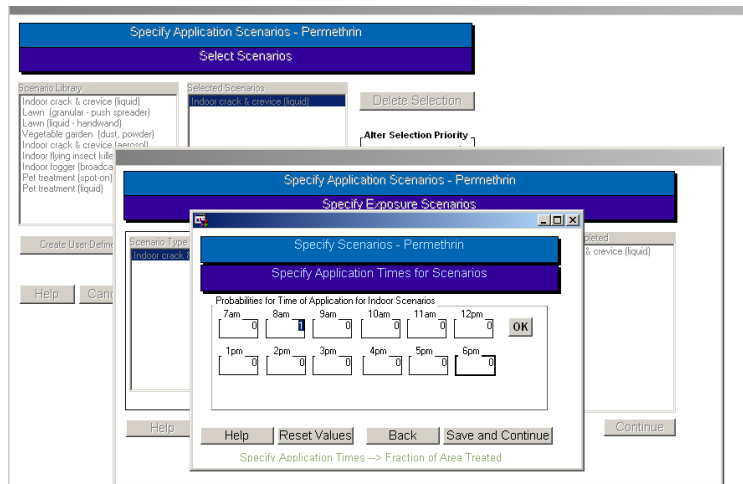
The next screen appears only when an indoor scenario is included in the run. Accept the default fraction of the house treated with the crack/crevice aerosol by clicking <Save and Continue>.

This proceeds to the Re-entry screen.

Detailed instructions for specifying these options are given in **Section 5.7.8 of the SHEDS-Residential User Guide**.

Only a re-entry time for indoor areas is available because this run only includes a single indoor scenario. If outdoor or pet scenarios were included in the run, this screen would contain more distributions to specify.

Click <Save and Return> to accept the default re-entry time and return to the Main screen.

Detailed instructions for specifying
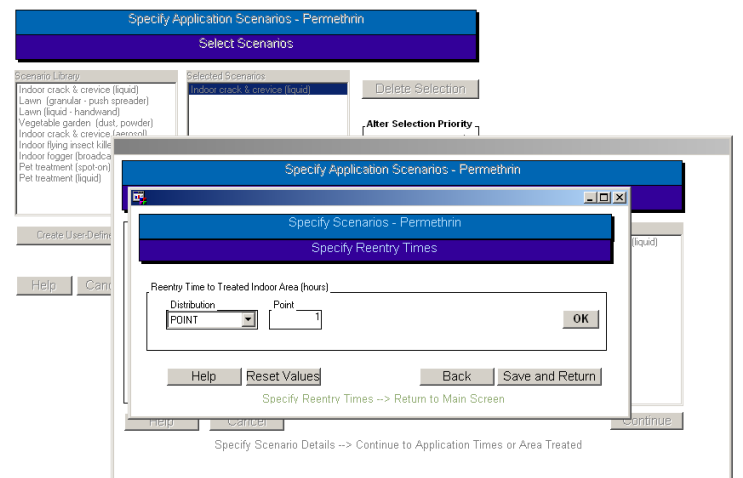
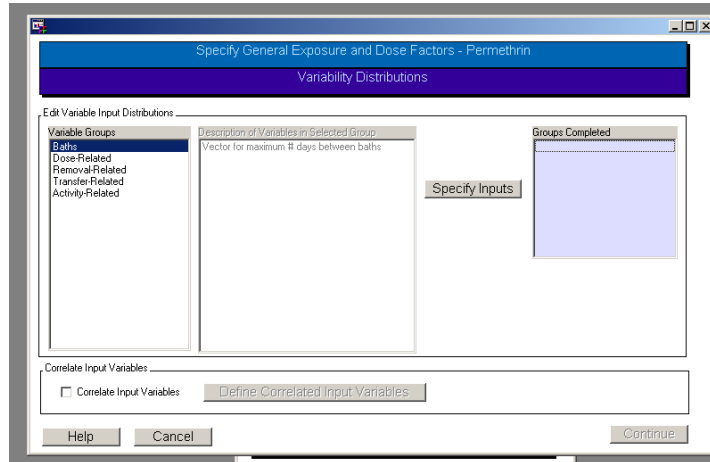|	
these options are given in **Section 5.7.9 of the SHEDS-Residential User Guide**.	
Click on <Specify Concentration Related Inputs> on the main screen. This initiates the Concentration screen cascade. After a warning related to chemical transfer, the first screen is the Decay and Dispersion Distributions. This screen is present because Decay and Dispersion was selected as the Source-to-Concentration Approach earlier in the run. Note that these variables are chemical-dependent; if there were more than one chemical present in the run, they would be included in the list box on the left side of the screen. Click <Save and Continue> to accept the defaults for Permethrin. Detailed instructions for specifying these options are given in **Section 5.8.1 of the SHEDS-Residential User Guide**.	Specify Concentration-Related Inputs - Permethrin Case Study Specify Decay and Dispersion Distributions - Permethrin Indoor crack _crevice (aerosol) Chemical(s) in this Scenario Permethrin Concentration in Air During 1st Hour Post-Application (ug/m3) Distribution UNIFORM Minimum 36 Maximum 150 OK Concentration in Air 24 Hours Post-Application (ug/m3) Distribution UNIFORM Minimum 0.05 Maximum 0.13 OK Initial Residue/Concentration on Hard Floors (ug/cm2) Distribution NORMAL Mean 1.51 Std. Dev. 0.38 Minimum 0.75 Maximum 2.27 OK Initial Residue/Concentration on Carpet (ug/cm2) Distribution NORMAL Mean 1.51 Std. Dev. 0.38 Minimum 0.75 Maximum 2.27 OK Initial Residue/Concentration in Dust (ug/g) Distribution POINT Point 0 OK Chemical Decay Rate (per Day) Distribution NORMAL Mean 0.03 Std. Dev. 0.005 Minimum 0.01 Maximum 0.06 OK Ratio of Treated to Untreated Room Concentration (unitless) Distribution POINT Point 0.01 OK Help Reset Values Back Save and Continue
This is the Background Screen. Background in SHEDS refers to chemical present due to applications in other homes. Only outside surfaces have background concentrations. Click <Save and Continue> to accept the default value of 0 for permethrin background concentration. This returns the user to the Main screen. Detailed instructions for specifying	Specify Concentration-Related Inputs - Permethrin Specify Decay and Dispersion Distributions Background- Permethrin Chemical(s) Permethrin Background Concentration for Outside Surfaces (ug/cm2) Distribution POINT Point 0 OK Help Cancel Back Save and Continue

