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

SHEDS-Dietary version 1

Draft User Guide

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Computing Issues, Disclaimer, and Support

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

It is highly recommended that the user pause or disable any automated anti-virus or back-up programs that access the SHEDS installation or data output directories, or place these directories in locations that are not virus-checked or backed up. Such programs may access SHEDS data files and interfere with model performance, causing unpredictable results.

Disclaimer
EPA's SHEDS-Dietary model is a probabilistic, population-based dietary exposure assessment model that simulates individual exposures to chemicals in food and drinking water over different time periods (e.g., daily, yearly). SHEDS-Dietary is one module (along with the separate SHEDS-Residential module) of EPA's more comprehensive human exposure model, the Stochastic Human Exposure and Dose Simulation model for multimedia, multipathway chemicals (SHEDS-Multimedia), which can simulate aggregate or cumulative exposures over time via multiple routes of exposure (dietary & non-dietary) for different types of chemicals and scenarios. SHEDS-Residential and SHEDS-Dietary will be merged together in a future version of SHEDS-Multimedia.

SHEDS-Dietary version 1 includes case study examples for illustrative purposes, as described in the the Technical Manual and User Guide. All input values used in the SHEDS-Dietary model for a given application should be entered or reviewed by the researcher so that the model results are based on appropriate data sources for the given application.

The United States Environmental Protection Agency through its Office of Research and Development developed and funded the SHEDS-Dietary model with assistance from contractor Alion Science and Technology. SHEDS-Dietary Version 1 will undergo external peer review by EPA's Scientific Advisory Panel July, 2010, and should be considered draft at this time.

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

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ACRONYMS AND ABBREVIATIONS

aRfD – acute reference dose
cancer Q – cancer potency factor
CDFs – cumulative distribution functions
EDFs – empirical distribution functions
FCID – Food Commodity Intake Database
NOEL – no observed effect level
aPAD – acute population adjusted dose
cPAD – chronic population adjusted dose
PDFs – probability density functions
PF – processing factor
RDF – residue distribution file
RPF – relative potency factor
RfD – reference dose
SHEDS – Stochastic Human Exposure and Dose Simulation
ug (in SAS printout or variable names) – microgram

1 Overview of SHEDS-Dietary

SHEDS-Dietary is a stochastic dietary exposure model that can be used to estimate population estimates of dietary exposure, based on food consumption data from either the United States Department of Agriculture's Continuing Surveys of Food Intake by Individuals (CSFII) for the years 1994-1996 and 1998 or the National Health and Nutrition Examination Survey (NHANES). Exposure is determined from food consumption through the stochastic assignment of chemical residues to food commodities.

SHEDS-Dietary Version 1 is a stand-alone module that can be used in conjunction with the SHEDS-Multimedia Version 4 residential module (also referred to as 'SHEDS'), a sophisticated but user-friendly cumulative human exposure model for chemicals contacted in a residential setting (Isaacs et al. 2010, Glen et al. 2010).

This document is intended to be a practical guide to performing a SHEDS-Dietary model simulation using the stand-alone SHEDS-Dietary interface. The interface provides a user-friendly environment for:

- Creating the required SHEDS-Dietary input files, including creation of residue distribution data, assignment of residue distributions to food commodities, and definition of population risk parameters.
- Running the SHEDS-Dietary model.
- Viewing the model output in chart, graph, and tabular form.

Section 7 of this User Guide presents four illustrative case studies intended to guide the user completely through multiple examples of running SHEDS-Dietary from start to finish. A full description of the technical aspects of the SHEDS-Dietary model, including all model data and algorithms, is given the in SHEDS-Dietary Technical Manual (Xue et al., 2010).

2 Installation

2.1 Requirements

SHEDS-Dietary was developed under SAS version 9.1 on computers running MS Windows 2000 and XP Professional.

To install and use SHEDS-Dietary, you will need a computer running 32-bit SAS version 9.1 or higher. A version of SHEDS for 64-bit SAS is available upon request. SAS must be installed prior to installing SHEDS. Your computer hardware needs to be adequate to run SAS and MS Windows. Additionally you should have:

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

However, it is recommended that you have:

a faster processor,
128 MB or more RAM, and
more than 2 GB of free disk space.

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

WARNING: It is highly recommended that the user pause or disable any automated anti-virus or back-up programs that access the SHEDS installation or data output directories, or place these directories in locations that are not virus-checked or backed up. Such programs may access SHEDS data files and interfere with model performance, causing unpredictable results.

2.2 Installation under MS Windows

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

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

2.2.1 Starting with a CD

If you have a CD, do the following:

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

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

2.2.2 Starting with a Downloaded File

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

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

2.2.3 The Standard Installation Process

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

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

Figure 2-1. Setup Screens: Initial Screen.

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

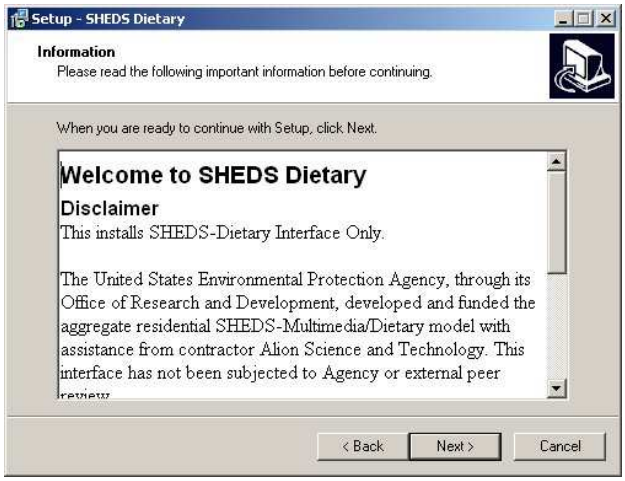


Figure 2-2. Setup Screens: Welcome and Information Screen.

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

Figure 2-3. Setup Screens: Installation Directory Screen.

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

Figure 2-4. Setup Screens: Shortcut Folder Name.

The next window allows the user to set the name of the program group in the Start Menu. The user should not need to change this.

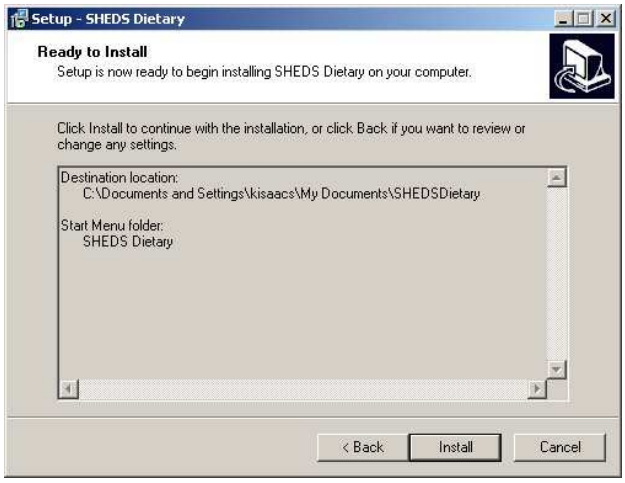


Figure 2-5. Setup Screens: Confirmation Screen.

This is the final window before install begins. The user has the chance to review installation specifications on this screen before the installation begins.

Figure 2-6. Setup Screens: Completion Confirmation.

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

2.2.4 Starting the Model Interface

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

Figure 2-7. SHEDS Dietary Desktop Icon.

2.2.5 Removing SHEDS-Dietary

If SHEDS was installed using the installation wizard, the user can uninstall it in a manner similar to other Windows programs. **Removal of the program will remove all of the user's output files unless these were saved elsewhere.** To start the removal process, click on the "Uninstall SHEDS Dietary" choice in the SHEDS-Dietary group of the Programs menu.

3 The SAS User Interface

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

3.1 The SAS Screen

Assuming one uses the link in the MS Windows Programs menu or the screen icon to start the model, the main graphical user interface (GUI) screen will start inside the main SAS window (Figure 3-1). By default, the SAS log window also starts.

The SAS window is split into a number of distinct areas. The main area for viewing documents, forms, data sets, and graphs is in the middle (the gray area). This area may have multiple windows active at one time. The user may activate a particular window by clicking on the title of the window. The bar immediately below this area contains one button for each window in the main area. The buttons indicate which window is active, and allow one to activate a different window. In Figure 3-1, the main SHEDS screen is active as can be seen by the colored title bar and the depressed appearing button. Note that since the main SHEDS screen does not have a title on the title bar, its button is unlabeled. As the SHEDS GUI and model are run, informational and error messages will be displayed in the log window. The pull-down menus are on the top of the screen, just under the title. The toolbar is below this. At the very bottom of the SAS window is a status bar.

Additional SAS windows can be opened using the SAS View menu (Figure 3-2). The Graph window displays all graphical output generated. The interface uses a separate output window for this purpose so the Graph window will generally not be needed. It should also be noted, that since the model interface overwrites images of the same type, SAS's graph window may appear unreliable.

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

The Explorer window (Figure 3-3) is used to navigate through SAS libraries and files, data sets, forms, and programs. It can be used to access the raw files used as input or output to the model. This screen may float in SAS's main area or it may be locked on the left side of the SAS window and be accessed via a tab on the bottom of this area. This screen may be toggled between tree mode (shown) and a single pane, similar to MS Windows Explorer.

A number of SAS libraries are created upon installation of SHEDS-Dietary. The names and contents of these libraries are discussed in Appendix A.

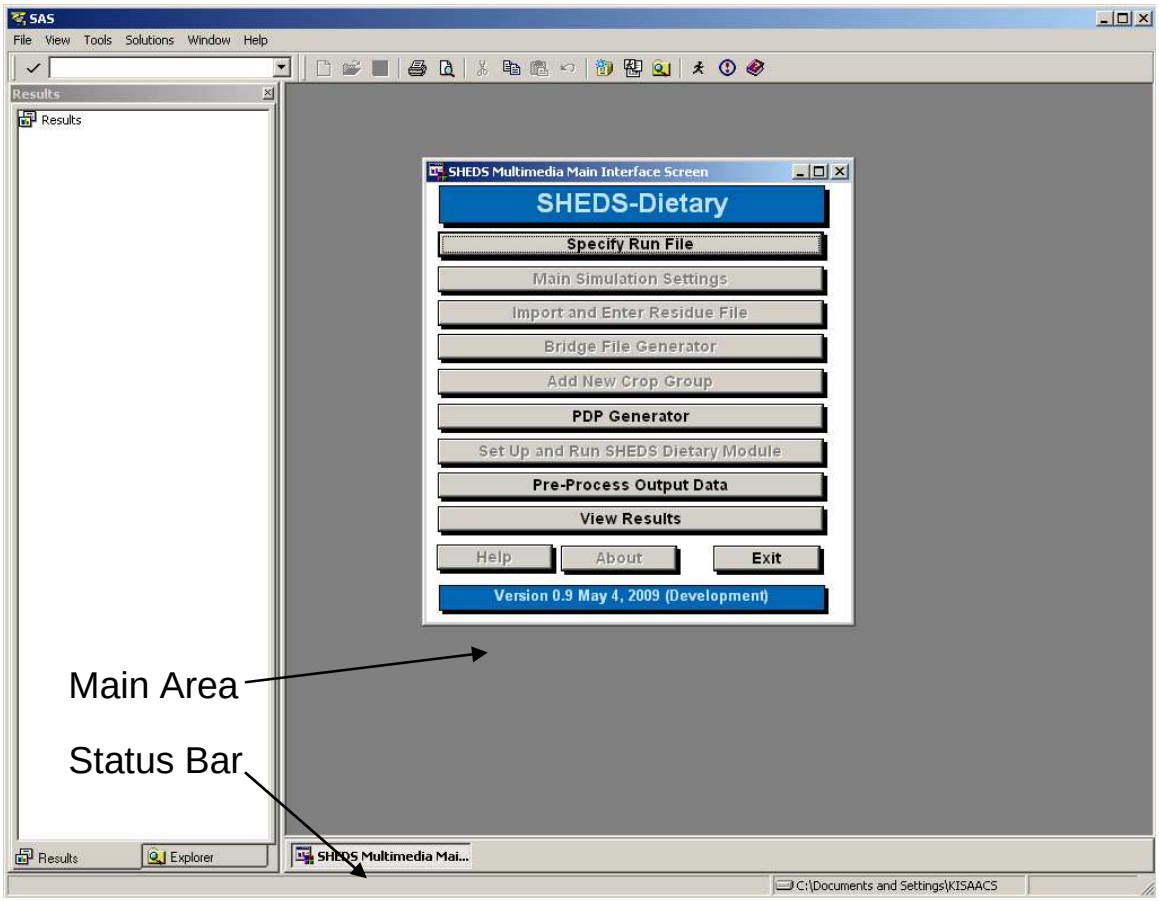


Figure 3-1. The Main SHEDS-Dietary Interface Screen in the SAS Window on Startup.

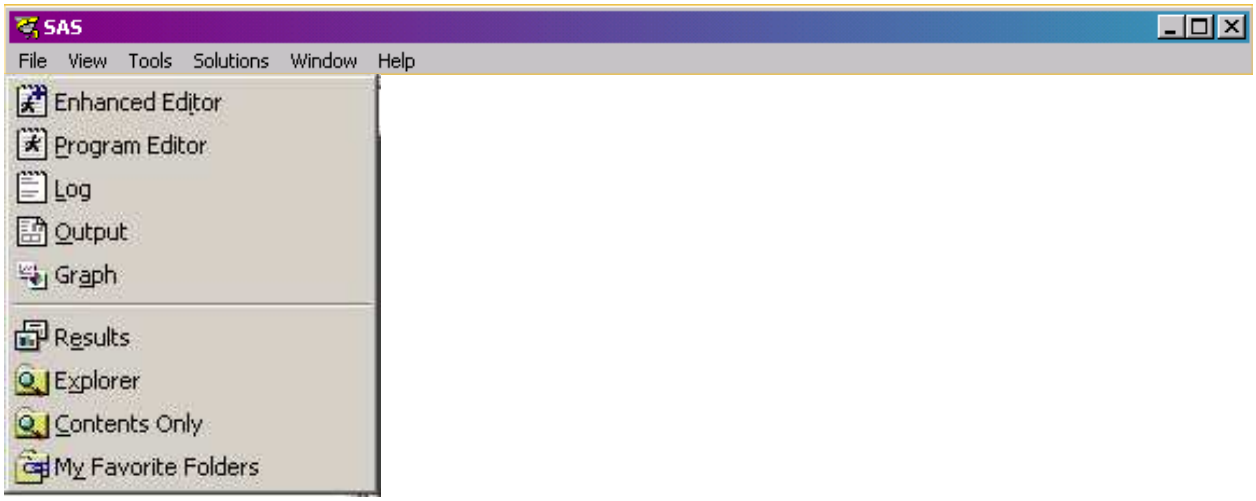


Figure 3-2. The SAS Menu Bar and the View Menu.

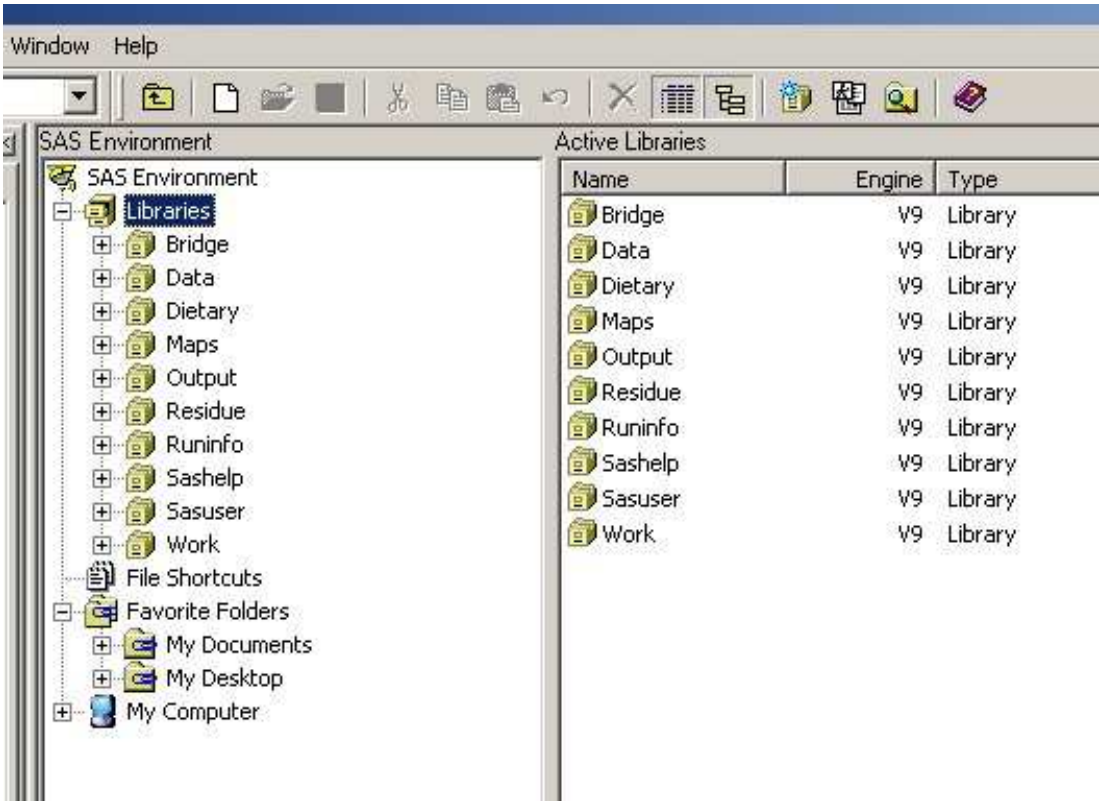


Figure 3-3. The SAS Explorer Window.

4 General Interface Hints

4.1 Display Issues

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

4.2 Grayed Out Buttons or Widgets

Figure 4-1. Sample of Two Buttons, One Normal and One Grayed Out (Bottom).

Occasionally buttons will be grayed out (displayed with muted text, see Figure 4-1). This may mean that a function has not been implemented. In version 1 the Help and About buttons have not been implemented. In some cases a grayed out button means that additional steps are required before the user is permitted to enter certain data.

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

5 SHEDS-Dietary: The Graphical User Interface

5.1 Overview of the SHEDS-Dietary Interface

A flow chart of the SHEDS-Dietary interface is provided in Figure 5-1. This figure may be useful when navigating the interface screens. The main SHEDS-Dietary screen serves as jumping-off point for navigating the other interface windows.

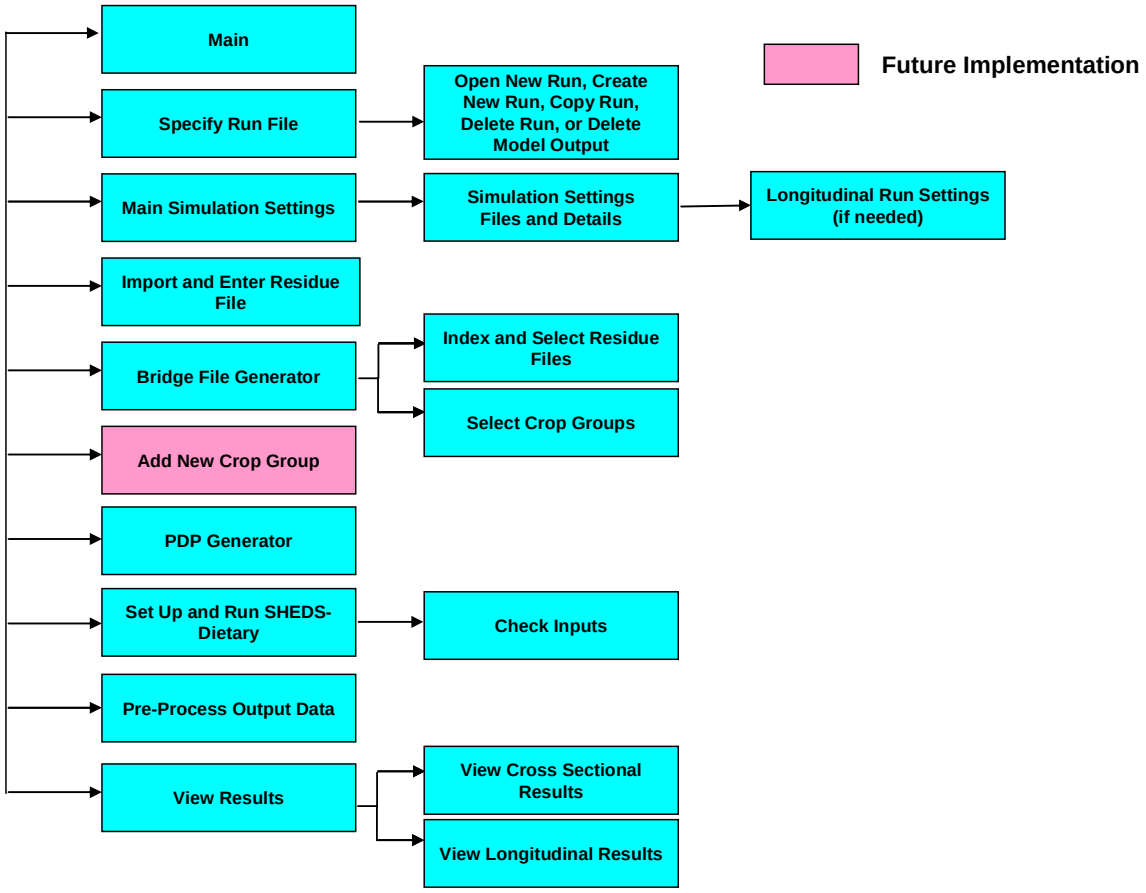


Figure 5-1. Overview of the SHEDS-Dietary Interface.