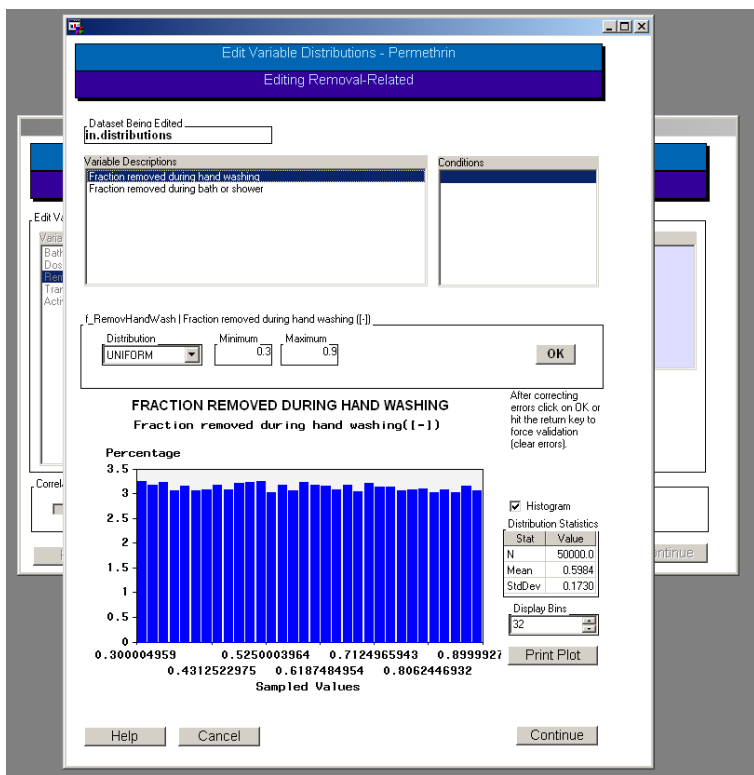|	
these options are given in **Section 5.8.4 of the SHEDS-Residential User Guide**.	
Click <Specify General Exposure and Dose Variables> on the Main screen. This opens the Variability Distributions screen. The user will need to visit each of the variable groups before being allowed to continue. Click <Specify Inputs> to view/edit the Baths variable group. Detailed instructions for specifying these options are given in **Sections 5.9.1 and 5.9.2 of the SHEDS-Residential User Guide**.	
The Baths group is a special case: it consists of a single probability vector for days between baths. Accept the defaults by clicking <Save>. Detailed instructions for specifying these options are given in **Section 5.9.2.1 of the SHEDS-Residential User Guide**.	
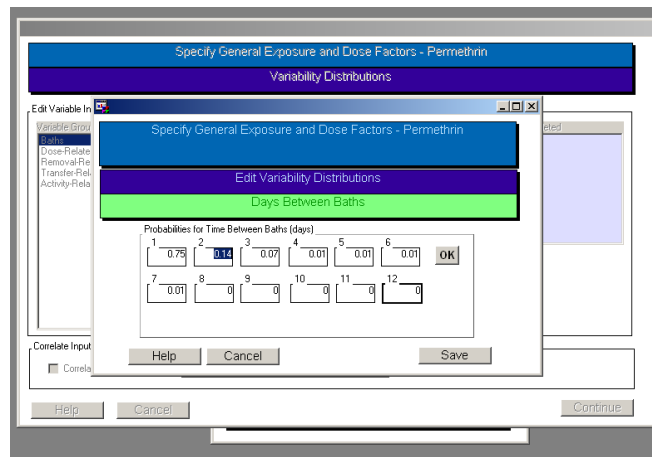
When the user is returned to the prior screen, the next Variable group, "Dose-Related," should be highlighted. Click <Specify Inputs> again to edit this group. This opens the Edit Variable Distributions window, which allows the user to view or edit any of the distributions in the group, for any available conditions.

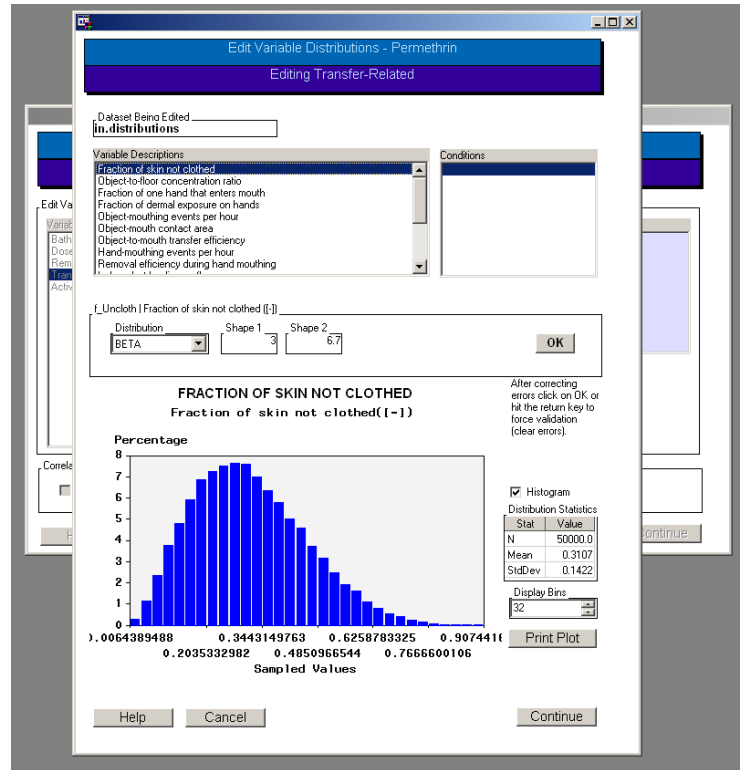Click <Continue> to accept the defaults for permethrin and return to the prior screen.
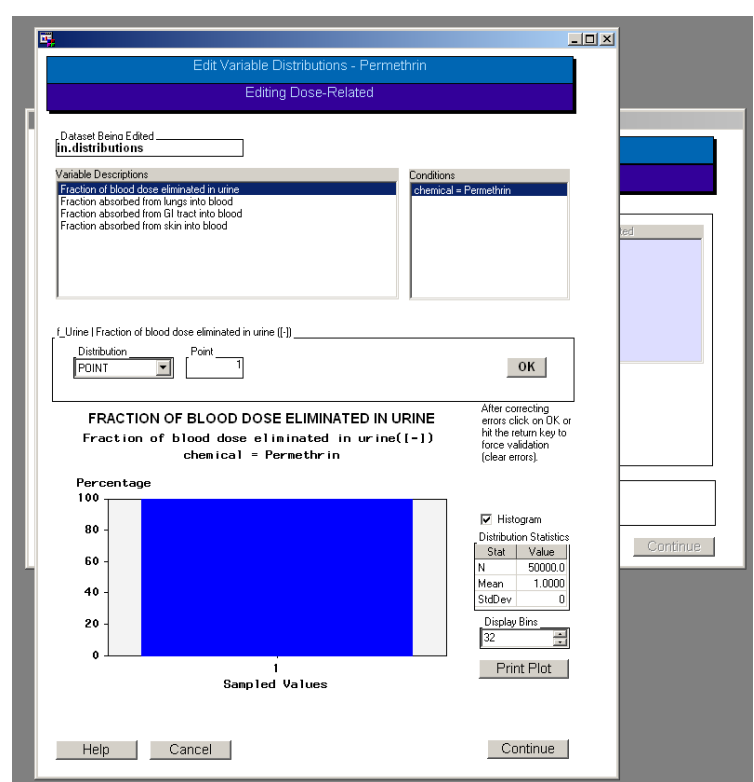
Click <Specify Inputs> to edit variables in the "Removal-Related" group.

Click <Continue> to accept the defaults and return to the prior screen.

Click <Specify Inputs> to edit variables in the "Transfer-Related" group.
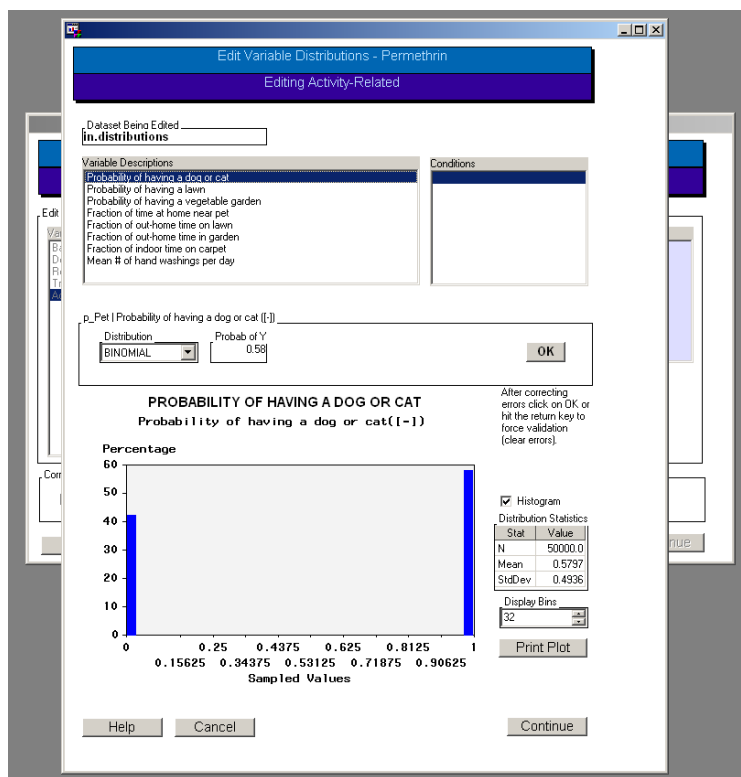
Click <Continue> to accept the defaults and return to the prior screen.

Click <Specify Inputs> to edit variables in the "Activity-Related" group.