5.2 SHEDS-Dietary Main Interface Screen

When SHEDS-Dietary is started the main screen will be displayed (Figure 5-2). This is the main interface window that the user will be returned to after completing each main step. It contains the following buttons:

Specify Run File: Create a new SHEDS-Dietary run, open an existing run, copy an existing run to a new run, delete an existing run, or delete model output data.

Main Simulation Settings: Select the main settings for the current run, including single chemical versus multi-chemical, cross-sectional versus longitudinal output**.**

Import and Enter Residue File: Import and edit existing single-chemical residue files for foods, or create new residue files from scratch.

Bridge File Generator: Create the file that maps residue files or point values to food commodities.

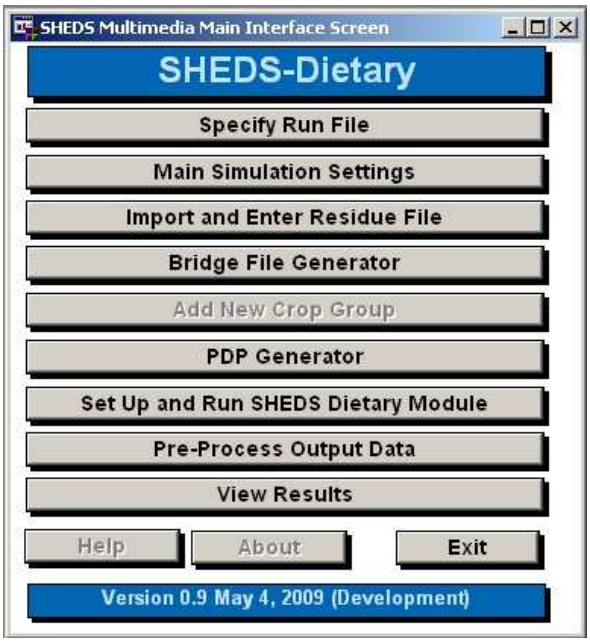


Figure 5-2. SHEDS-Dietary Main Screen.

Add New Crop Group: This is a future feature of SHEDS-Dietary and is currently inactive.

PDP Generator: Create chemical, residue, and processing factor files from the United States Department of Agriculture Pesticide Data Program (PDP) database. (Currently, the created files assume a processing factor equal to 1.)

Set Up and Run SHEDS-Dietary Module: Set general run parameters for the simulation and save the file that governs the run. Run the simulation.

Pre-Process Output Data: Produce summary data from raw SHEDS-Dietary output.

View Results: View results from cross-sectional or longitudinal SHEDS-Dietary runs.

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

About: Bring up the help screen describing this version of the model (to be implemented in future).

Exit: Close the SHEDS-Dietary user interface.

5.3 Specify Run File

Clicking the Specify Run File button from the Main SHEDS-Dietary screen opens the dialog shown in Figure 5-3. From this window, the user may select a number of options related to creating or deleting Run Information Files. Run Information files (or "Run Files" for short) are the SAS datasets that contain all the required main settings for the SHEDS-Dietary run. The files can be created in SHEDS and then saved, so that they can be reopened, edited, and run at a later time. In such a way, the user can create a library of different Run Files with different settings to meet their needs. The details of the information contained in the Run Files are included in Appendix A. The interface screens guide the user through the process of creating and editing the information in these files. Normally, the user should have no reason to edit Run Files outside of the interface.

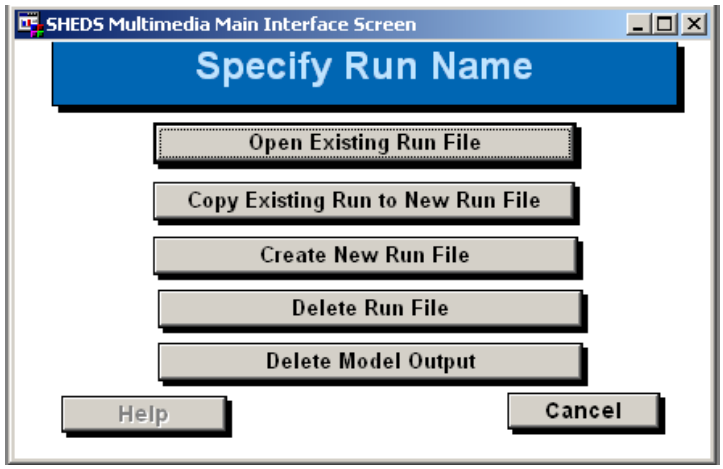


Figure 5-3. The Specify Run Screen.

The first button on the Specify Run File Screen is the Open Existing Run File button. Clicking it opens the file selection dialog shown in Figure 5-4. The dialog automatically opens in the R_info library, which is the SAS library where all the Run Information Files are stored. When the user selects a files from the dialog, the interface loads the information from the Run File and returns to the main SHEDS-Dietary screen. The other buttons on the main screen will be enabled when the file is loaded.

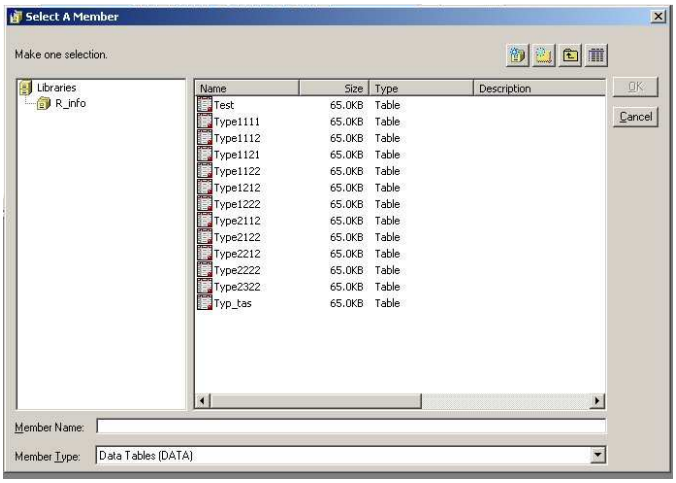


Figure 5-4. Selecting a Run File.

The screen shown in Figure 5-5 opens when the user selects the Copy Existing Run to New Run button. This screen allows the user to copy an existing Run File to a new run for editing without changing the original Run File. The user clicks the Select Existing Run File button, and a file selection dialog identical to the one in Figure 5-4 opens. After selecting the file to copy, the user also provides a name for the new file. The run name must not contain any spaces or odd characters; SHEDS will warn the user if the name is invalid and prompt for a new name.

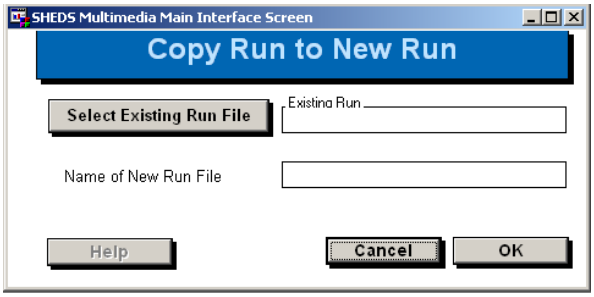


Figure 5-5. Copy Run to New Run

The interface also provides a means to create Run Files from scratch by selecting the Create New Run File button. This button initiates the screen in Figure 5-6. The user provides a new name for the run. The run name must not contain any spaces or odd characters; SHEDS will warn the user if the name is invalid and prompt for a new name.

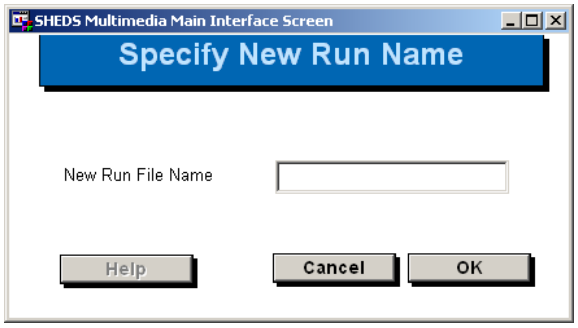


Figure 5-6. Specify New Run Name

The last two buttons on this screen provide tools for deleting Run Files and model output. While these tasks can also be performed using the SAS explorer window, the bookkeeping tools provided here may be of help to those unfamiliar with SAS. Selecting the Delete Run File button will open the window seen in Figure 5-7. Clicking the Select Existing Run File button will open a dialog identical to Figure 5-4. The user selects a file, and then clicks the Delete File button. SHEDS will prompt the user to confirm the delete before continuing.

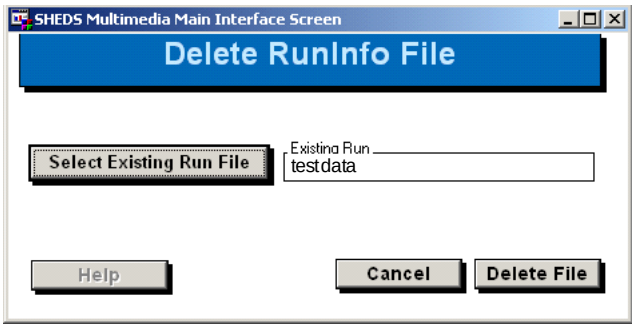


Figure 5-7. Delete Run Information File

Similarly, the user can select model output to delete by clicking the Delete Model Output button, which will open the window seen in Figure 5-8. The user selects the SAS library where the data is located via the Select Output Library button, and then selects a prefix that identifies the data. As will be explained later in this manual, output from all models runs (cross-sectional data, summary data, and longitudinal data) are assigned a text prefix by the user when the model is run. The user can then access the data via the prefix in order to select run data to delete. The user will be prompted before the run is deleted.

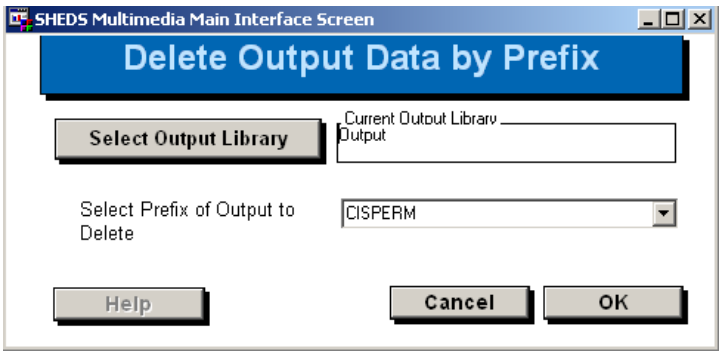


Figure 5-8. Delete output Data by Prefix

5.4 Main Simulation Settings

The first window that a user encounters after creating a new run is the Main Simulation Settings window (Figure 5-9). In this window, the user selects the four main simulation options for performing a SHEDS-Dietary Run: the simulation type (single chemical or cumulative), the study design (cross-sectional or longitudinal), the exposure pathways to model (food exposure or food and water), and an option that determines the type of input residue information the user will be providing.

If the user selects “Longitudinal Run,”, then two other options become available in the “Study Design” box (Figure 5-10). The user has the option of creating cross-sectional data and longitudinal diaries at the same time, or constructing longitudinal diaries from existing cross-sectional data (that was created earlier with the model).

There are two options for providing residue information in SHEDS-Dietary. In the first option, the user provides individual food residue files (RDF files), which are linked to food commodity groups via the Bridge File. The details of this mapping procedure are discussed later in this manual. This option is currently only available for single-chemical cross-sectional runs. The second option is for the user to provide a pre-constructed SAS dataset (a Final or "Processed" Residue File) that contains the residue measurements of interest for different foods. The foods in this file are then also linked to food commodity IDs or commodity groups via a Bridge File. This option is available for any type of run, including cumulative or longitudinal runs. The interface will limit the choices of these options to valid combinations. The contents and formats of all these files are detailed in the Appendix.

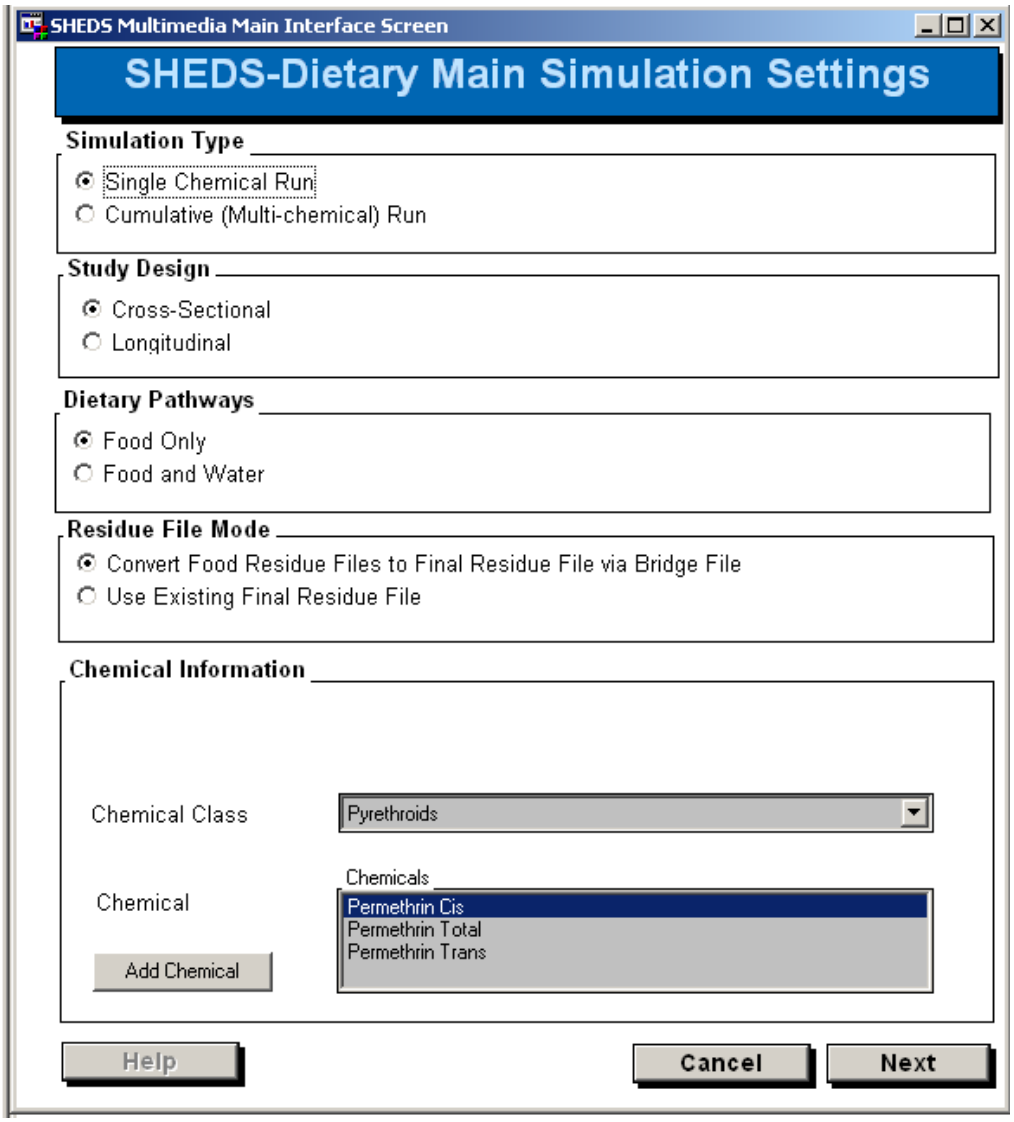


Figure 5-9. The Main Simulation Settings Screen.

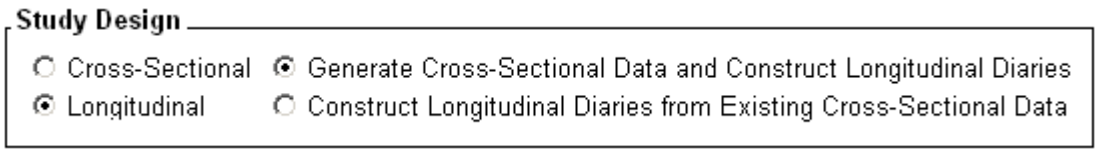


Figure 5-10. The Study Design Options for a Longitudinal Run.

The final information that is entered on this screen is the chemical information for the run. For single chemical runs, the user may select from the current list of chemical classes (currently

Pyrethroids and Other Compounds). If the user selects "Other Compounds" they may add a chemical of their own via the Add Chemical button, (it will become visible when "Other Compounds" is selected). Clicking "Add Chemical" will open a screen that will prompt the user to enter a chemical name. When the user selects OK, the chemical will be added to the selection list, which will allow the user to select it. For multiple chemical runs, however, the user must select a Chemical Code file (see Figure 5-11). Chemical Code files contain a list of chemicals that the user may include in the current run. These files are saved in the m_pest library, and their format is described in Section A.2.6. These files can be created in the PDP Generator (see Chapter 6). SHEDS-Dietary contains an example default Chemical Code file for pyrethroids, called b_pestcode. For multiple chemicals, the chemical class is automatically determined by the chemicals contained in the Chemical Code file. If more than one class of chemicals is included in the file, the class will read "Multiple Classes."

Once the desired options and chemicals are selected on the first Main Simulation Settings screen, the user can continue to a second screen of simulation settings. NOTE: This screen is bypassed if the user is creating longitudinal data from an existing cross-sectional run; in this case this input information is not needed since the cross-sectional data has already been generated. However, if the user is generating cross-sectional data and constructing longitudinal diaries, the screen is not bypassed.

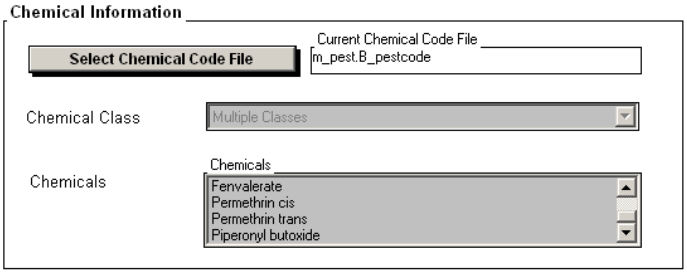
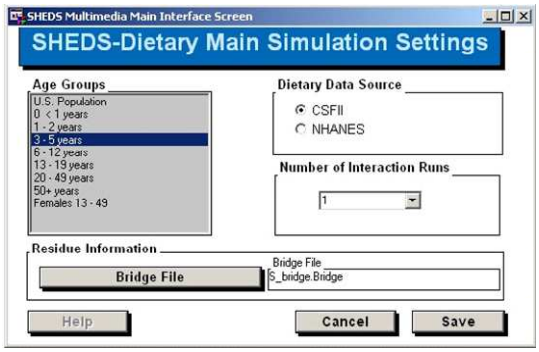
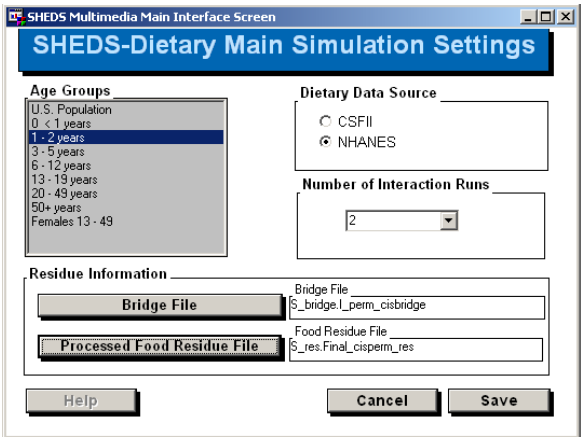


Figure 5-11. The Chemical Information Section of the Main Simulation Settings Screen for a Cumulative Simulation.