Click <Continue> to accept the defaults and return to the prior screen.
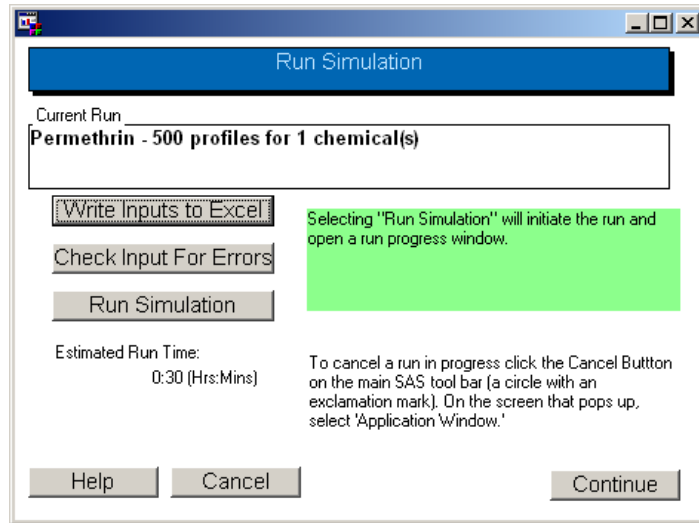
Then click <Continue> once more to return to the Main screen.

Click <Run Simulation> on the Main screen. This brings up the Run Simulation Screen. The screen should indicate that 500 profiles will be run for one chemical.
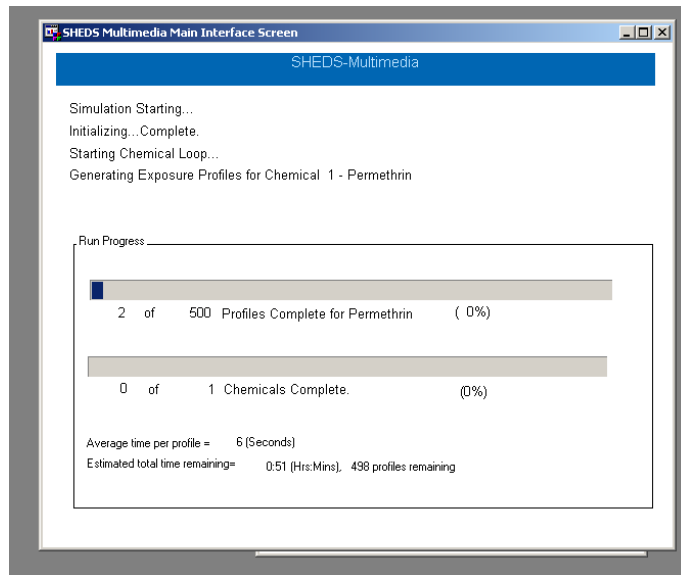
Click <Run Simulation> to initiate the simulation.

Detailed instructions this screen are given in **Section 5.10 of the SHEDS-Residential User Guide**.

This opens the SHEDS-Residential Run Progress screen. This gives the user an idea how long the simulation will take to complete. This run should take between 20 minutes and an hour depending on the age/configuration of the user's computer. When the run is complete, this window will close automatically and return to the Run screen.
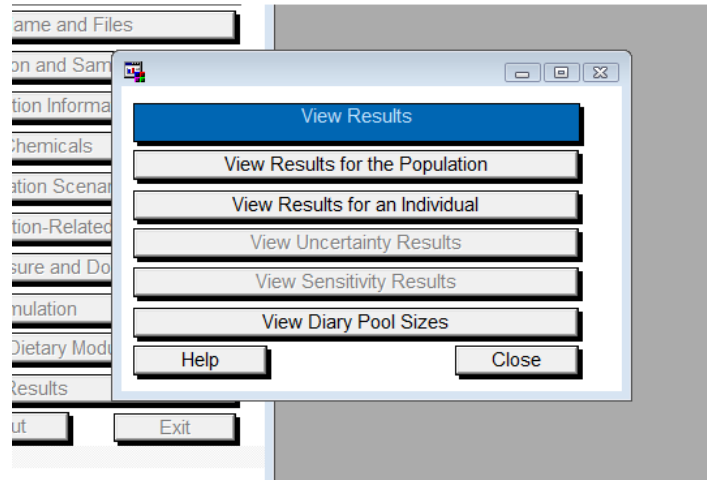
Click <Continue> to return to the Main screen.

|	
Select <View Results> from the Main screen. Then click <View Results for the Population>. Detailed instructions for this screen are given in **Section 5.11 of the SHEDS-Residential User Guide**.	
Select "New Dose" as the Variable Group. Select "Total New Dose", and the New Dose variables for "Hands", "Body", and "Dermal" from the available variables. Click <Display> to view the default output type, CDF, for the default Output Variable Type, Personal Means. This creates a CDF of the 500 mean daily exposure values (one for each person). The other output variables types are personal maxes (explores the 500 daily maximum exposures for the population) and all person days, which visualizes the distribution of all person-days (500 * 365 exposures in this case). Detailed instructions for specifying these options are given in **Section 5.11.2 and 5.11.2.2 of the SHEDS-Residential User Guide**.	
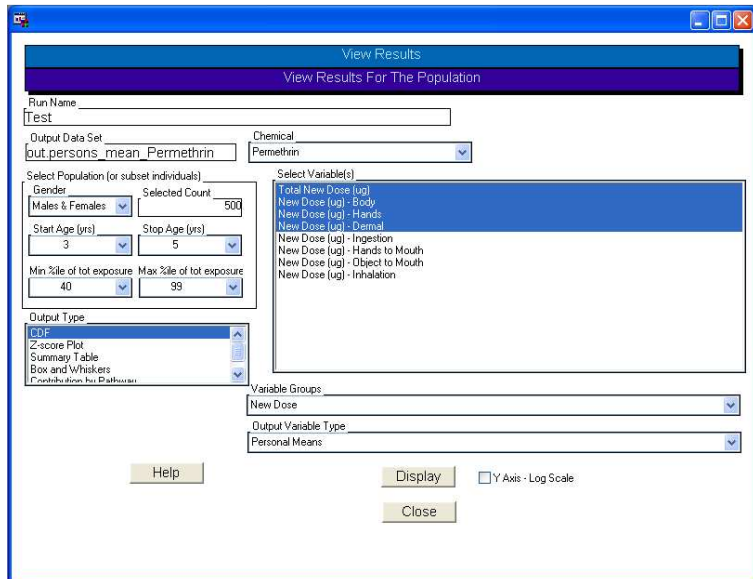
This draws a plot with CDFs for the 4 variables that were selected.

Click <Close> to return to View Results for the Population.

Detailed instructions for specifying these options are given in **Section 5.11.2.2 of the SHEDS-Residential User Guide**.
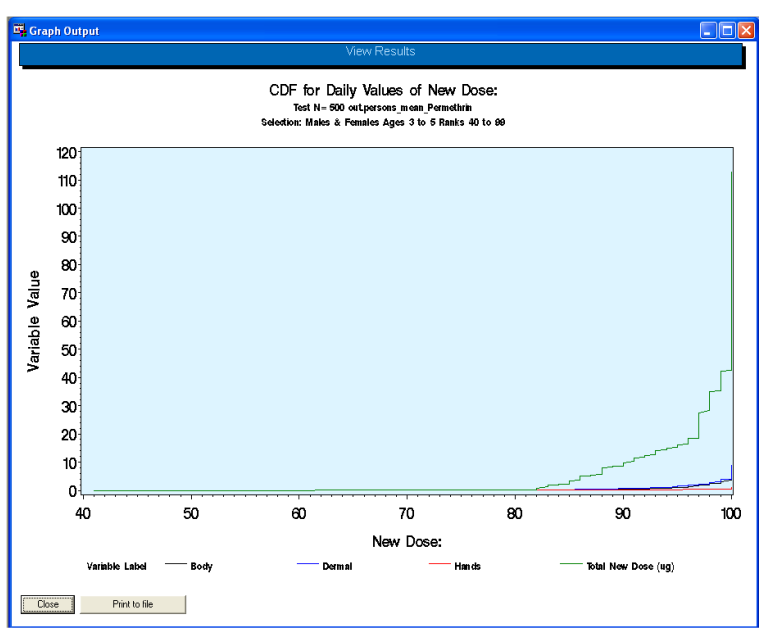
Select "Summary Table" as the output type. Select "New Exposure" as the variable group, highlight all the available variables, and click <Display>. This creates the table.

Click<Close> to return to the previous screen.

Detailed instructions for specifying these options are given in **Section 5.11.2.1 of the SHEDS-Residential User Guide**.

Select "Box and Whiskers" as the output type. Select "New Dose Normalized to Body Mass" as the variable group, highlight all the available variables, and click <Display>. This creates the box plot.

Click<Close> to return to the previous screen.

Detailed instructions for specifying these options are given in **Section 5.11.2.3 of the SHEDS-Residential User Guide**.
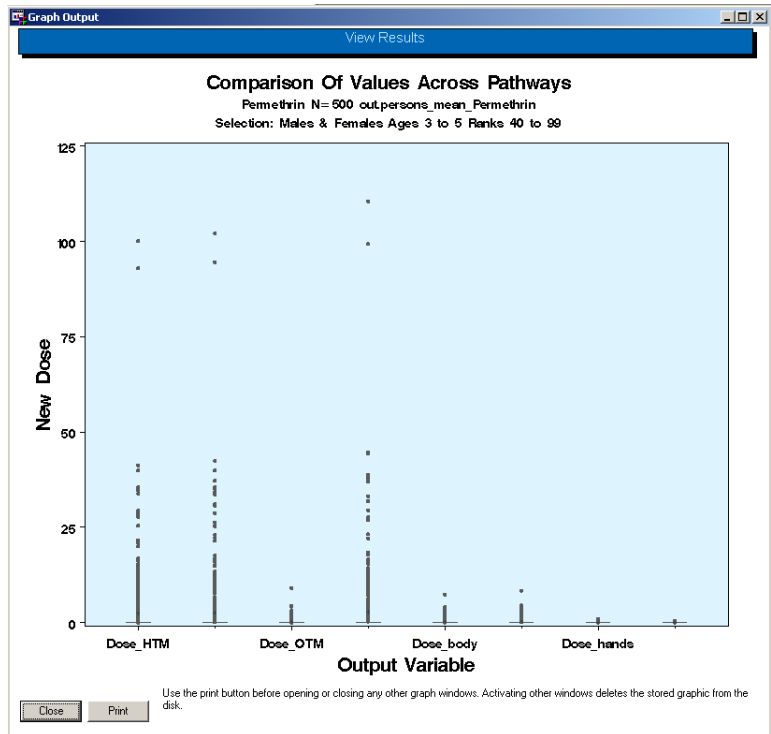

Select "Contribution By Pathway" as the output type. Select "New Exposure as" as the variable group and click <Display>. This creates the pie chart.

Click<Close> to return to the previous screen.