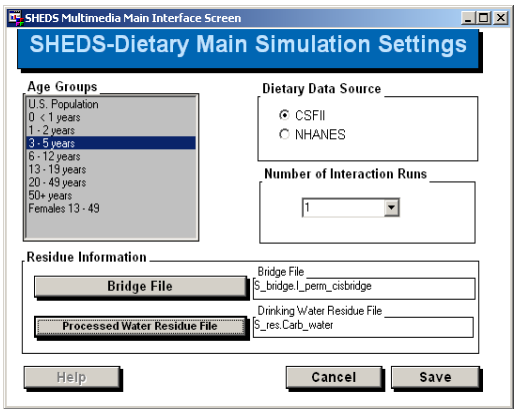
The appearance of this screen is different depending on the options selected on the first screen; different input settings are required from the user for different types of SHEDS-Dietary runs. The screens for different combinations of the four main settings are shown in Figure 5-12 and Figure 5-13. The settings that the user must potentially select in this window are described below.



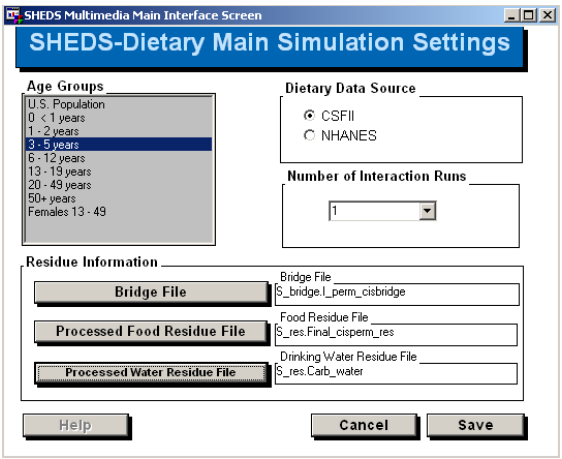
Single chemical run, cross -sectional, converting using Bridge file, food pathway



Single chemical run, using final residue file, food pathway



Single chemical run, cross -sectional, converting using Bridge file, food and water pathways



Single chemical run, using final residue file, Food and water pathways

Figure 5-12. The Second Main Settings Screen for Single-Chemical Runs.

Age Groups. Required for all runs. The user selects the age groups to be considered in the current SHEDS-Dietary run. Multiple groups may be selected.

Dietary Data Source. Required for all runs. The source of the dietary food consumption diaries that form the basis of the simulation. The options are diaries from either the Continuing Survey of Food Intakes by Individuals (CSFII) or National Health and Nutrition Examination Survey (NHANES).

Number of Interaction Runs: Required for all runs. This is the number of simulations performed per food diary for all diaries in the selected age group. Multiple runs can be performed to increase the total number of cross-sectional exposure outcomes that are generated.

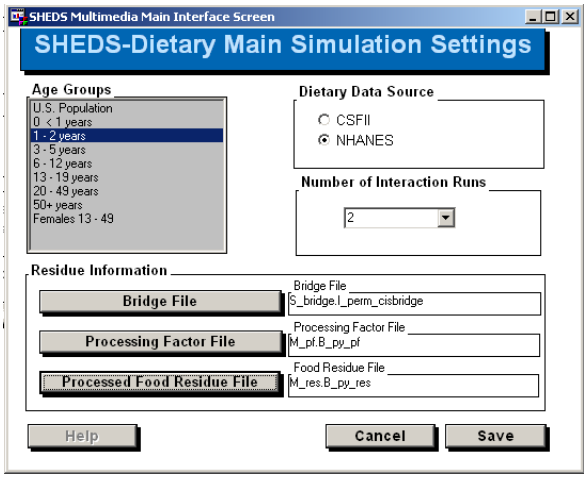
A number of files are also specified in this window. Clicking the button associated with each file opens a selection dialog in the appropriated SHEDS library where the file type is stored. The specific location, contents, and formats of all files are provided in the Appendix.

Bridge File: Required for all runs. The main purpose of the Bridge File is to map residue information to different EPA FCID commodity codes. FCID is the Food Commodity Intake Database which refers to food recipes; it is also known as the 100 g tables. The residue information may be saved in individual food residue files (residue distribution, or "RDF" files) or in a pre-constructed SAS dataset (a final, or "processed" residue file).

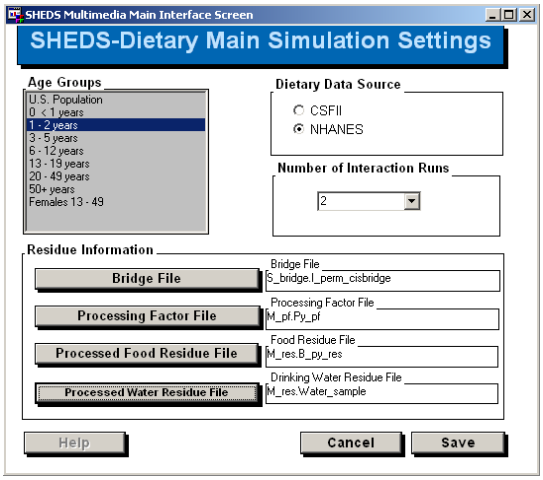
Processed Food Residue File: Required for runs using a final (processed) residue file, thus all cumulative runs require this type of file. This file contains a database of residue measurements from different food items, indexed by number (single chemicals) or measured food commodity code (multiple chemicals). The residue measurements from the different food items are linked to specific EPA food commodity IDs via a Bridge File.

Processed Water Residue File: Required for all runs modeling water exposure. A file containing water residue measurements is required for all water exposure runs.

Processing Factor File: Required for all cumulative runs. If no processing factor data available, then this file can contain values all equal to 1 so that the processing factor will have no effect on the exposure estimates.



Multi-chemical run, food exposure only



Multi-chemical run, with water exposure

Figure 5-13. The Second Main Settings Screen for Multi-Chemical (Cumulative) Runs.

After the user selects all the settings and files on this screen with valid values, the button on the right of the screen can be selected. In the case of a cross-sectional run, the button will read "Save," and clicking it returns the user to the main SHEDS screen. When the "Generate Cross-Sectional Data and Construct Longitudinal Diaries" option is being used, the button will read "Next," and clicking it will send the user to the Longitudinal Settings screen.

The Longitudinal Settings screen is the final screen in the Main Simulation Setting screen cascade (Figure 5-14). This screen will appear only for longitudinal runs (i.e. when the longitudinal option was selected on the first main settings screen). It contains the following settings related to creating longitudinal data.

Simulation Dates: The start and stop dates for the longitudinal simulation.

Diary Assembly Method: SHEDS provides three different methods for assembling longitudinal diaries. The first is an eight-diary method that uses repeats of eight daily diaries for a person (two diaries per season, a weekday and a weekend) to construct the longitudinal diary. The second method is a method that reproduces certain population variance (diversity) and autocorrelation statistics for individuals and the population. The final method uses the results from the cross-sectional analyses – interleaving the outcomes from each person's two diaries to construct a longitudinal exposure pattern.

Key Diary Variable: Only required if the Diversity and Autocorrelation method is selected. This is the variable on the dietary diaries to which the variance-based method is applied.

Diversity: Only required if the Diversity and Autocorrelation method is selected. This variable is the desired value of the ratio of between-person variance to total variance in the key diary variable.

Autocorrelation: Only required if the Diversity and Autocorrelation method is selected. This variable is the desired value of the ratio of mean day-to-day autocorrelation in the key diary variable.

Cross-Sectional Output Library: The library where the cross-sectional output data is located. If the option "Generate Cross-Sectional Data and Construct Longitudinal Diaries" is selected, this setting determines the library where the current run will write the cross-sectional data. If the option "Generate Longitudinal Diaries from Existing Cross-Sectional Data" is selected, this library specifies where the existing data are stored. Clicking the button for this library opens a SAS selection dialog to select a library (directory). The default SAS output library for cross-sectional data is called "Output". The location and names of all built-in SHEDS-Dietary libraries are given in the Appendix. However, the user may also define a new library via the Create New Library button. Clicking this button opens a small screen (Figure 5-15) that lets the user select a directory where they want to store data, and assign it a SAS library name. However, the user must have already created the directory of the new library somewhere under the SHEDS-Dietary installation tree. For example, if the program was installed in C:/Dietary, then any directory or subdirectory starting with C:/Dietary… would be valid.

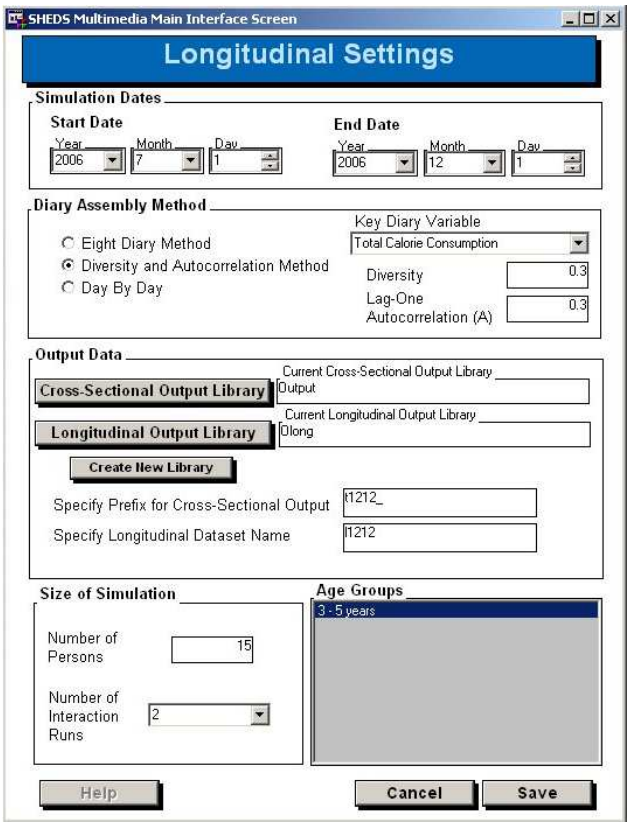


Figure 5-14. Longitudinal Settings Screen.

Longitudinal Output Library: This is the library where the dataset containing the longitudinal output data will be stored. The default SHEDS library for longitudinal output data is "Olong", but as before, the user may create a new library, provided that the directory is created under the SHEDS-Dietary directory tree.

Prefix for Cross-Sectional Output: All SHEDS output datasets are assigned a prefix. In this manner all datasets from a single run can be identified. If the option "Generate Cross-Sectional Data and Construct Longitudinal Diaries" was selected, this widget will be a text box; the user enters a prefix for the cross-sectional data to be created. If the option "Generate Longitudinal Diaries from Existing Cross-Sectional Data" was selected, this widget will be a selection

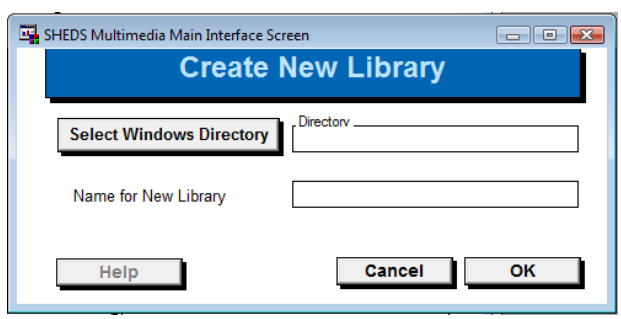


Figure 5-15. Create New Library

list of available cross-sectional runs; the selected prefix will identify the cross-sectional data to be used to create the longitudinal diaries.

Longitudinal Dataset Name: This is the name of the dataset where the longitudinal exposure diaries will be stored. Any food exposures are saved in this file, while any water exposures are given the same name, with the added suffix "_w". The default location for longitudinal datasets is the Olong library, but the user may select any defined SAS library.

Age Groups. The age groups for which to create longitudinal diaries. The displayed age groups will be a subset of those selected for the corresponding cross-sectional run.

Number of Persons: The number of persons for which longitudinal diaries will be created.

Number of Interaction Runs: The number of interactions runs to use when constructing the longitudinal diaries. Must be equal to or smaller than the number of runs used to generate the corresponding cross-sectional data.

When the option "Construct Longitudinal Runs from Existing Cross-Sectional Data" has been selected, there must be existing cross-sectional data available in the cross-sectional directory, or a message box will appear that reads "Error: No Available Multiple Chemical Cross-Sectional Datasets in Output Library."

5.5 Import and Enter Residue File

5.5.1 The Residue File Editor and Residue File Format

Residue files are text files that contain residue measurements for a particular food group. The measurements define an empirical distribution of residue values from which samples are made.

Selecting the "Import and Enter Residue File" button on the Main Screen brings up the Residue File Editor screen (Figure 5-16). This screen can be used to edit existing Residue files or create new files from scratch.

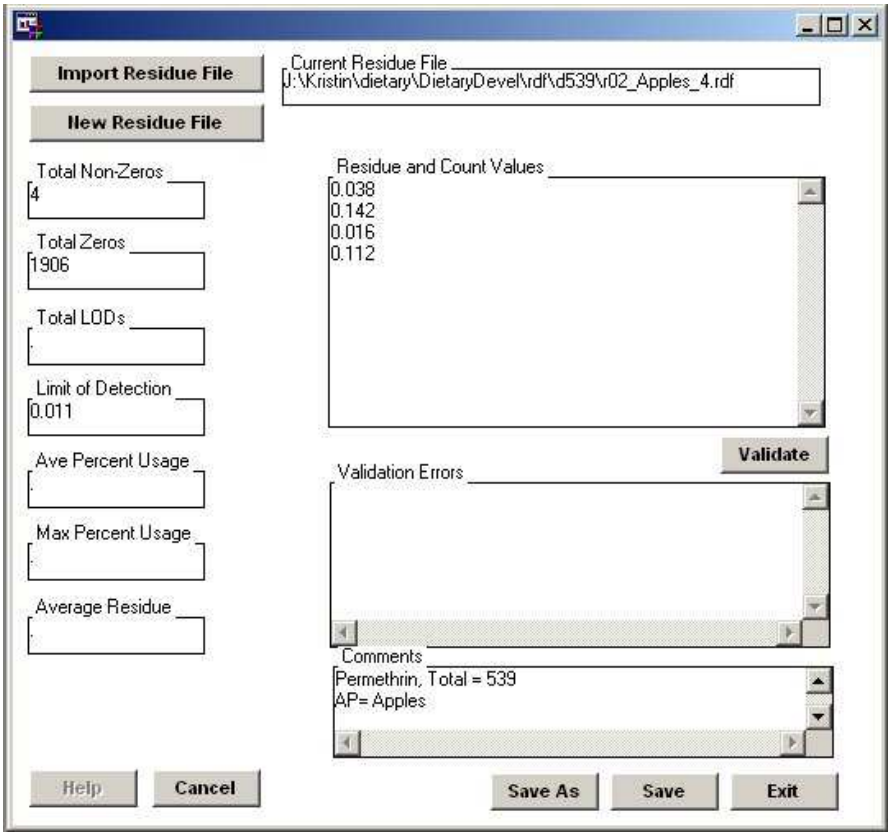


Figure 5-16. The Residue File Editor Screen.

Residue files can be created in the SHEDS-Dietary Residue Editor or in any text editor. However, the following formatting rules apply:

1. The file may contain comments; they must be marked with a leading single apostrophe (‘).

2. The file may contain the following descriptive variables, using the keywords below. These variables must be entered each on a line, using the format KEYWORD=value.

TOTALNZ	- total non-zero residue values in file
TOTALZ	- total zero residue values
LODRES	- limit of detection
TOTALLOD	- total number of limit of detections in file
USAGE	- pesticide usage percent
AVGPCT	- average percent of crop treated
MAXPCT	- maximum pesticide usage percent

3. Of the above keywords, only TOTALNZ and TOTALZ are required by SHEDS to be present. NOTE: Currently, MAXPCT is not used by the model.

4. Residue values may be entered as single numerical values (one on each line) in units of parts per million (ppm). They may also be entered as a block of values using the format NUMBER, RESIDUE where NUMBER is the number of measurements at a particular value, and RESIDUE is the value. Note that NUMBER and RESIDUE must be separated by a comma. The two methods of entering residues (single values and blocks) may both be used in the same file. The total number of measurements (all the single values plus any measurements contained in blocks) must be equal to the TOTALNZ variable (see above). **All residue values must be greater than zero**. Any zeros should be included in the TOTALZ variable (see above) and **not** entered as residues. As an example, the following is a valid Residue file:

```
'Example Residue File
TOTALZ=10
TOTALNZ=20
15, 0.002
0.005
0.005
0.004
0.002
0.006
```

5.5.2 Importing and Editing a Residue File

An existing Residue file can be imported and edited using the Residue File Editor Screen. A file is imported by clicking the "Import Residue File" button. This action opens a standard Windows File selection dialog. The user selects the file to be edited, and then selects "OK". The values in the residue file are read in to the corresponding widgets on the Residue File Editor. The residue values are loaded into the "Residue and Count Values" text pad. Residue values can be added or edited within this text pad using the formatting rules described above. Any comments in the file (i.e. the lines marked by a leading apostrophe) are displayed in the "Comments" text pad. Comments may be edited or added in this field.

The variables listed in the previous section are loaded into the corresponding text boxes along the left side of the Editor. The values for Total Zeros and Total Non-Zeros must be updated to reflect any changes made to the residue values, or else an error will result (see Validating a Residue File, below).

The user may elect to save the edited file with the same name by clicking the "Save" button, or save it with a different name using the "Save As" button. Exiting the Editor without saving discards any changes to the Residue file; the user will be prompted to confirm the exit in this case.

5.5.3 Creating a New Residue File

When the "New Residue File" is clicked, a standard Windows File Selection dialog opens and the user is prompted for a name of the new file. As an alternative, the user may also select an existing Residue file to overwrite. Once the file selection is complete, the user is presented with an entirely blank Editor which can then be populated with residue values, comments, and values for the descriptive variables. The user then proceeds as described above to save the new file when it is complete.

5.5.4 Validating a Residue File

Clicking the "Validate" button in the Residue File Editor checks the current values within the Editor (including residue values and the descriptive variables) for errors. Validation is also performed prior to any Save or Save As action. If errors exist, the Editor widget containing the error will be colored yellow, and a description of the error will be printed in the "Validation Errors" text pad.

The following are the possible validation errors:

- **Count of residue values entered does not equal value input to Total Non-Zeros text box**. The correct number of non-zero values will be noted in the Validation text pad. The user must update the Total Non-Zeros text pad to match this value.

- **A zero residue value is entered in the text pad**. Zero values cannot be added to the list of residue measurements; they must be entered in the Total Zeros text box. For all zero values added to the text pad, the user will be asked if they would like to increment Total Zeros.

- **Value too large for percentage.** Max Percent Usage and Average Percent Usage must be less than or equal to 100.

- **Invalid or negative value.** None of the descriptive variables can have negative values.

- **Invalid number format.** A line with a comma is missing either the residue or count value, or an invalid character or character combination has been entered.

- **Error: Fractional counts are not allowed.** A non-integer count value is entered on a line with a comma.

- **Negative count and residue values are not allowed**. A negative count or residue has been entered.

5.6 Bridge File Generator

The Bridge File Generator screen is accessed from the corresponding button on the main screen. The Bridge File Generator is an interactive screen that is used to create the file that maps RDF files or residue values to food commodities. The Bridge File generator is only active for single-chemical cross-sectional runs.