Detailed instructions for specifying these options are given in **Section 5.11.2.4 of the SHEDS-Residential User Guide**.
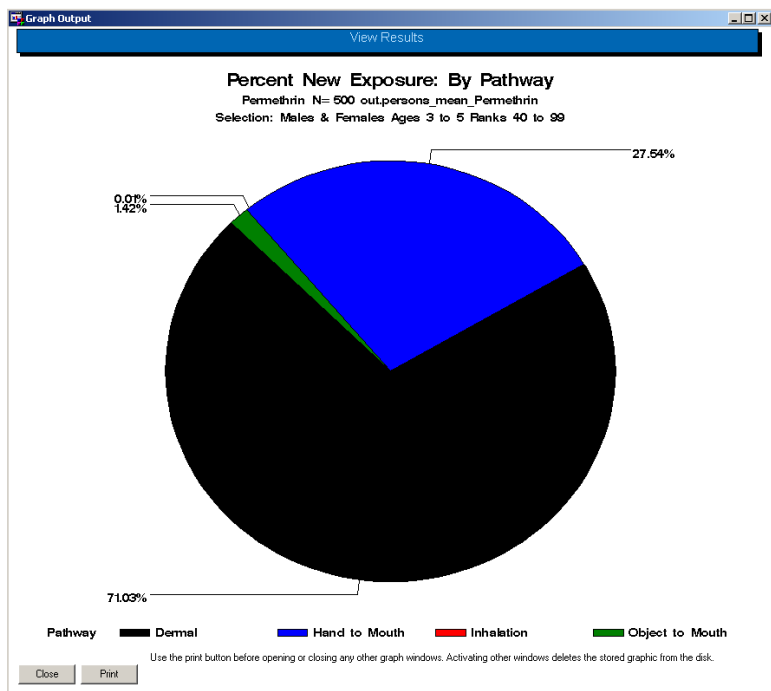
Click <Close> to return to the View Results screen.

Click <View Results for an Individual>.

Select person 5, or any other person with a higher percentile (Rank) of total exposure (lower percentile persons may not have non-zero exposures). Select "Time Series" as output type, "New Exposure" as variable group, and "Hands to Mouth" as the variable.

Detailed instructions for specifying these options are given in **Section 5.11.3 and 5.11.3.1 of the SHEDS-Residential User Guide**.

Click <Display> to view the time series plot. Note: The plot show here may differ from the one you see due to the stochastic nature of SHEDS.

Click <Close> to return to the previous screen.

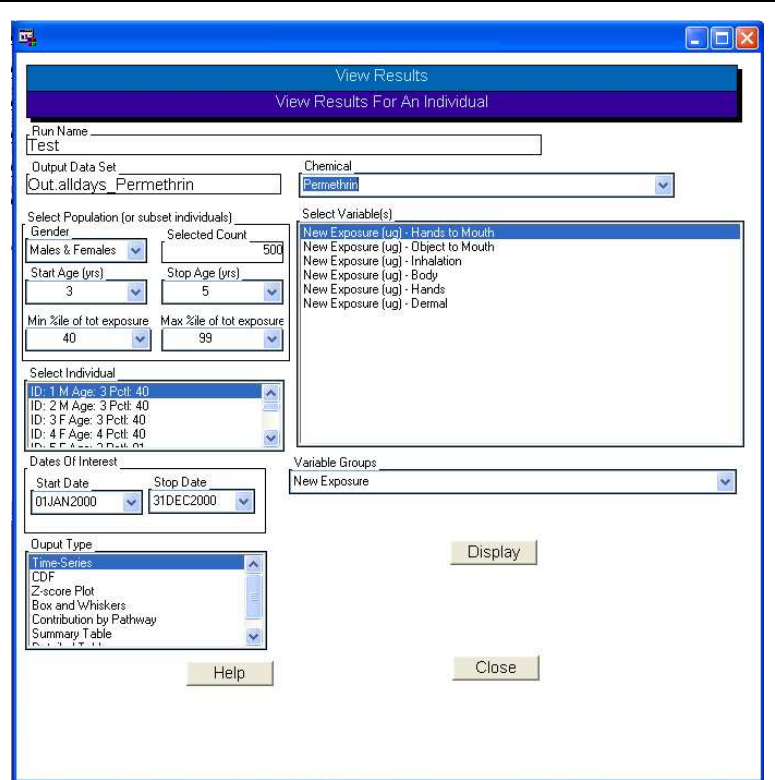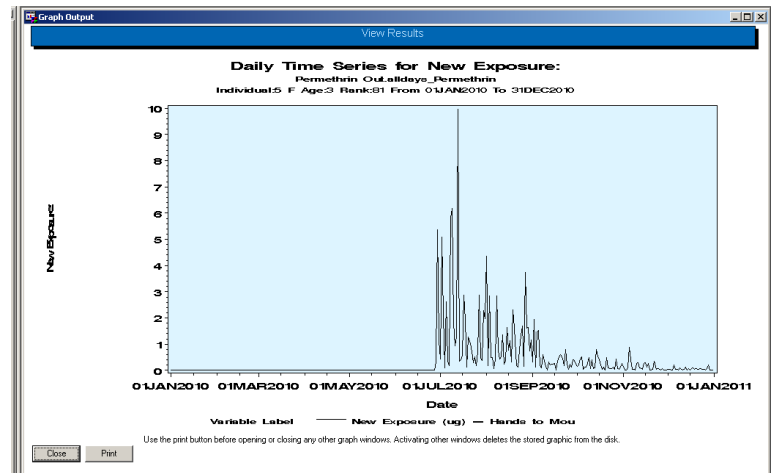|	
Select "CDF" as the output type. Select "New Exposure" as the variable group, highlight dermal and hand to mouth exposure, and click <Display>. This creates the CDF. Note: The plot show here may differ from the one you see due to the stochastic nature of SHEDS. Click<Close> to return to the previous screen. Detailed instructions for specifying these options are given in **Section 5.11.3.2 of the SHEDS-Residential User Guide**.	
Select "Box and Whiskers" as the output type. Select "Chemical and Metabolite Entering Blood" as the variable group, highlight all the available variables, and click <Display>. This creates the box plot. Note: The plot show here may differ from the one you see due to the stochastic nature of SHEDS. Click<Close> to return to the previous screen. Detailed instructions for specifying these options are given in **Section 5.11.3.3 of the SHEDS-Residential User Guide**.	
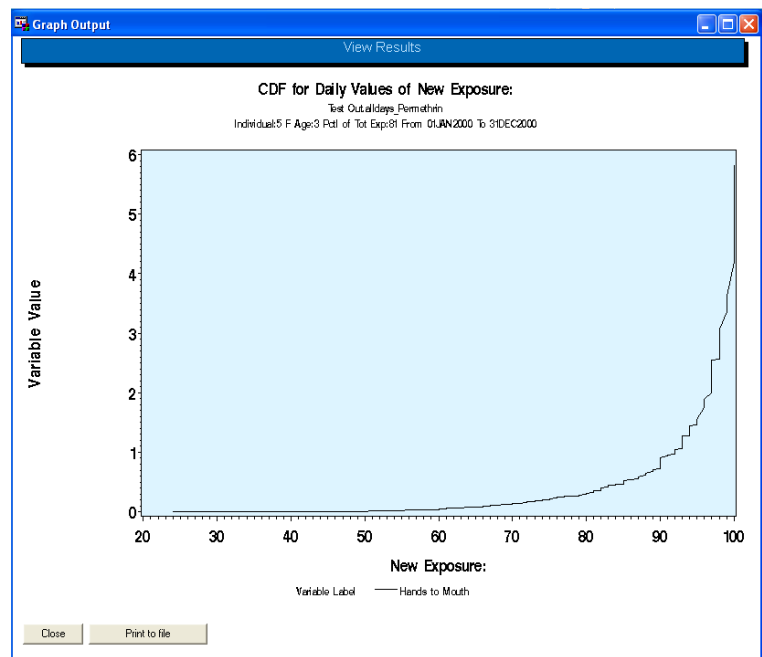
Select "Contribution by Pathway" as the output type. Select "New Dose Normalized to Body Mass" as the variable group and click <Display>. This creates the pie chart. Note: The plot show here may differ from the one you see due to the stochastic nature of SHEDS.

Click<Close> to return to the previous screen.

Detailed instructions for specifying these options are given in **Section 5.11.3.4 of the SHEDS-Residential User Guide**.

Select "Summary Table" as the output type. Select "Eliminated Chemical" as the variable group, highlight all variables, and click <Display>. This creates the table. Note: The plot show here may differ from the one you see due to the stochastic nature of SHEDS.

Click<Close> to return to the previous screen.

Detailed instructions for specifying these options are given in **Section 5.11.3.5 of the SHEDS-Residential User Guide**.

Select "Detailed Table" as the output type. Select "New Exposure" as the variable group, and click <Display>. This creates the table. You may need to page down to see the non-zero exposure estimates. Note: The plot show here may differ from the one you see due to the stochastic nature of SHEDS.
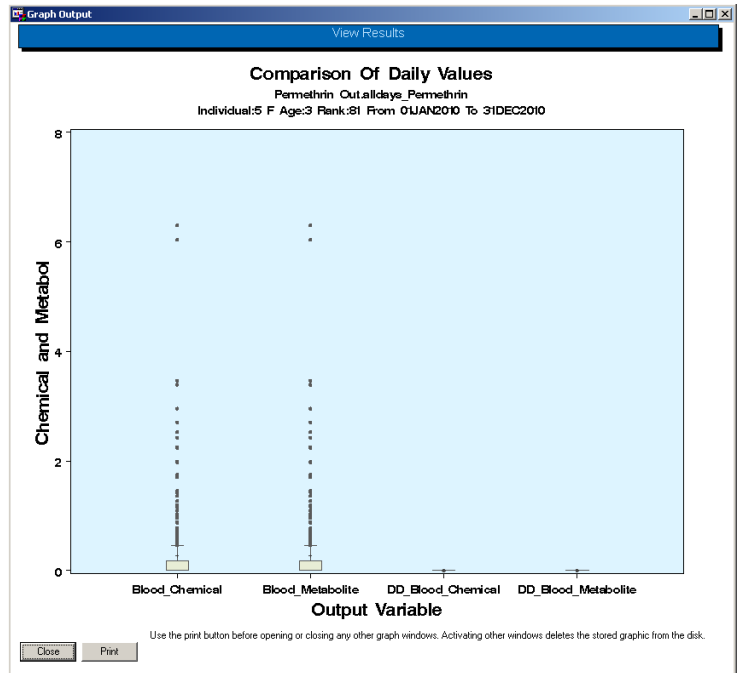
Click <Close> to return to the previous screen.