5.6.1 Overview of the Bridge File

The Bridge File is the SHEDS-Dietary input file that maps the food commodities available in the model to either residue value distributions (via assigning them to one or more corresponding Residue files) or to point residue values. It is a SAS dataset that contains the food commodities available in the model along with a number of other variables that define how residues should be sampled for each food. The available options for mapping residues to foods in SHEDS-Dietary are illustrated in Figure 5-17. Note that the use of "File Indices" is simply a convenient way of referring to Residue files. The indices are integer numbers that are assigned to each individual Residue file. See Section 5.6.4 for details of how files are assigned indices for use in SHEDS-Dietary.

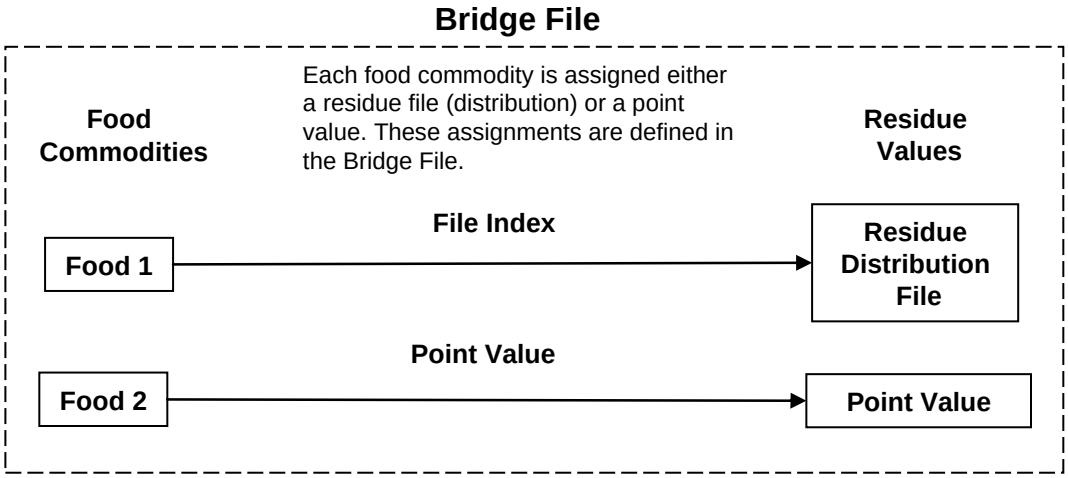


Figure 5-17. Options for Mapping Residue Values to Food Commodities in the Bridge File.

The available options are:

- **File Index**. The file index associated with a Residue file is assigned to a food commodity. All samples of residues for that food will come from the distribution defined in the file.

- **Point Value.** The user may assign a single residue point value to the food commodity.

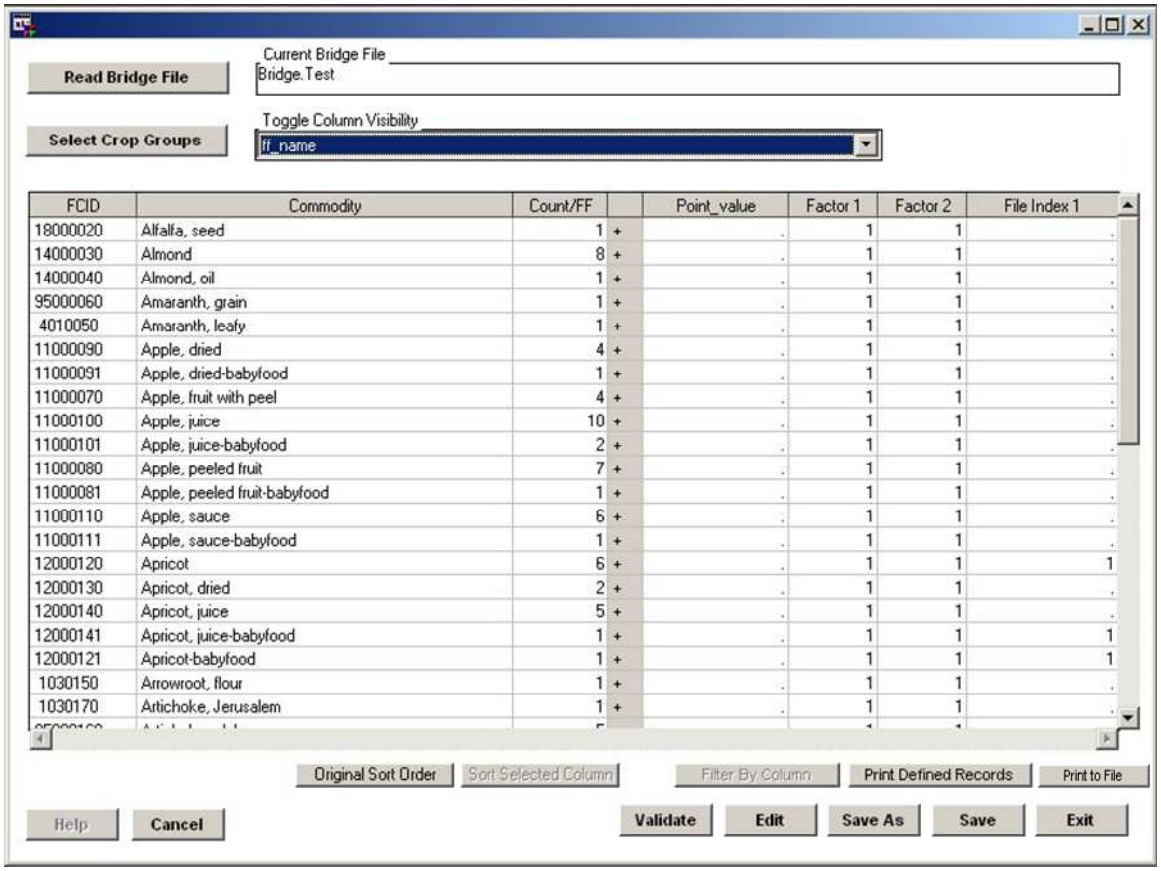
Note that assigning file indices or point values to all foods in the Bridge File is not required. If a food is not a significant source of the chemical being studied, then it may be ignored.

5.6.2 The Bridge File Generator Screen

The Bridge File Generator screen is shown in Figure 5-18. The generator displays the Bridge File, which contains an indexed list of all the food commodities available in SHEDS-Dietary (the "Commodity" column). The other columns of the file contain information related to the assignment of residue values to foods. The variables in the file are given in Table 5-1. Not all of the variables listed here must be displayed at one time. Although the screen has scroll bars that can be used to view variables that are off the display, the user may also elect to hide some select variables from view. This is done using the "Toggle Column Visibility" menu. Selecting a variable from this list either hides or redisplays the column containing the variable.

Table 5-1. Variables (Columns) in the Bridge File

Variable Name	Variable Label	Description
CropGroup	CG (hidden by default)	USDA crop group number associated with the Commodity
FCID	FCID	FCID food commodity code
Commodity	Commodity	FCID commodity name
ff_name	CondName (hidden by default)	FCID Food Form
Count/FF	Count/FF	Number of food forms for commodity
Point Value	Point_Value	Residue point value assigned to commodity
Factor 1	Factor 1	Processing factor 1
Factor 2	Factor 2	Processing factor 2
use_pct	use_pct (hidden by default)	AvgPCT, MaxPCT, or AvgResTrtd
File Index 1	File Index 1	Residue file index associated with the food commodity.



FCID	Commodity	Count/FF		Point_value	Factor 1	Factor 2	File Index 1
18000020	Alfalfa, seed	1	+	.	1	1	.
14000030	Almond	8	+	.	1	1	.
14000040	Almond, oil	1	+	.	1	1	.
95000060	Amaranth, grain	1	+	.	1	1	.
4010050	Amaranth, leafy	1	+	.	1	1	.
11000090	Apple, dried	4	+	.	1	1	.
11000091	Apple, dried-babyfood	1	+	.	1	1	.
11000070	Apple, fruit with peel	4	+	.	1	1	.
11000100	Apple, juice	10	+	.	1	1	.
11000101	Apple, juice-babyfood	2	+	.	1	1	.
11000080	Apple, peeled fruit	7	+	.	1	1	.
11000081	Apple, peeled fruit-babyfood	1	+	.	1	1	.
11000110	Apple, sauce	6	+	.	1	1	.
11000111	Apple, sauce-babyfood	1	+	.	1	1	.
12000120	Apricot	6	+	.	1	1	1
12000130	Apricot, dried	2	+	.	1	1	.
12000140	Apricot, juice	5	+	.	1	1	.
12000141	Apricot, juice-babyfood	1	+	.	1	1	1
12000121	Apricot-babyfood	1	+	.	1	1	1
1030150	Arrowroot, flour	1	+	.	1	1	.
1030170	Artichoke, Jerusalem	1	+	.	1	1	.

Figure 5-18. The Bridge File Generator Screen.

The FCID food form variable specifies the commodities' cooking status (1=cooked, 2=uncooked), food form (1=fresh or not specified; 2=frozen; 3=dried; 4=canned; 5=cured, pickled, smoked, salted; 6=no applicable), and cooking method (0=not specified,1=baked, 2=boiled, 3=fried, 4=fried or baked, 5=boiled or baked). For example, the food form 211 (as for banana in Figure 5-19), indicates "Cooked", "Fresh or Not Specified" and "Baked."

The number of different food forms for each commodity is given in the "Count/FF" column. The "+/-" column that is located to the immediate right of the food form column may be used to expand or collapse the viewing of the food form list for a commodity. An example is shown in Figure 5-19; in this case the food commodity "banana" has been expanded to list all of its food forms, and the display food form name (CondName) column has been toggled on.

FCID	Commodity	CondName	Count/FF	
1030150	Arrowroot, flour	Cooked;Fresh or N/S;Baked	1	+
1030170	Artichoke, Jerusalem	Uncooked;Fresh or N/S;N/S	1	+
95000160	Artichoke, globe	Cooked;Fresh or N/S;N/S	5	+
4010180	Arugula	Uncooked;Fresh or N/S;N/S	1	+
95000190	Asparagus	Uncooked;Fresh or N/S;N/S	5	+
95000200	Avocado	Uncooked;Fresh or N/S;N/S	2	+
9020210	Balsam pear	Cooked;Fresh or N/S;N/S	2	+
95000220	Bamboo, shoots	Uncooked;Fresh or N/S;N/S	5	+
95000230	Banana	Uncooked;Fresh or N/S;N/S	110	-
95000230	Banana	Uncooked;Frozen;N/S	120	
95000230	Banana	Uncooked;Dried;N/S	130	
95000230	Banana	Cooked;Fresh or N/S;Baked	211	
95000230	Banana	Cooked;Fresh or N/S;Boiled	212	
95000230	Banana	Cooked;Fresh or N/S;Fried	213	
95000230	Banana	Cooked;Frozen;Fried	223	
95000230	Banana	Cooked;Canned;N/S	240	
95000240	Banana, dried	Uncooked;Dried;N/S	3	+
95000241	Banana, dried-babyfood	Cooked;Dried;N/S	1	+

Figure 5-19. An Expanded Food Commodity with Food Forms (Banana).

In addition to the “Toggle Column Visibility” menu, there are several other tools on the screen that can aid in viewing and editing the Bridge File. By using the “Sort Selected Column” and “Original Sort Order” buttons, the user can sort the Bridge File by any field. A column must be selected by clicking on the column title will enable the sort button. In addition, the user can limit the Bridge File rows visible by selecting “Filter by Column” after selecting a column. This button will filter the Bridge File to show only the records for which the selected column (variable) is defined. This feature may be particularly useful when the user is only assigning residues to a small number of commodities, and would like to see them all at once.

The user can also limit the food commodities listed in the Bridge File Generator by crop group. This is accomplished by clicking the “Select Crop Groups” button. This will bring up the Select Crop Groups dialog (Figure 5-20).

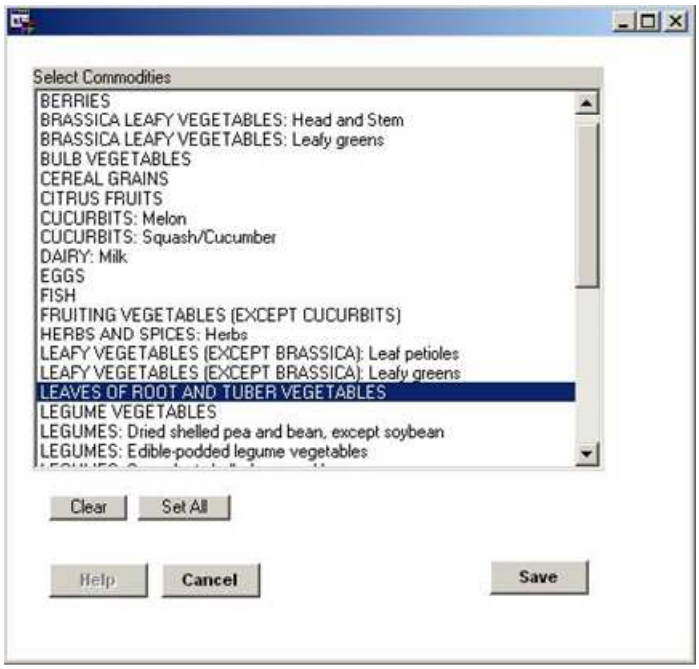


Figure 5-20. Select Crop Groups Dialog.

The user may select multiple crop groups by holding down the "Shift" key and clicking with the mouse. When the user selects "Save," the dialog closes and returns to the Bridge File Generator, which will then have food commodities in the selected Crop Groups visible. Note that selecting only certain crop groups does not delete non-selected crop groups from the Bridge File; crop/groups commodities that are not selected are maintained and can be reselected and viewed at any time.

Finally, the user may print only the records for which residue values or file indexes are defined by clicking the "Print Defined Records." This action will print a copy of the defined Bridge File records to the default printer. The data can also be printed to a comma-separated value (*.csv) file via the "Print to File" button.

5.6.3 Read Bridge File

All Bridge Files must be stored in the Bridge library (see Appendix A-1 on page 129 for information on the SHEDS-Dietary libraries). By default, the Bridge File Generator opens and displays the Bridge File named "Bridge," which is the SHEDS-Dietary default Bridge File. However, the user can alter this default file and save other Bridge Files using the "Save As" option. For example, the user may create different Bridge Files for different chemicals. Then in future SHEDS-Dietary sessions the user may read and edit any of these Bridge Files. SHEDS-Dietary provides an empty Bridge File, called "Bridge_empty" that users can use as a starting

point for creating their own Bridge Files with the Bridge File editor. The file is stored in the s_bridge library, which is the default library for single chemical Bridge Files.

Selecting the “Read Bridge File” button brings up a SAS library dialog box, which will display all the Bridge Files in the Bridge library for selection (Figure 5-21).

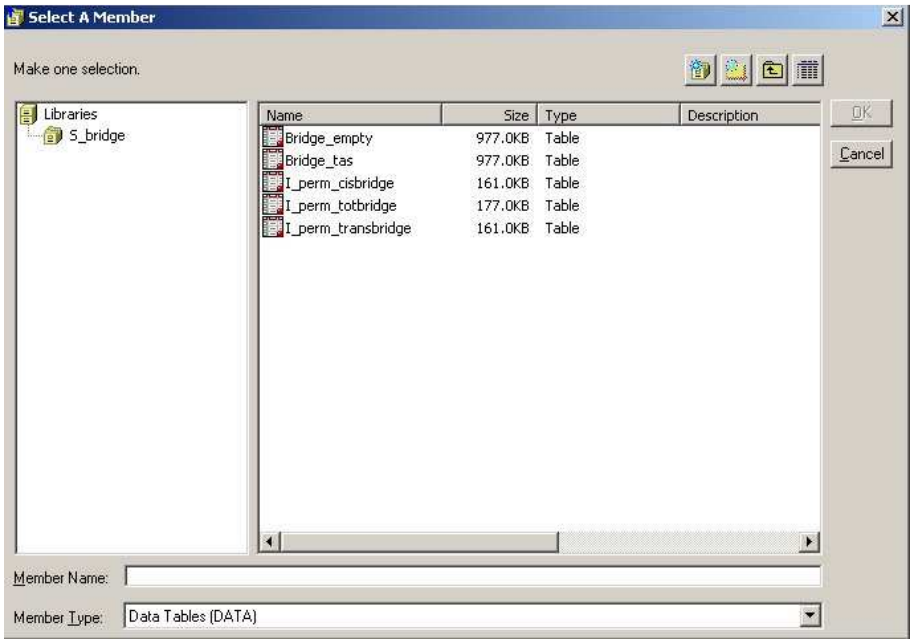


Figure 5-21. Selecting a Bridge File.

5.6.4 Editing the Bridge File

Once the user has opened a Bridge File for editing, they may then begin making edits to the file (i.e. adding point residue values or residue files to food commodities). In order to edit the file, the user must first select the “Edit” button on the main Bridge Generator screen. This puts the file into edit mode. Once it is pushed button label will become “Stop Editing”; selecting it again will disable editing.

Edits made to the variables for a food commodity (for example, the point value, file index, or probability) when the food form list is collapsed will automatically be applied to all food forms. However, when the list is expanded the values for each food form can be set independently. However, if the list is subsequently collapsed and edited, the changes will overwrite any previously entered values.

Editing any variables (columns) other than file indices is extremely straightforward; the user simply clicks on the column and row and enters the desired value. Editing the file indices is unique; in this case, clicking on any field in any of the File Index columns will open the Residue File Index Screen. The purpose of this screen is two-fold: 1) It allows the user to "index" Residue Files so that they can be assigned to food commodities in the Bridge File and 2) it provides the list of currently "indexed" Residue Files to the user. The user makes a selection from this list for the current food commodity.

Figure 5-22 shows what the Residue Index screen looks like the first time it is accessed by the user. The screen displays the Index File, which is a list of the Residue Files to be used in a run and their corresponding indexes. Since at this point in time the user has not indexed any residue files, the list of files/indexes is empty.