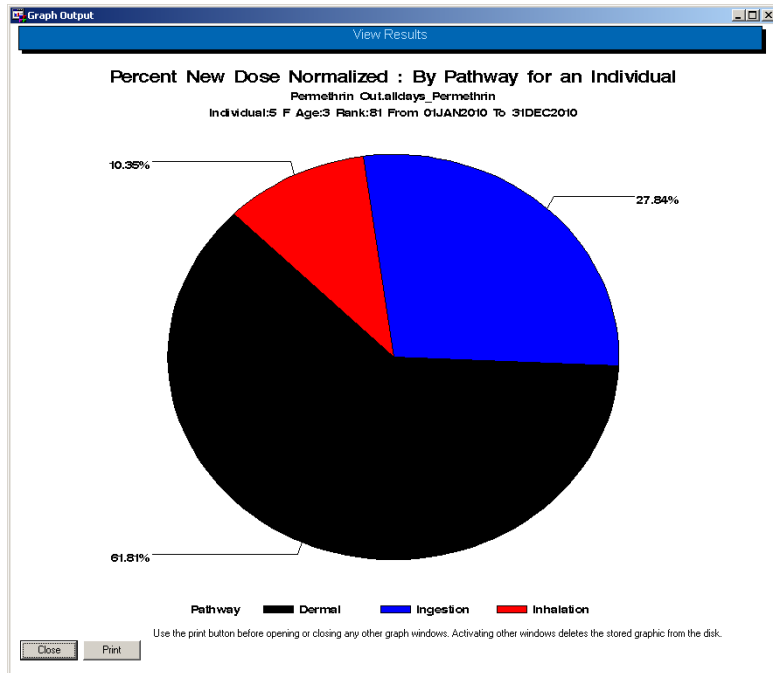Detailed instructions for specifying these options are given in **Section 5.11.3.6 of the SHEDS-Residential User Guide**.

View Results

New Exposure:

Permethrin Out.alldays_Permethrin

Individual:5 F Age:3 Rank:81 From 01JAN2010 To 31DEC2010

	day_num	chadid	New Handler Exposure [ug] Dermal	New Handler Exposure [ug] - Hands	New Handler Exposure [ug] - Body	New Exposure [ug] - Dermal	New Exposure [ug] - Hands	New Exposure [ug] - Body	PostApp_dermal	PostApp_hands	PostApp_body	New Dose - Dermal
169	169	NHW/18518A	0	0	0	0	0	0	0	0	0	0
170	170	UMC00014A	0	0	0	0	0	0	0	0	0	0
171	171	CAC03176A	0	0	0	0	0	0	0	0	0	0
172	172	CAC01639A	0	0	0	0	0	0	0	0	0	0
173	173	CAC03631A	0	0	0	0	0	0	0	0	0	0
174	174	UMC01429A	0	0	0	0	0	0	0	0	0	0
175	175	0AB00031C	0	0	0	0	0	0	0	0	0	0
176	176	UMC01954B	0	0	0	0	0	0	0	0	0	0
177	177	NHA17440A	0	0	0	0	0	0	0	0	0	0
178	178	UMC00573A	0	0	0	0	0	0	0	0	0	0
179	179	CAC02240A	0	0	0	45.313801048	26.192317238	19.12148381	45.313801048	26.192317238	19.12148381	>>>>>>>>>
180	180	0AB00599D	0	0	0	522.82375869	291.00147727	231.82228142	522.82375869	291.00147727	231.82228142	>>>>>>>>>
181	181	0AB00238A	0	0	0	312.89340066	179.49033865	133.40306201	312.89340066	179.49033865	133.40306201	>>>>>>>>>
182	182	0AB00602A	0	0	0	29.179189224	16.896604487	12.282584737	29.179189224	16.896604487	12.282584737	>>>>>>>>>
183	183	0AB00009A	0	0	0	1181.2102597	675.96747114	505.24278851	1181.2102597	675.96747114	505.24278851	>>>>>>>>>
184	184	UMC00848B	0	0	0	238.83223297	140.09985213	98.732380839	238.83223297	140.09985213	98.732380839	>>>>>>>>>
185	185	CAC01191A	0	0	0	24.162327448	13.969032897	10.19329455	24.162327448	13.969032897	10.19329455	>>>>>>>>>
186	186	UMC00195B	0	0	0	334.92744852	186.75219743	148.17525109	334.92744852	186.75219743	148.17525109	>>>>>>>>>
187	187	0AB00307A	0	0	0	45.806406801	26.489216865	19.31718936	45.806406801	26.489216865	19.31718936	>>>>>>>>>
188	188	CIN12313C	0	0	0	80.810836633	46.723375717	34.087460916	80.810836633	46.723375717	34.087460916	>>>>>>>>>
189	189	0AB00304B	0	0	0	998.97454008	575.29521524	423.67932484	998.97454008	575.29521524	423.67932484	>>>>>>>>>
190	190	UMC00246A	0	0	0	168.14227923	69.574983117	98.567296118	168.14227923	69.574983117	98.567296118	>>>>>>>>>
191	191	NHA17440A	0	0	0	178.066731	101.94410949	76.122621506	178.066731	101.94410949	76.122621506	>>>>>>>>>
192	192	CIN11300C	0	0	0	48.812728357	27.895658539	20.917069818	48.812728357	27.895658539	20.917069818	>>>>>>>>>
193	193	CAC01076A	0	0	0	337.77531242	192.01230611	145.76300631	337.77531242	192.01230611	145.76300631	>>>>>>>>>
194	194	0AB00279A	0	0	0	704.13278028	397.63920443	316.49357596	704.13278028	397.63920443	316.49357596	>>>>>>>>>

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

5 Recommended Next Steps

Once the new user has worked through this tutorial, it is recommended that they read through the User's Guide to better understand the capabilities and options of SHEDS. Specifically, the user may want to explore further the following SHEDS topics, to determine which SHEDS Settings will be optimal for their own modeling investigations:

- The differences among methods for estimating concentrations in the residential media (interval chemical distributions versus the decay-dispersion approach)

- The differences among methods for specifying dates (fixed versus model-selected).

- Chemical co-occurrence

- The different methods for constructing longitudinal activity diaries