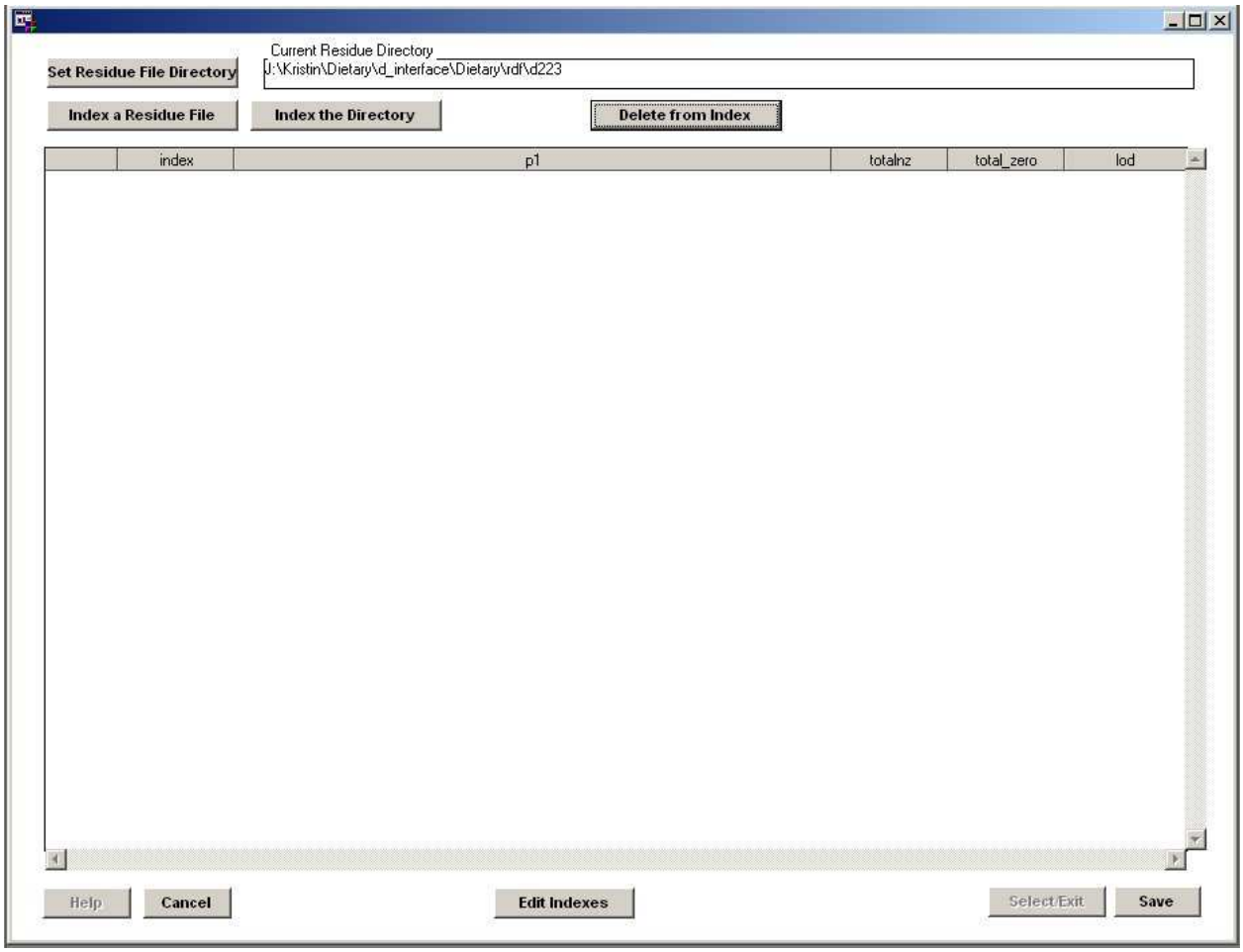
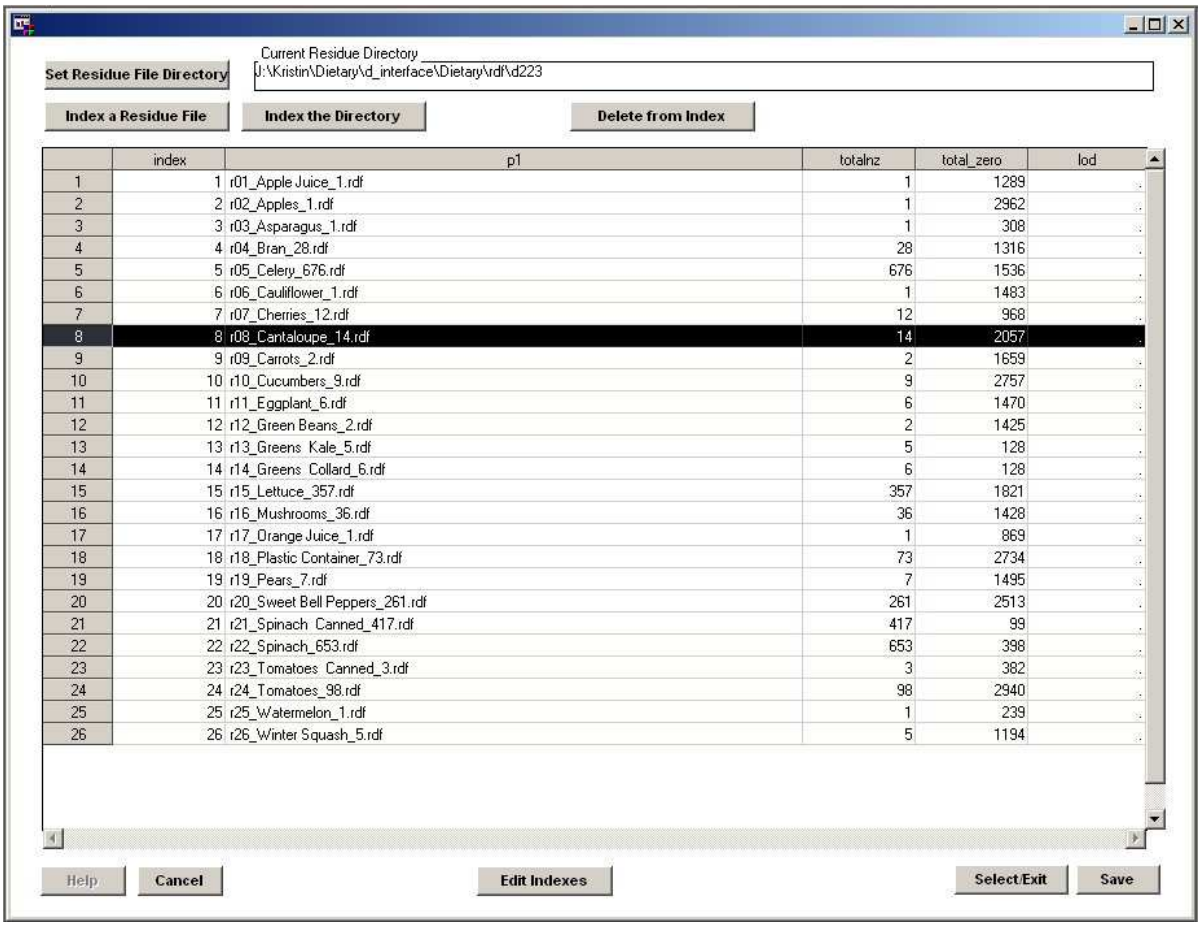


Figure 5-22. An Empty Index Residue File Screen

The user can tell the interface where to look for Residue Files by selecting “Set Residue File Directory”. This opens a standard Windows file section dialog. By default, the residue file directory is the folder ./Dietary/rdf under the SHEDS-Dietary main installation directory.

The user then adds residue files to the index by selecting either the “Index a Residue File” or “Index the Directory”. Clicking “Index a Residue File” opens up yet another standard Windows file selection dialog box. The user then selects a Residue file, which will then appear listed in the index window. “Index the Directory” will automatically index all the *.rdf files in the current Residue directory. Note that if there are many files in the directory or if the files have many residue values, then this action may take a few minutes to complete. Utilizing “Index a Residue File” may be easier for the user if only a few Residue files are going to be assigned to foods; indexing the entire directory is more efficient if many files are going to be used.

After many Residue files have been indexed, the Index File will look as it does in Figure 5-23.



	index	p1	totalnz	total_zero	lod
1	1	r01_Apple Juice_1.rdf	1	1289	.
2	2	r02_Apples_1.rdf	1	2962	.
3	3	r03_Asparagus_1.rdf	1	308	.
4	4	r04_Bran_28.rdf	28	1316	.
5	5	r05_Celery_676.rdf	676	1536	.
6	6	r06_Cauliflower_1.rdf	1	1483	.
7	7	r07_Cherries_12.rdf	12	968	.
8	8	r08_Cantaloupe_14.rdf	14	2057	.
9	9	r09_Carrots_2.rdf	2	1659	.
10	10	r10_Cucumbers_9.rdf	9	2757	.
11	11	r11_Eggplant_6.rdf	6	1470	.
12	12	r12_Green Beans_2.rdf	2	1425	.
13	13	r13_Greens Kale_5.rdf	5	128	.
14	14	r14_Greens Collard_6.rdf	6	128	.
15	15	r15_Lettuce_357.rdf	357	1821	.
16	16	r16_Mushrooms_36.rdf	36	1428	.
17	17	r17_Orange Juice_1.rdf	1	869	.
18	18	r18_Plastic Container_73.rdf	73	2734	.
19	19	r19_Pears_7.rdf	7	1495	.
20	20	r20_Sweet Bell Peppers_261.rdf	261	2513	.
21	21	r21_Spinach Canned_417.rdf	417	99	.
22	22	r22_Spinach_653.rdf	653	398	.
23	23	r23_Tomatoes Canned_3.rdf	3	382	.
24	24	r24_Tomatoes_98.rdf	98	2940	.
25	25	r25_Watermelon_1.rdf	1	239	.
26	26	r26_Winter Squash_5.rdf	5	1194	.

Figure 5-23. Index Residue File Screen with Files Indexed.

Once the user has added one or more files to the Index file, they can select a record (that is, a file) to assign to the current food. Selecting a record will highlight it in the index (as in Figure 5-23). The user then clicks the "Select/Exit" button to close the screen and assign the file index to the current food. The file index will automatically be present in the Bridge File editor in the current file index field (ex. File Index 1).

Note that the user can select the Save button in the Index Residue File screen at any time to save the current Index file. However, the file will also be saved automatically when the user leaves the screen via "Select/Exit." The index file is saved in the Bridge library with the name XXX_idx, where "XXX" is the name of the current Bridge File. The user should have no reason to edit this file outside the interface.

Residue files can be deleted from the Index file at any time using the "Delete from Index" Button. The files to delete may be selected by highlighting one or more rows. Clicking on the row number will select a single row; hold down the SHIFT key while clicking to select more than one row.

If the user chooses, the index numbers may be edited. By default, the residue files are numbered in which they are indexed (which is alphabetical order when "Index the Directory" is used); however, the user may decide to assign different unique indexes to files after they are loaded. This is accomplished by selecting the "Edit Indexes" button. This button turns on the edit mode of the screen; after it is clicked the user should be able to directly edit the index fields.

The user assigns point values, file indexes, and probability values (if needed) to every food commodity of interest for the chemical being studied.

5.6.5 Validating the Bridge File, Index File, and Residue Files

After the Bridge File has been constructed (through adding point values and/or file indexes to every food commodity of interest), the user can validate the Bridge File, the Index File, and any Residue Files that are included in the Index File. The validation process will identify any errors in the assignment of point values, mapping of file to indexes, or creation of residue files. Note that the validation procedure that is performed on the Residue Files is the same that is performed on the Residue File Editor screen, but the process is required here as well since the user may create Residue Files outside of the SHEDS-Dietary editor.

The validation process is initiated by clicking the "Validate" button on the Bridge File Generator Screen. Any errors are written to the SAS log. The potential errors are given below.

Index File Errors:

- **RDF file FILENAME does not exist.** The residue file indexed in the file does not exist. This could occur if a user deletes a residue file after it has been indexed.

Residue File Errors:

- **TotalNZ missing in FILENAME**. The descriptive variable TOTALNZ, the total number of non-zero residues in the file, must be defined.

- **TotalZ missing in FILENAME**. The descriptive variable TOTALNZ, the total number of zero residue values in the file, must be defined.

- **TotalNZ not compatible with number of non-zero residue values in FILENAME**. The value of TOTALNZ and the number of actual non-zero residues in the file (including those defined in blocks) must be equal.

- **Invalid character in FILENAME**. Only numeric values and commas can appear in the residue file data lines.

- **Error: Zero or negative residue measurement in FILENAME**. All residue values must be greater than 0. Any zero residue measurements must be defined via the TOTALZ variable.

- **Error: Number of residues in block must be >0 in FILENAME**. A block definition of residue values (i.e., one defined using the form "NUMBER, RESIDUE") must have at number>zero.

- **TOTALNZ, TOTALZ, LODRES, TOTALLOD, USAGE, AVGPCT, MAXPCT, or AVGRESTRTD negative in FILENAME.** Values for these descriptive variables must be greater than or equal to zero.

Bridge File Errors:

- **Invalid point value.** Point values must be greater than zero.

- **Missing index for at least 1 season.** If using the "By Season" option, indexes must be defined for all seasons. (Note that all four seasons can be missing, but if one season is defined the others must be as well).

- **Invalid factor1 or factor2**. These values must be greater than 0.

- **Invalid probability**. These values must be greater than 0.

- **Warning: Point value will be ignored; file index used.** The Bridge File editor allows the user to enter both point values and one or more file indexes for a food. However, the file index will supersede the point value. This is just a warning to that effect.

- **Invalid RDL file index**. The Bridge File contains a file index that is not defined in the index file (i.e., is not assigned a residue file).

5.7 Set Up and Run SHEDS-Dietary Module

Selecting "Set Up and Run SHEDS-Dietary Module" from the Main Screen opens the Run Screen (Figure 5-24). This screen is used to set a number of options for the current SHEDS-Dietary run, which are then saved in the Run file. This screen is also used to initiate the actual SHEDS-Dietary simulation. In this screen, the user can both confirm settings that have already been selected for the run, and set risk parameters and other options.

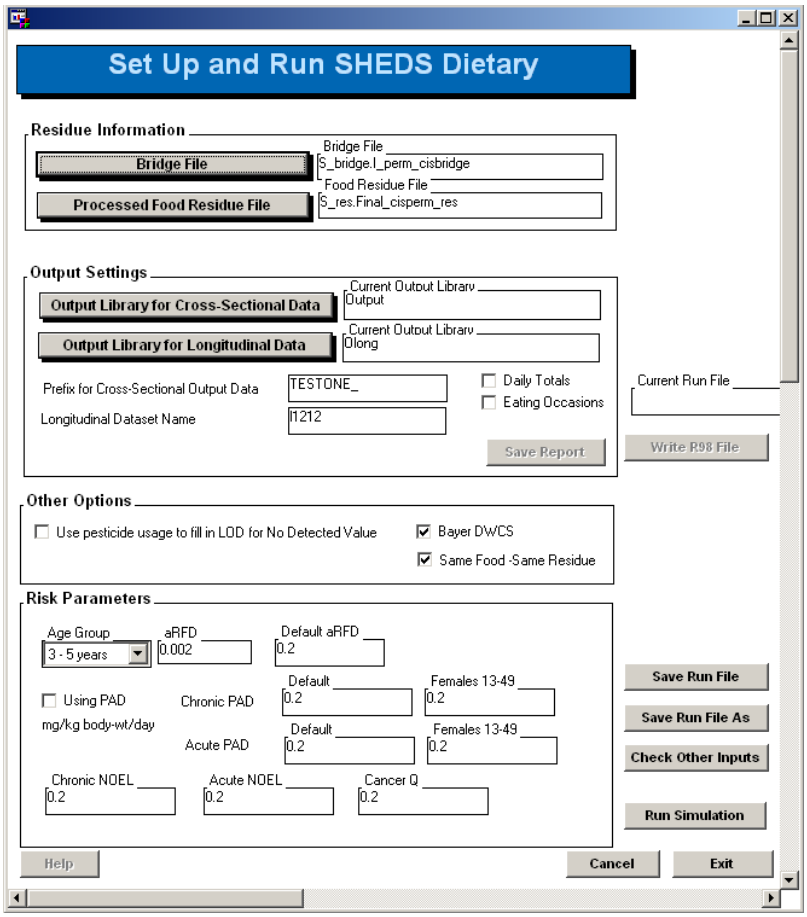


Figure 5-24. The Run SHEDS-Dietary Screen: Single Chemical Longitudinal Run

The appearance of this screen is also dependent on the run settings. All of the required files designated in the Main Settings Screen can also be updated here prior to running the simulation. The types of files that are present depend on the run type. In the case of a run where the "Convert Via Bridge File" option is used, the residue file location (directory) is also present. The

selection widgets for these files will be pre-populated with the values chosen earlier; this screen gives the user a chance to make any final changes.

In addition, the output file libraries and prefixes for cross-sectional and (if present) longitudinal data are also present. A note about prefixes: if the prefix designated does not end with an underscore, SHEDS will add one. This underscore is necessary for constructing the filenames. When the user visits the screen again, the underscore will be present. Again, these values are populated with any prior selections of these values that were made on the Longitudinal Settings screen. In the case of a solely cross-sectional run, the output library and prefix are first specified here. The user may also indicate which outputs should be written for the run using three checkboxes: Daily Totals and/or Eating Occasions.

5.7.1 Other Options

There are three additional options provided in this section.

- **Use Pesticide Usage to Fill in LOD for No Detected Value.** Use any pesticide usage information included in the residue files to fill in limit-of-detection values.

- **Bayer DWCS**. Use data from the Bayer Drinking Water Consumption Survey (Barraj and Daniels, 2004) to model direct drinking water consumption (the default). If this box is unchecked, CSFII data will be used to model water consumption (spread equally over 6 drinking occasions per day).

- **Same Food-Same Residue.** When this option is selected, any instance of the same RAC of the same food being eaten more than one time in day will use the same sampled value from the residue distribution.

5.7.2 Risk (Toxicological) Parameters

Risk (toxicological) parameters are also entered on the Set Up and Run screen. NOTE: Currently these risk factors are not used by the model, therefore risk values have not been linked with exposure values in this version. The parameters are given in Table 5-2. By default, all risk (toxicological) parameters are initially given a value of 0.002.

Table 5-2. Risk (Toxicological) Parameters in the Run Information File

Risk (Toxicological) Parameter	Description
aRFD	Acute reference dose
aRDF: Default	Default acute reference dose
Chronic PAD: Default	Chronic population adjusted dose
Chronic PAD: Females 13-49	Chronic population adjusted dose for females 13-49
Acute PAD: Default	Default acute population adjusted dose for females 13-49
Acute PAD: Females 13-49	Acute population adjusted dose for females 13-49
Chronic NOEL	Chronic no observed effect level
Acute NOEL	Acute no observed effect level
Cancer Q	Cancer potency factor

Reference dose is assigned to each age group; the user must select each defined age group from the Age Group menu and enter appropriate values for the parameter. If an invalid value has been assigned for any age group, the field will be colored yellow, indicating an error. Note that this may occur, even if the value for the currently displayed age group is valid. If an error exists, a text field will appear at the bottom of the Run Screen and the current errors will be displayed (Figure 5-25). All errors in this field need to be resolved before the user can save the Run File or run the SHEDS-Dietary simulation.

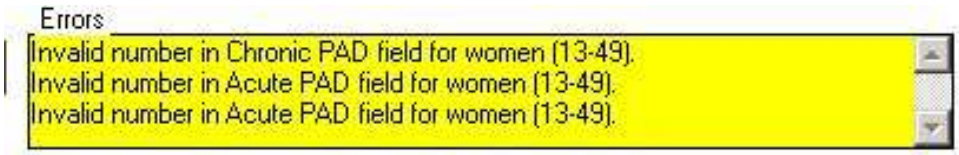


Figure 5-25. Run Screen Error Field

Advanced users of SHEDS-Dietary may want to directly view or edit values of the Run Files variables. This can be done using the Check Run Variables screen (Figure 5-26), which is initiated via the “Check Other Inputs” button on the Set up and Run screen. This screen will display all the relevant Run File variables for the current run, editable as text. Note that any changes made to the Run File from this dialog is not subjected to the rigorous error testing that is provided by the other interface screens.

When all the fields in the run screen are completed with valid values, then the “Save Run File”, “Save As Run File” and “Run Simulation” buttons are active. Clicking the Save Run File button

will save all the current values of the Run file variables. The Save As Run File button performs the same function as the Save Run File button, with the exception that is always opens a dialog in order for the user to designate a filename different from the current Run file name. Finally, selecting the "Run Simulation" button will initiate the SHEDS-Dietary Run. The model outputs are discussed in Appendix A of this manual.

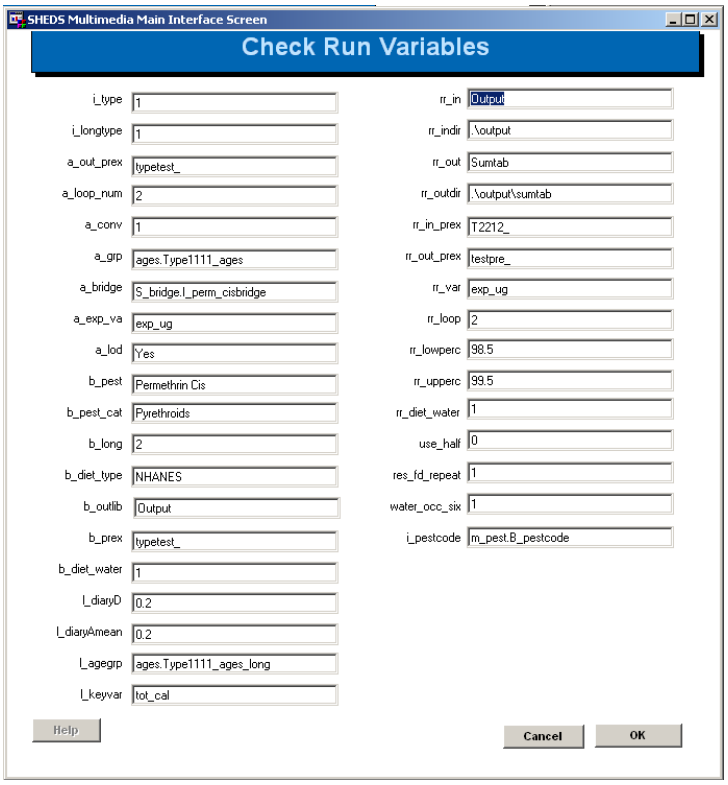


Figure 5-26. Check Run Variables

5.8 Pre-Process Output Data

Once cross-sectional data is generated by a SHEDS-Dietary run, it must be processed to generate summary and percentile data tables. The contents of these tables are described in the Appendix. This step is accomplished via the Pre-Process Output Data screen (Figure 5-27), which is accessed via a button on the Main SHEDS Screen. If the user has a Run File open when the screen is initiated, much of the data in this screen will be populated with valid values. The user may also open a new Run File via the Runinfo file button at the top of the screen.

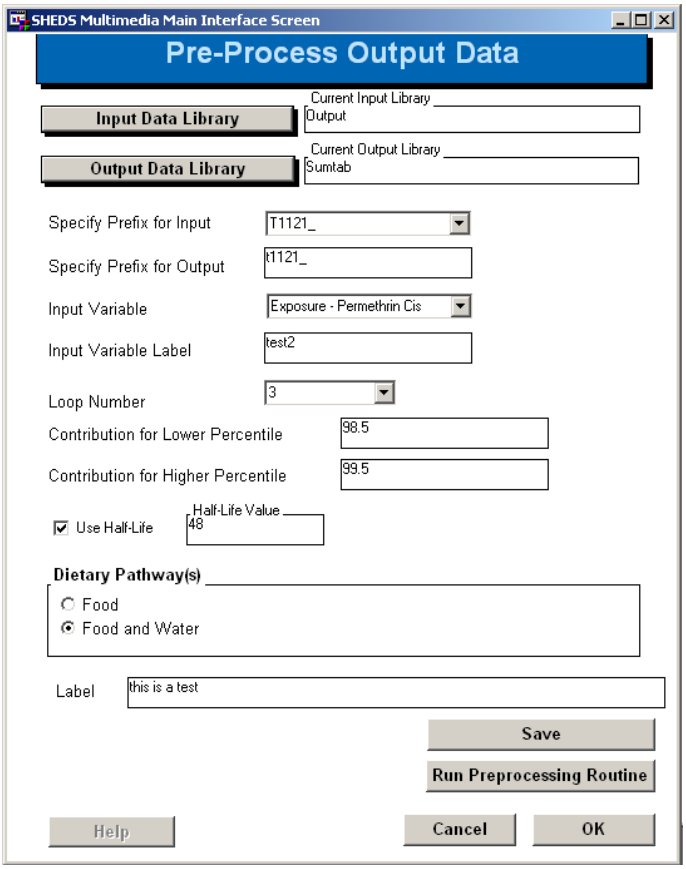


Figure 5-27. The Preprocess Output Data Screen.

The following variables must be specified in this window in order to successfully preprocess cross-sectional output data.

Input Data Library: This is the library where the data that is to pre-processed (the cross-sectional model output) is located. Selecting a library will populate the Input Data Prefix widget with a list of the available cross-sectional runs.

Input Data Prefix: The user selects the prefix of the model output data they would like to preprocess from the list. (Recall that all model runs are supplied a output prefix for identifying unique sets of data). This selection will populate several of the other widgets on the screen with default values.

Output data Library: This is the library where the SHEDS summary datasets will be created. By default, the data is written to the Sumtab library, but the user may select any library.

Output Data Prefix. This is the prefix for the output data table filenames. The interface will add a underscore to all prefixes before they are used to create filenames.

Input Variable: The variable to be processed. In a single chemical run, this variable is always called "Exposure: XXX" where XXX is a chemical name. In a multi-chemical run, the variables will be identified as either "Total Exposure" (total cumulative exposure) or Exposure: XXX, where XX X is a chemical name.

Use Half-Life. If this option is selected, SHEDS uses a half-life value (in hours) when estimating exposures, otherwise, SHEDS uses the Maximum Exposure-Eating Occasion to calculate per capita exposures.

Input Variable Label. Label to give the input variable in the processed datasets. (Not currently required).

Loop Number: Number of interaction runs (loops) to include in the summary statistics. For example, if 4 repetitions were run in the original simulation, the user may choose any number less than 4 to include in the summary statistics.

Contribution for Lower Percentile and Contribution for Upper Percentile. Specify lower and upper range for contribution analyses.

Pathway. Pathways to include in the analysis.

Label. Label for the output datasets. (Not currently required).

5.9 View Results

Selecting the "View Results" button on the Main SHEDS-Dietary screen opens the View Results window (Figure 5-28), which contains two option buttons: View Cross-Sectional Results and View Longitudinal results. Clicking either of these buttons will open a screen to that provides to the user tools for viewing and exploring the results of the current SHEDS-Dietary run or previous runs. Details of the View Results windows are discussed in the next two sections.

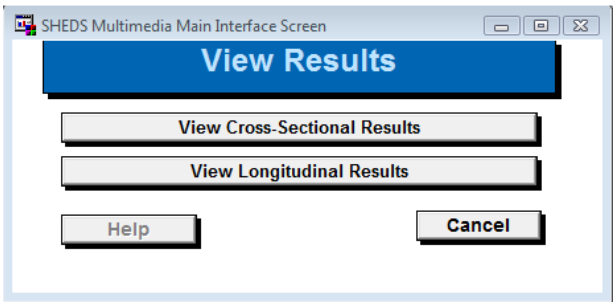


Figure 5-28. The View Results Screen.

5.9.1 The View Cross-Sectional Results Window

The View Cross-Sectional Results window is used to view the summary datasets that are generated using the Pre-process output screen. This screen has two sections, the control section and the display window. The control section (Figure 5-29) contains the widgets and menus that control the creation of the tables and figures. The display window is directly beneath the control section; it is the area of the screen where the selected figure or table is displayed. After the user selects the desired settings from the control section, he or she can select the "Update Display" button to render the figure or table in the display window. Selecting the "Print the Figure" button sends whatever figure or table is currently displayed to the default printer.

There are several widgets and menus that are used to select the figure or table to display. The "Set Output Library" button is used to designate which SAS library contains the output data of interest. By default, this is the main SHEDS-Dietary library named "output." Clicking this button will bring up a SAS library dialog box, in which the user may select other available SAS libraries, if desired.

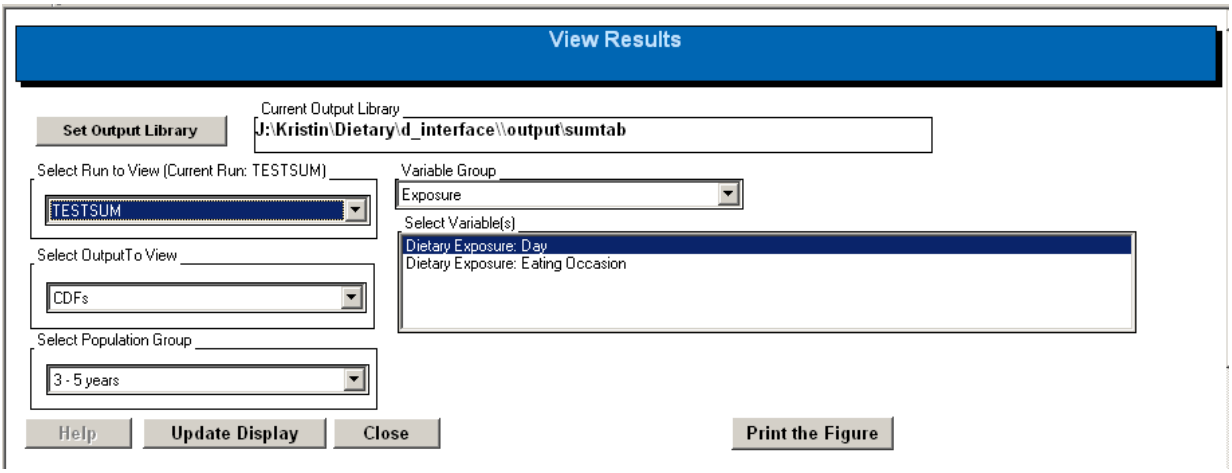


Figure 5-29. The View Cross-Sectional Results Control Section

The "Select Run to View" menu will be populated with a list of all of the runs whose outputs are saved in the current run library. By default, the first run in the list will be selected. As is normal in SHEDS, the output is selected by choosing the prefix for the run of interest.

The "Select Output to View" menu provides 5 different methods of visualizing the results of a model run. These output types are:

- **CDFs.** Plot cumulative distribution functions for one or more exposure or dose variables.
- **Exposure: Percentile Table**. Display a table containing selected population statistics for one or more exposure variables.
- **Exposure and %APAD: Summary Table.** Display a table containing percentiles and statistics for both exposure and % APAD.
- **Contribution by Commodity: Bar or Pie Chart**. Plot the contribution of each food commodity to either the amount of food or chemical consumed, either in bar or pie chart format.
- **Contribution by Commodity: Summary Table**. Display a table listing the contribution of each food commodity to either the amount of food or chemical consumed.

These output types are defined in detail (with examples) in the next five subsections.

For each of the above output types, the population group of interest must be set using the Select Population Group Menu. The population groups available are only those that were included in the run. If either Exposure: Percentile Table and Exposure and %APAD: Summary Table is

selected as the output to view, there will an All Groups option available and the resulting table will include entries for all of the population groups in the run. All the other output types can only display one population group at a time.

The last two menus in the control section of the screen are the Variable Group and Select Variable(s) menus. These control which variables are displayed on the current figure or table. The contents of these menus will differ for each output type; they are discussed below.

When viewing a figure, a "Print Figure" button will be visible. Clicking this button will print a copy of the current figure to the default printer. When viewing a table, a "Print to File" button is visible. This button can be used to save the current table in *.csv format. The table can also be printed to the default printer by right-clicking on the table and selecting "Print."

5.9.2 CDFs

By selecting the CDFs option on the Select Output to View menu the user can plot cumulative distribution functions of exposure and dose variables. Multiple CDFs (exposure or dose variables) can be displayed at one time.

The user first selects either Exposure or Percent Acute Population Adjusted Dose from the Variable Group menu. This selection will populate the Select Variable(s) menu with either a list of exposure or %APAD variables. For exposure, the available variables are:

- Dietary Exposure: Day
- Water Exposure: Day
- Combined Exposure: Day
- Dietary Exposure: Eating Occasion
- Water Exposure: Eating Occasion
- Combined Exposure: Eating Occasion

For % APAD, the available variables are:

- Dietary % APAD: Day
- Water % APAD: Day
- Combined % APAD: Day
- Dietary % APAD: Eating Occasion
- Water % APAD: Eating Occasion
- Combined % APAD: Eating Occasion

One or more of these variables are then selected from the Select Variable(s) menu. The user also designates the age group of interest using the Select Population Group menu, and then updates the display window by clicking the Update Display button.

An example of a CDF plot is given in Figure 5-30. This CDF plot contains three exposure variables (Dietary Exposure: Day, Water Exposure: Day, and Water Exposure: Eating Occasion) for children 3-5 years.

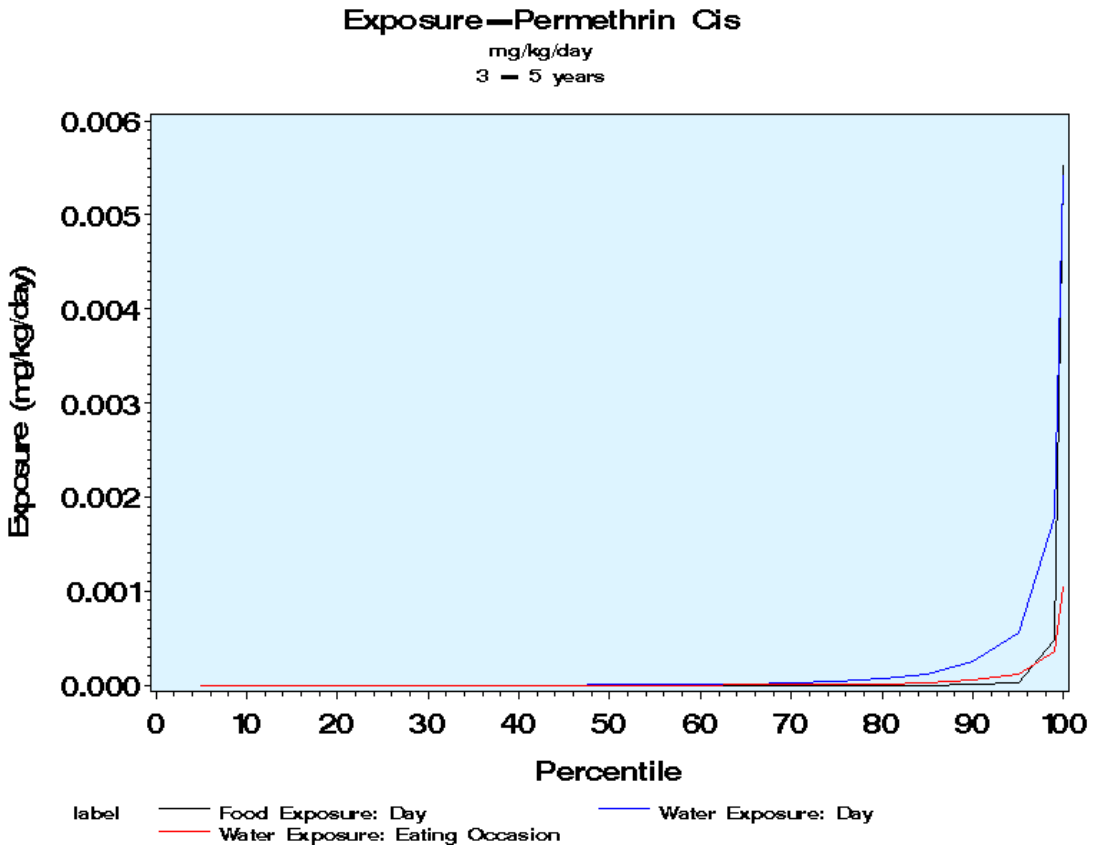


Figure 5-30. Example of a CDF Plot Created with View Results

5.9.3 Exposure: Percentile Table

The user can create a table of exposure statistics by selecting Exposure: Percentile Table from the Select Output to View menu. One or more exposure variables can be selected for inclusion in the table via the Select Variable(s) menu. The available variables are:

- Dietary Exposure: Day
- Water Exposure: Day
- Combined Exposure: Day
- Dietary Exposure: Eating Occasion
- Water Exposure: Eating Occasion
- Combined Exposure: Eating Occasion

One or more of these variables are then selected from the Select Variable(s) menu. The user also designates the age group of interest using the Select Population Group menu. For this output type, the user can choose to include all available population groups in the table by selecting All Groups from the menu. The table is created by clicking the Update Display button.

This type of output table includes the following information (columns):

- Exposure Type: Food (Dietary), Water, or Combined
- Exposure Category: Daily or Eating Occasion
- Age Group: One or more Population age groups as defined using the Select Population Group menu
- Sample size: number of simulated persons (number of person days = number of daily food diaries times the number of interactions runs) in age group
- Mean, Standard Deviation, Median, and 5th, 25th, 75th, 95th and 99th percentiles: statistics of the corresponding exposure variable for age group

An example of an exposure percentile table is given in Figure 5-31. In this example, daily food (dietary) and water exposures are given for all population groups.

	Exposure Type	Exposure Category	Age Group	sample size	Mean	Standard Deviation	Median	5th Percentile	25th Percentile	75th Percentile	95th Percentile	99th Percentile
1	Dietary	Daily	U.S. Population	82428	8.5E-07	1.7E-04	3.3E-07	7.3E-09	6.7E-08	1.0E-06	3.2E-06	6.9E-06
2	Dietary	Daily	0 < 1 years	5944	1.1E-06	2.0E-04	1.9E-07	0.0E+00	1.0E-08	7.3E-07	5.9E-06	1.5E-05
3	Dietary	Daily	1 - 2 years	8384	1.9E-06	2.4E-04	3.6E-07	2.9E-08	1.3E-07	1.6E-06	9.5E-06	1.9E-05
4	Dietary	Daily	3 - 5 years	17564	1.2E-06	1.3E-04	3.2E-07	3.6E-08	1.4E-07	9.3E-07	6.3E-06	1.1E-05
5	Dietary	Daily	6 - 12 years	8356	7.3E-07	1.8E-04	2.0E-07	2.4E-08	8.8E-08	5.2E-07	3.8E-06	7.3E-06
6	Dietary	Daily	13 - 19 years	4888	3.9E-07	1.4E-04	9.3E-08	3.8E-09	3.6E-08	2.7E-07	2.0E-06	4.6E-06
7	Dietary	Daily	20 - 49 years	18708	7.9E-07	2.0E-04	3.2E-07	5.6E-09	4.9E-08	1.1E-06	3.0E-06	5.7E-06
8	Dietary	Daily	50+ years	18584	9.5E-07	1.3E-04	6.5E-07	1.1E-08	2.0E-07	1.3E-06	3.0E-06	5.0E-06
9	Dietary	Daily	Females 13 - 49	11752	7.1E-07	1.9E-04	2.0E-07	3.9E-09	4.0E-08	9.5E-07	2.9E-06	5.7E-06
10	Water	Daily	U.S. Population	82428	7.2E-05	3.2E-02	1.3E-06	7.0E-09	1.2E-07	2.4E-05	3.7E-04	1.2E-03
11	Water	Daily	0 < 1 years	5944	1.4E-04	3.1E-02	1.2E-06	0.0E+00	6.5E-08	3.6E-05	7.0E-04	2.4E-03
12	Water	Daily	1 - 2 years	8384	1.0E-04	2.4E-02	1.6E-06	0.0E+00	1.4E-07	3.3E-05	5.3E-04	1.9E-03
13	Water	Daily	3 - 5 years	17564	1.1E-04	2.3E-02	1.9E-06	5.6E-10	1.6E-07	3.6E-05	5.8E-04	1.7E-03
14	Water	Daily	6 - 12 years	8356	7.7E-05	3.4E-02	1.3E-06	6.1E-10	1.2E-07	2.5E-05	3.9E-04	1.3E-03
15	Water	Daily	13 - 19 years	4888	6.1E-05	3.4E-02	9.2E-07	0.0E+00	7.5E-08	1.7E-05	3.3E-04	1.1E-03
16	Water	Daily	20 - 49 years	18708	6.6E-05	4.1E-02	1.2E-06	7.5E-09	1.1E-07	2.1E-05	3.4E-04	1.1E-03
17	Water	Daily	50+ years	18584	7.1E-05	3.0E-02	1.7E-06	2.0E-08	1.5E-07	2.9E-05	3.7E-04	1.1E-03
18	Water	Daily	Females 13 - 49	11752	6.8E-05	3.9E-02	1.3E-06	6.1E-09	1.1E-07	2.3E-05	3.6E-04	1.1E-03

Figure 5-31. Example of an Exposure Percentile Table

5.9.4 Exposure and aPAD: Summary Table

The user can create a summary table of exposure and dose (%APAD) statistics by selecting Exposure and aPAD: Summary Table from the Select Output to View menu. One or more exposure variables (and the corresponding doses) can be selected for inclusion in the table via the Select Variable(s) menu. The available variables are:

- Dietary Exposure: Day
- Water Exposure: Day
- Combined Exposure: Day
- Dietary Exposure: Eating Occasion
- Water Exposure: Eating Occasion
- Combined Exposure: Eating Occasion

One or more of these variables are then selected from the Select Variable(s) menu. The user also designates the age group of interest using the Select Population Group menu. For this output type, the user can choose to include all available population groups in the table by selecting All Groups from the menu. The table is created by clicking the Update Display button.

The Exposure and APAD Summary Table includes the following information (columns):

- Exposure Type: Food (Dietary), Water, or Combined
- Exposure Category: Daily or Eating Occasion
- Age Group: One or more Population groups as defined using the Select Population Group menu
- Sample Size: number of simulated persons in age group
- The 95th , 99th, and 99.9th percentiles

An example of an exposure and APAD Summary Table is given in Figure 5-32. In this example, daily combined exposures are given for all population groups.

Exposure Type	Exposure Category	Age Group	sample size	95th exposure mg/kg/day	99th exposure mg/kg/day	99.9th exposure mg/kg/day	95th %APAD mg/kg/day	99th %APAD mg/kg/day	99.9th %APAD mg/kg/day
Combined	Daily	U.S. Population	82428	3.8E-04	1.2E-03	3.5E-03	188.08	591.20	1732.73
Combined	Daily	0 < 1 years	5944	7.0E-04	2.4E-03	8.3E-03	935.06	3206.39	11021.64
Combined	Daily	1 - 2 years	8384	5.3E-04	1.9E-03	4.6E-03	711.17	2483.24	6117.40
Combined	Daily	3 - 5 years	17564	5.8E-04	1.8E-03	5.5E-03	771.49	2338.60	7385.55
Combined	Daily	6 - 12 years	8356	3.9E-04	1.3E-03	4.2E-03	518.65	1708.70	5556.37
Combined	Daily	13 - 19 years	4888	3.3E-04	1.1E-03	3.1E-03	163.26	552.84	1544.33
Combined	Daily	20 - 49 years	18708	3.5E-04	1.1E-03	3.1E-03	172.85	534.16	1548.17
Combined	Daily	50+ years	18584	3.7E-04	1.1E-03	3.1E-03	184.38	572.09	1562.46
Combined	Daily	Females 13 - 49	11752	3.6E-04	1.1E-03	3.0E-03	181.46	558.08	1520.58

Figure 5-32. Example of an Exposure and %APAD Summary Table

5.9.5 Contribution by Commodity: Bar Chart or Pie Chart

By selecting the Contribution by Commodity: Bar Chart or the Contribution by Commodity: Pie Chart option on the Select Output to View menu the user can create plots of the contribution of individual food commodities to exposure.

The user selects the desired variable from the Select Variable(s) menu. The available variables are:

- **% Food:** For each food commodity, the percent of total food consumed.
- **% Chemical**: For each food commodity, the percent of total chemical consumed.

Only commodities accounting for greater than 1% of the total food or chemical consumed are included in the graphs.

The user selects one of these variables, and then designates the age group of interest using the Select Population Group menu. The chart is created in the display window by clicking the Update Display.

An example of a Contribution by Commodity Bar Chart is given in Figure 5-33. In this example, the age group of interest was children aged 3-5 years. An analogous pie chart for children 0-1 years is given in Figure 5-34.

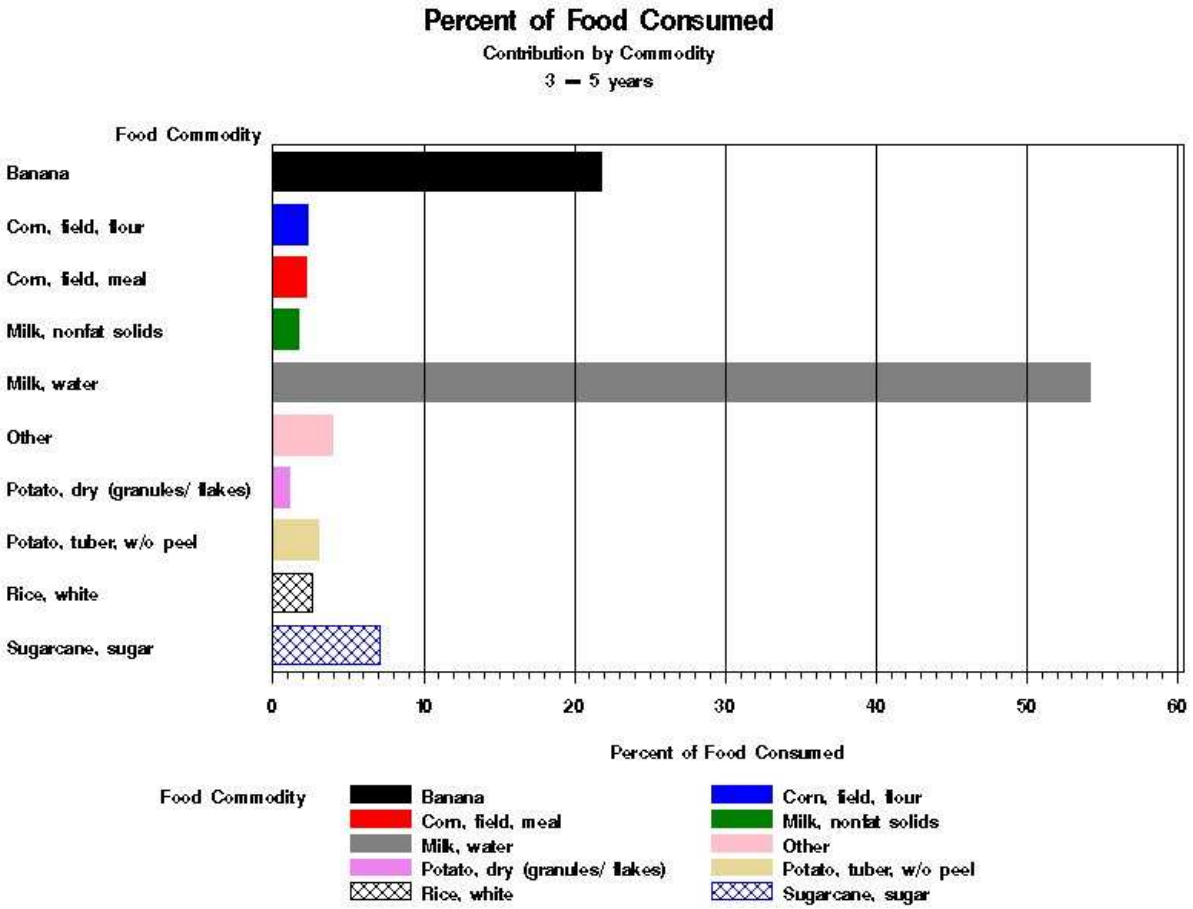


Figure 5-33. Example of a Contribution by Commodity Bar Chart

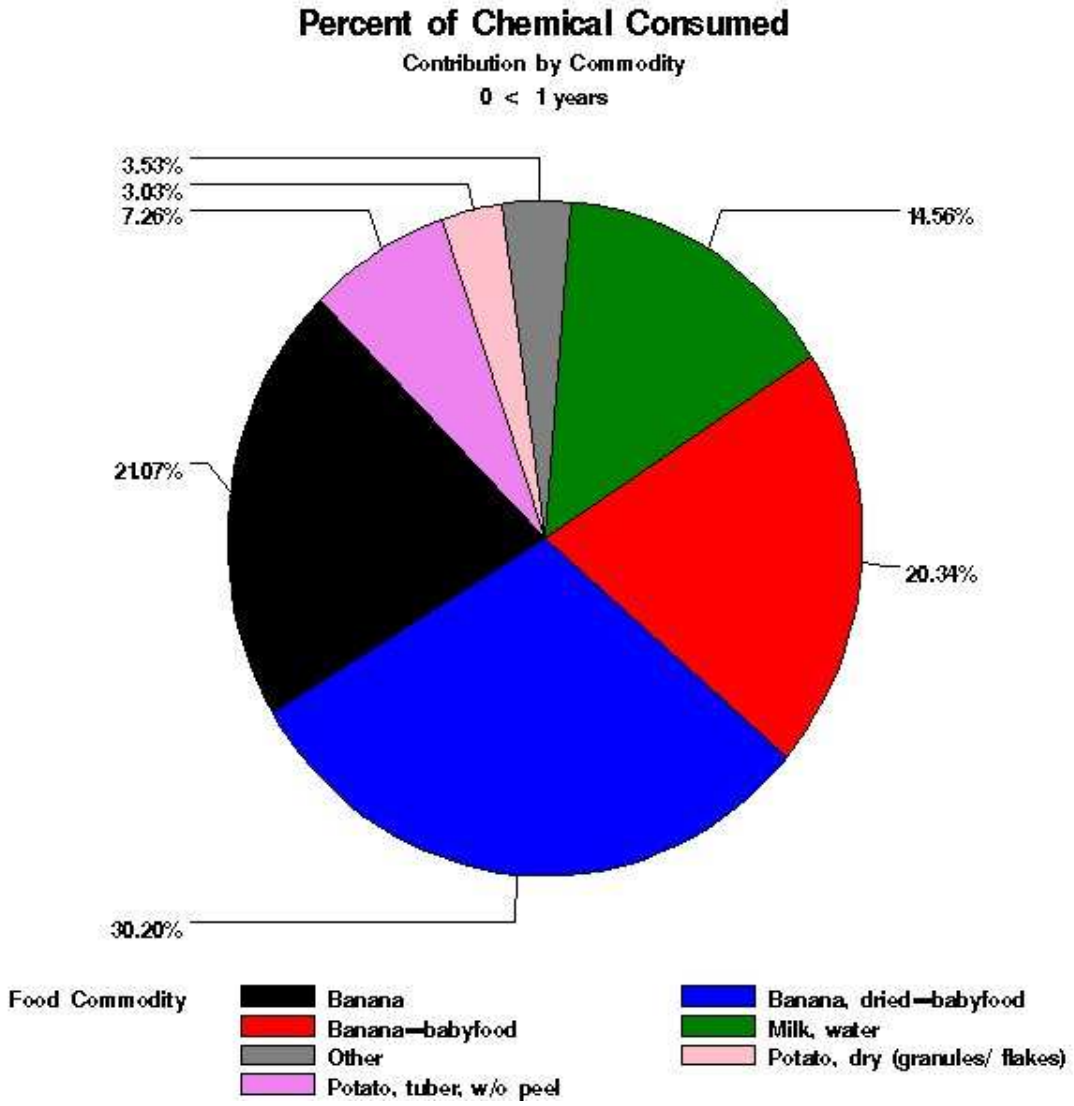


Figure 5-34. Example of a Contribution by Commodity Pie Chart

5.9.6 Contribution by Commodity: Summary Table

The user can create a summary table contribution by commodity statistics by Contribution by Commodity: Summary Table from the Select Output to View menu. For this output type there are no variables to select; information on both the percent of food and chemical consumed are included automatically in the table.

The Contribution by Commodity Summary Table includes the following information (columns):

- Age Group: One or more Population groups as defined using the Select Population Group menu
- Food Commodity
- FCID Code: EPA food commodity ID
- Percent of Food Consumed
- Percent of Pesticide Consumed

An example of a Contribution by Commodity Summary Table for children 6-12 years is given in Figure 5-35.

Age Group	Food Commodity	FCID_Code	Percent of Food Consumed	Percent of Pesticide Consumed
6 - 12 years	Milk, water	27022240	56.31	50.57
6 - 12 years	Banana	95000230	13.97	25.75
6 - 12 years	Potato, tuber, w/o peel	1033000	4.32	9.62
6 - 12 years	Sunflower, seed	20003640	0.48	3.31
6 - 12 years	Potato, tuber, w/peel	1032990	0.78	1.84
6 - 12 years	Potato, dry (granules/ flakes)	1032970	0.39	1.36
6 - 12 years	Corn, field, meal	15001210	4.14	1.12
6 - 12 years	Pumpkin	9023080	0.10	1.11
6 - 12 years	Sugarcane, sugar	95003620	8.71	1.07
6 - 12 years	Milk, nonfat solids	27012230	1.27	0.94
6 - 12 years	Banana, dried	95000240	0.10	0.75
6 - 12 years	Corn, field, flour	15001200	2.63	0.71
6 - 12 years	Plantain	95002830	0.34	0.61
6 - 12 years	Milk, fat	27002220	0.57	0.39
6 - 12 years	Pumpkin, seed	9023090	0.28	0.23
6 - 12 years	Corn, field, starch	15001230	0.74	0.20
6 - 12 years	Coffee, roasted bean	95001150	0.01	0.14
6 - 12 years	Rice, white	15003230	2.51	0.11
6 - 12 years	Potato, chips	1032960	1.10	0.09
6 - 12 years	Rice, flour	15003250	1.06	0.05
6 - 12 years	Coffee, instant	95001160	0.00	0.03
6 - 12 years	Rice, brown	15003240	0.11	0.00
6 - 12 years	Sugarcane, molasses	95003630	0.04	0.00
6 - 12 years	Potato, flour	1032980	0.03	0.00
6 - 12 years	Corn, field, bran	15001220	0.00	0.00
6 - 12 years	Rice, bran	15003260	0.00	0.00

Figure 5-35. Example of a Contribution by Commodity Summary Table

5.9.7 View Longitudinal Results

The longitudinal time series of daily exposures can be visualized using the View Longitudinal Results window. The View Longitudinal Results window (Figure 5-36) is similar in format to the cross-sectional window, in that it contains a control section and a display window. As discussed before, the user may select both an output data library (by default, the Olong library) and a run to view. The variable selection list is populated with the available exposure variables for the loaded run. For a single chemical run, food (dietary) exposure and water exposure (if present) are available. For a cumulative run, food (dietary) and water exposures for each chemical as well as total exposures will be present in the selection list. The user can limit the portion of the simulation to be viewed by selecting a start and ending date.

Each person in the run is listed in the Select Individuals list box. The user can choose a single individual to view by clicking on a single person ID, or view multiple individuals by clicking and dragging within the list box.

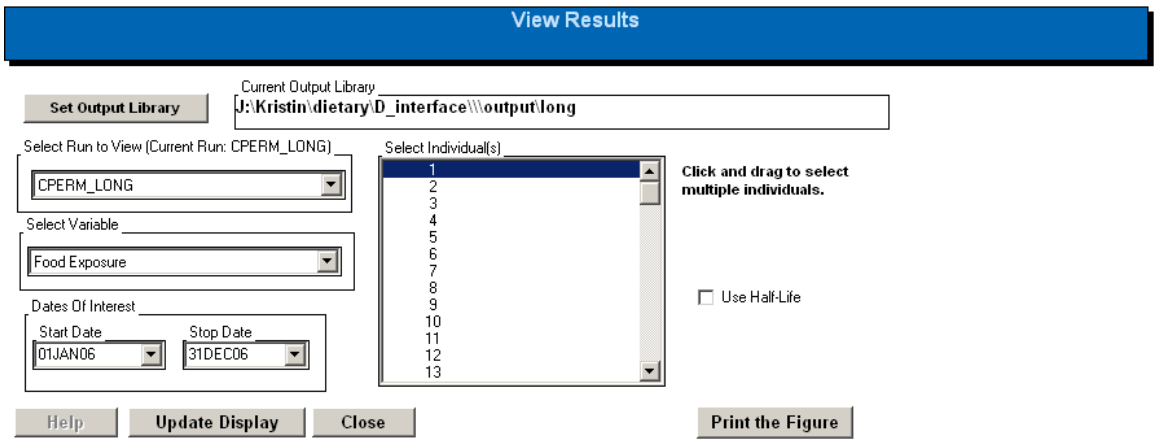


Figure 5-36. The Control Section of the View Longitudinal Results Window

An example of a daily exposure time series is shown in Figure 5-37.

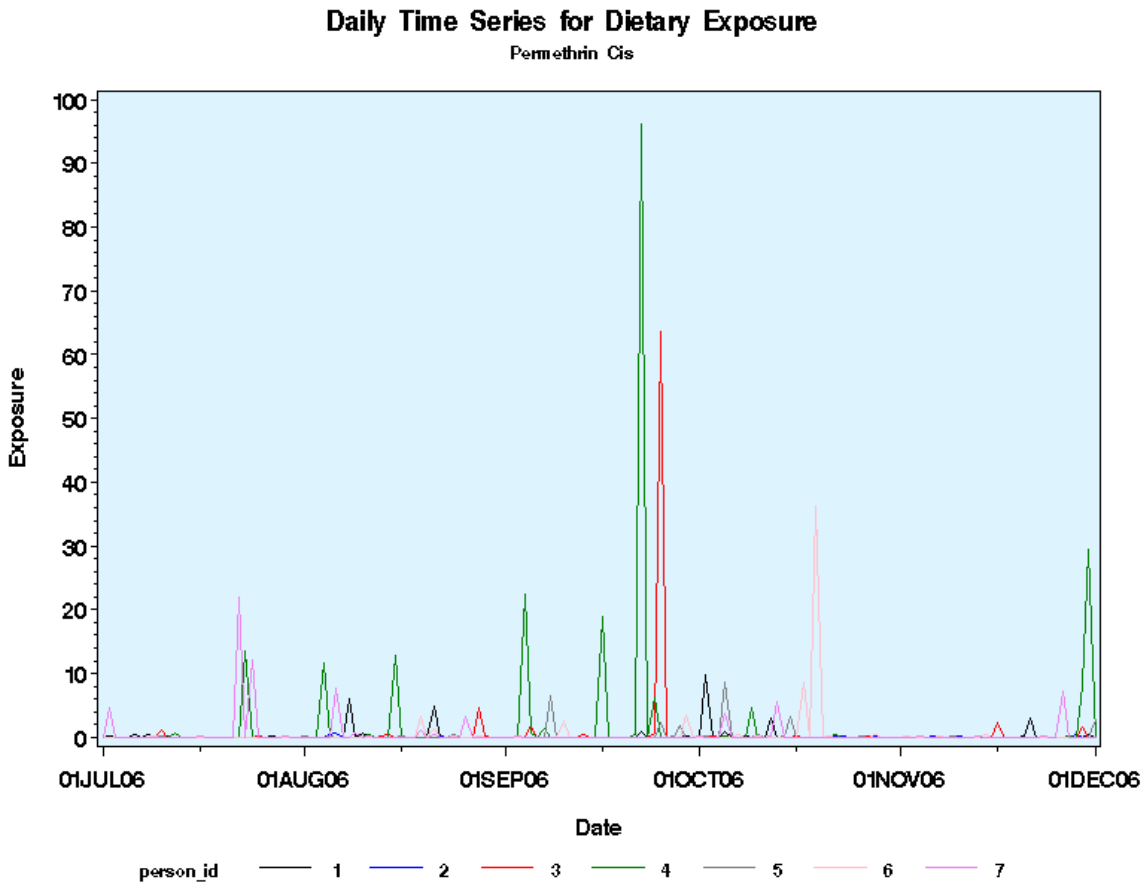


Figure 5-37. A Daily Exposure Time-Series for a Longitudinal Run.

If the "Use Half-Life" button is selected, the time-series of persistent exposure is also plotted on the graph. The user enters a half-life (in hours) and clicks the Update Display button. The persistent exposure will be added to the plot. An example for cis-permethrin using a half-life of 48 hours is shown in Figure 5-38.

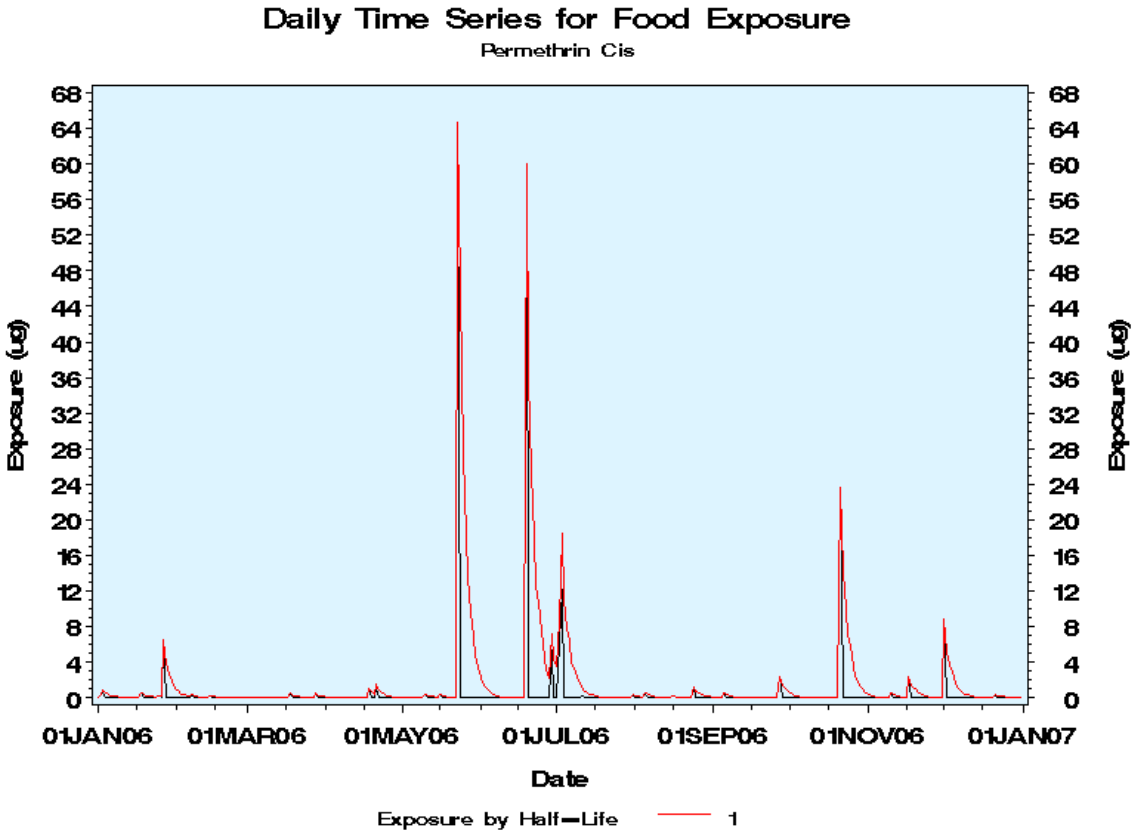


Figure 5-38. A Persistent Exposure Time Series Added to a Longitudinal Plot.

6 PDP Generator

The PDP Generator is a feature that allows the user to create multichemical input files for SHEDS-Dietary using data from the U.S. Department of Agriculture's Pesticide Data Program database. This database contains food residue measurements collected from 1996-present for dozens of chemicals. See the SHEDS-Dietary Technical Manual (Xue et al., 2010) for more information about the PDP database and the information it contains.

The PDP Generator screen is shown in Figure 6-1. The user first selects one or more chemical classes from the Select Chemical Classes to View list box. The chemicals available in the database in these classes are then listed in the Available Chemicals list box. The user then highlights one or more chemicals in the list box and uses the arrow keys to move them to the Chemicals to Use list. NOTE: Although the PDP Generator creates input files for cumulative (multi-chemical) runs, it is a valid choice in SHEDS-Dietary to perform runs in cumulative mode that contain a single chemical. Therefore, creating files with only one chemical is valid.

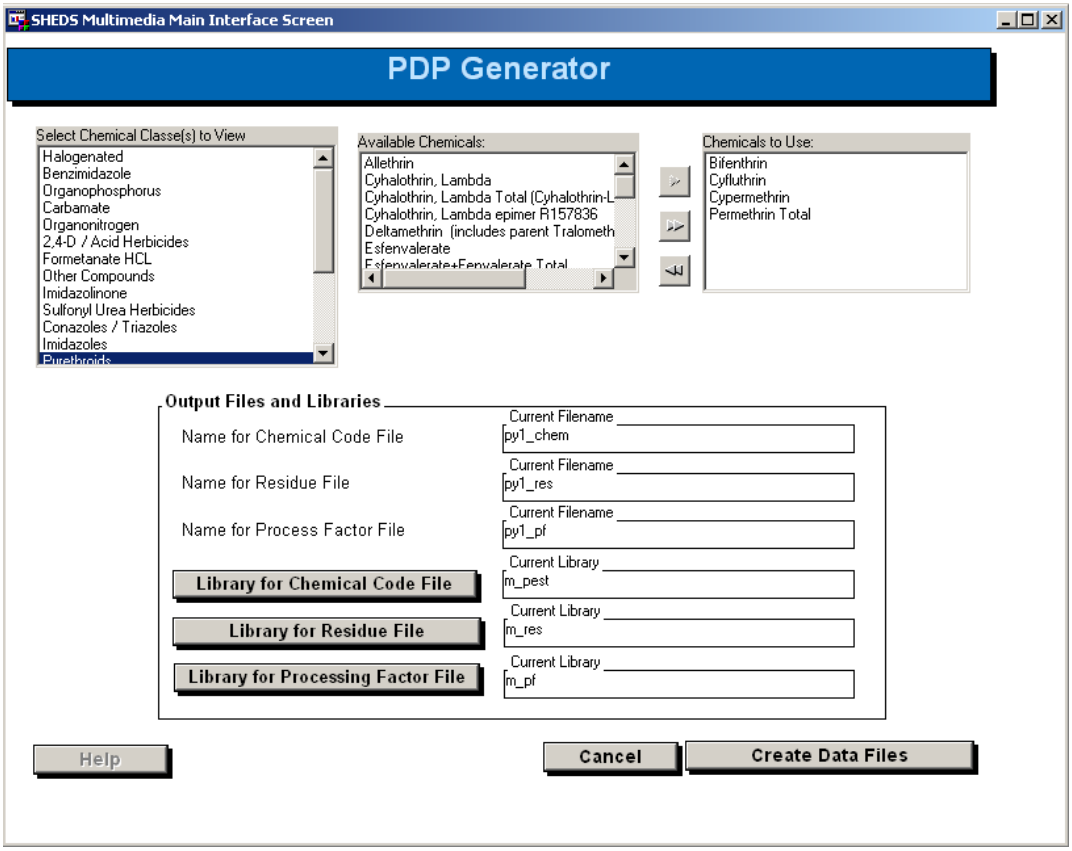


Figure 6-1. The PDP Generator Screen.

Once the list of chemicals to use is created, the user must then select names and locations for the three output files that the PDP generator creates:

1. A Chemical Code file. Chemical code files are discussed in Section 5.4 and Appendix A. By default, the code file is saved in the default SHEDS-Dietary multichemical chemical code library (m_pest).

2. A Residue file. Multichemical residue files are discussed in Section A.2.3. By default, the residue file is saved in the default SHEDS-Dietary multichemical residue library (m_res).

3. A Processing Factor file. Processing Factor files are discussed in Section A.2.5. By default, the residue file is saved in the default SHEDS-Dietary multichemical processing factor library (m_pf).

These files can then be used as input to future SHEDS-Dietary runs. When a multichemical run is created using these files, the user will also need to designate a bridge file. The bridge file B_py_bridge (that is included with the SHEDS-Dietary release) may always be used with files created with the PDP Generator.

WARNING: When using these files in a run, these three files must all be used together. These files may not be compatible with other files generated outside of SHEDS or made with different PDP generator settings. Therefore, it is a good idea to name them in such a way (with a prefix, for example) that makes it easy to recall which files are compatible.

7 Example Case Studies

The following case studies are meant to guide the user completely through multiple examples of running SHEDS-Dietary from start to finish. Each step in the examples are described briefly, and illustrated with accompanying screenshots. Any necessary input files are included with SHEDS-Dietary or created within the case study steps. The main run options for the included case studies included are as follows:

Case Study 1: Arsenic (As). Single chemical, cross-sectional run. Food exposure only. Convert food residue files via Bridge File.

Case Study 2: Cis-Permethrin. Single chemical, cross-sectional run. Food exposure only. Use final residue file.

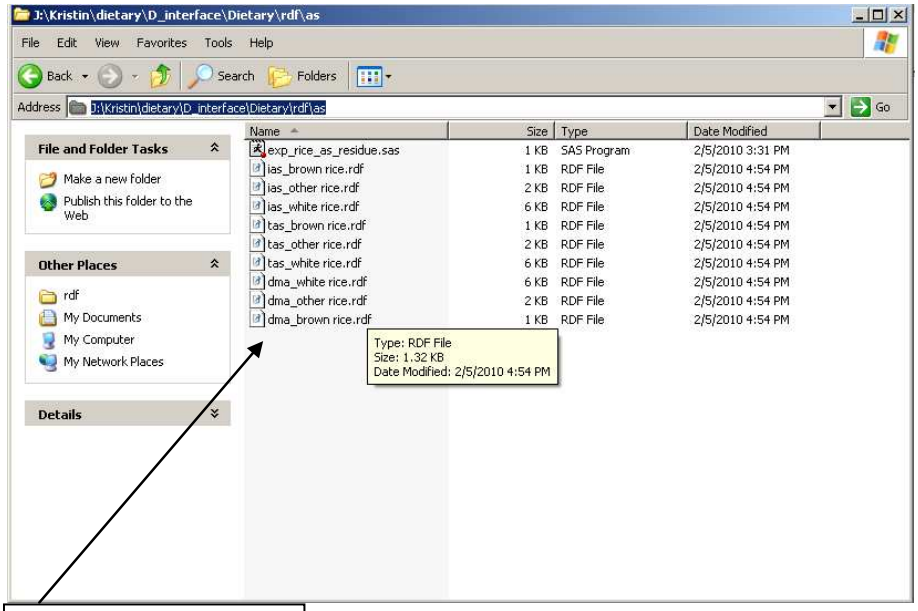
Case Study 3: Cis-Permethrin. Single chemical, longitudinal run. Food exposure only. Use final residue file.

Case Study 4: Pyrethroids. Multi-chemical, cumulative, cross-sectional run, using input files made with the PDP Generator. Food exposure only. Use final residue file.

7.1 Case Study 1: Arsenic

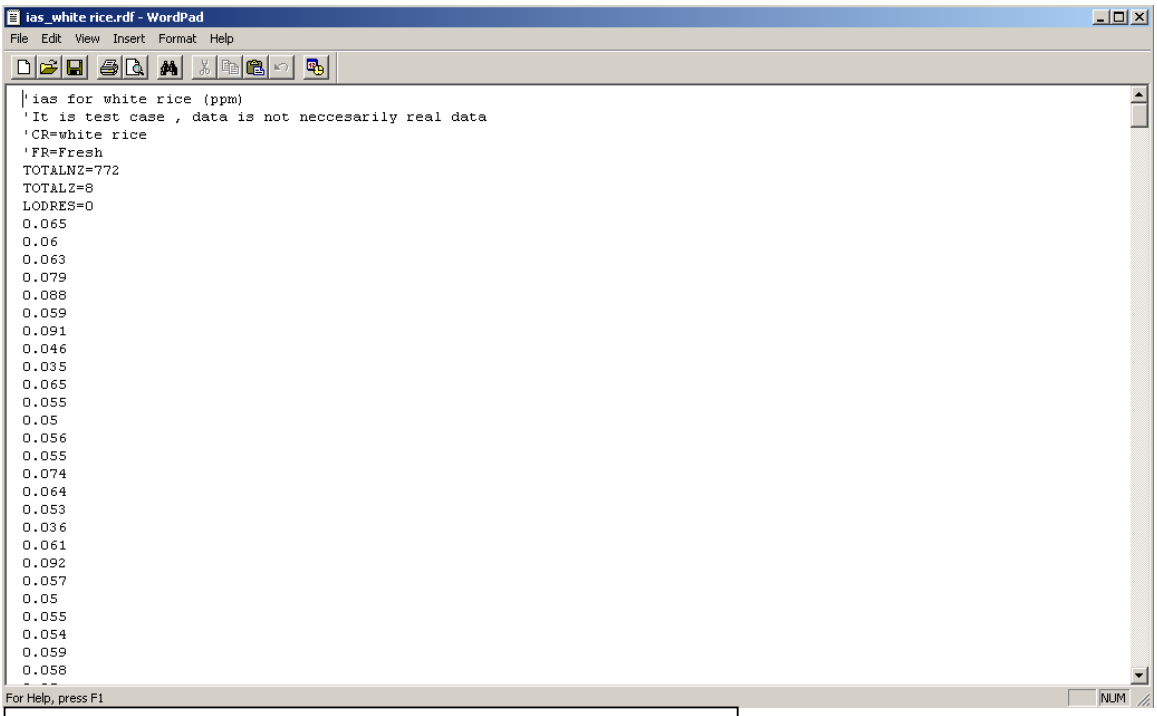
The first case study demonstrates the steps in creating a single chemical, cross-sectional run for arsenic. Food exposure is considered, and food residue files are converted via a Bridge File. The steps in setting up the run are enumerated below, followed by a corresponding screenshot.

1) Create the residue files of interest for the chemical. In this example, residue files were created for different rice food commodities using a plain-text editor. Store all the residue files in a single directory, under the SHEDS main directory tree. These files are included in the SHEDS-Dietary package in the directory .\ D_interface\Dietary\rdf\as.



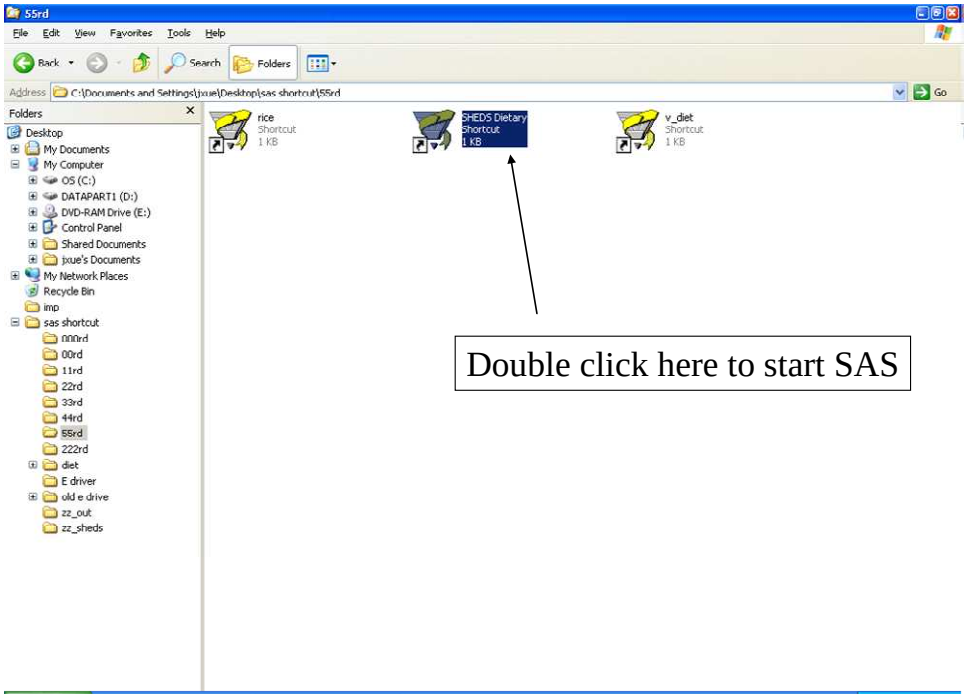
Residue Files

2) An example residue file is shown for white rice. The files follow the format described in detail in Section 5.5.2 of this manual.

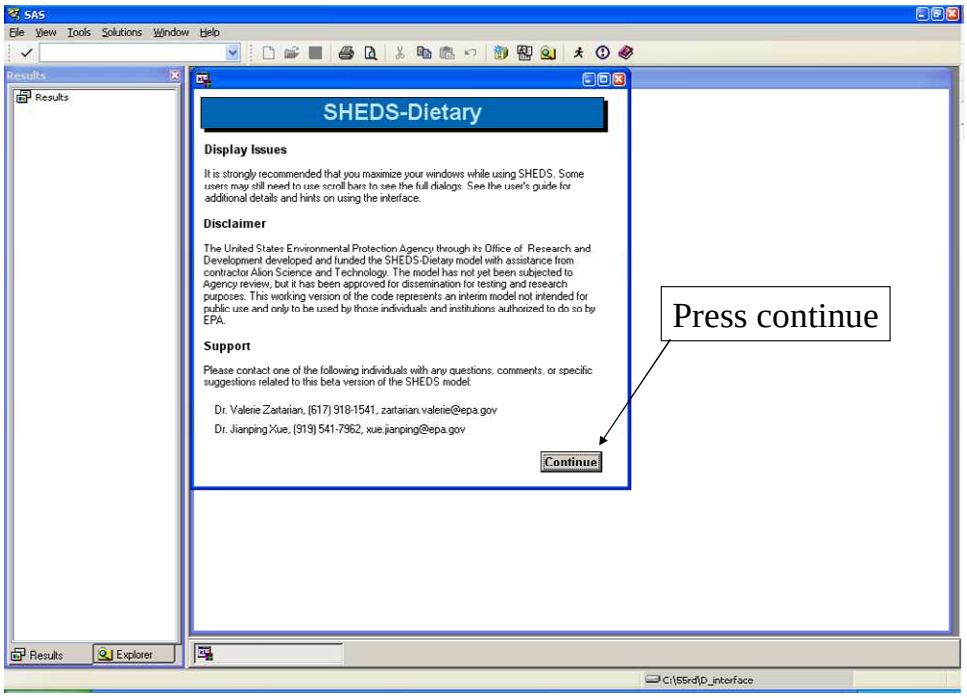


Example RDF file for white rice for As

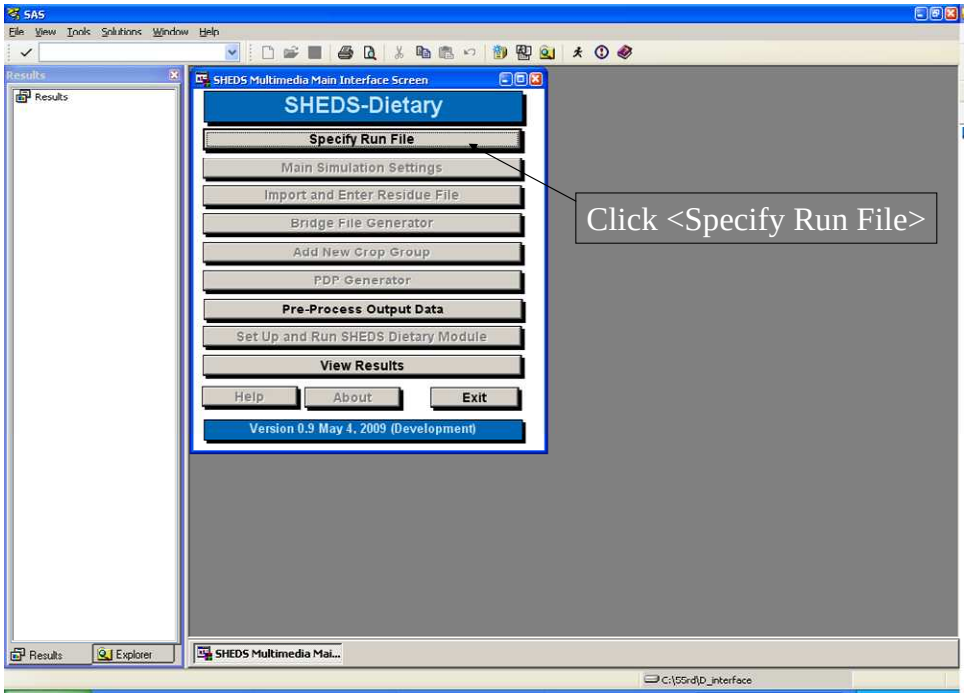
3) Initiate a SHEDS-Dietary session by double-clicking the SHEDS-Dietary SAS shortcut icon.

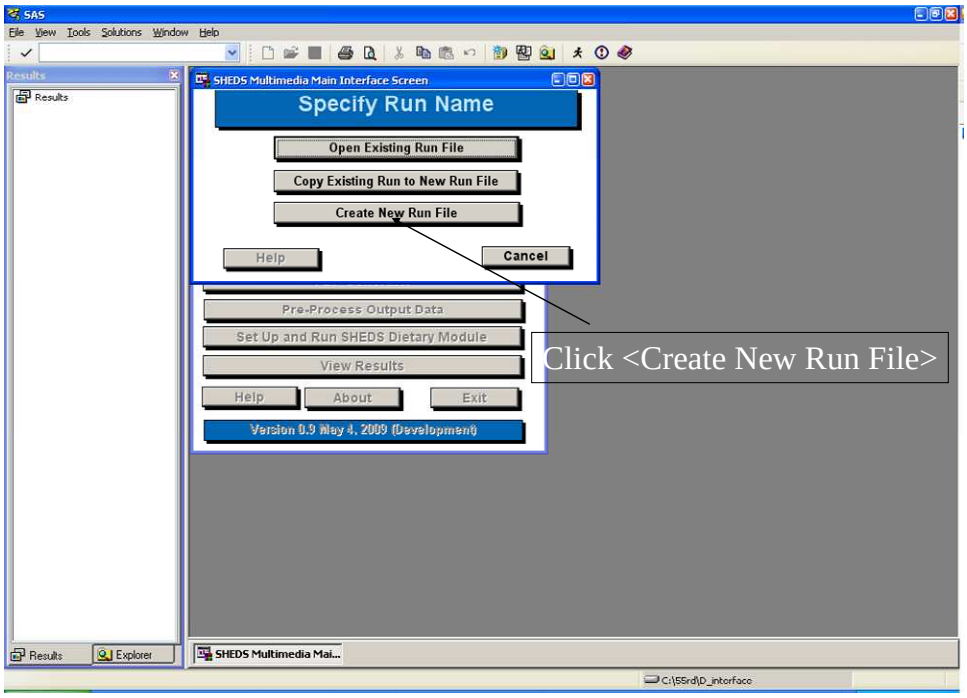


4) The SHEDS disclaimer screen appears first; select <Continue> to proceed to the main SHEDS screen.

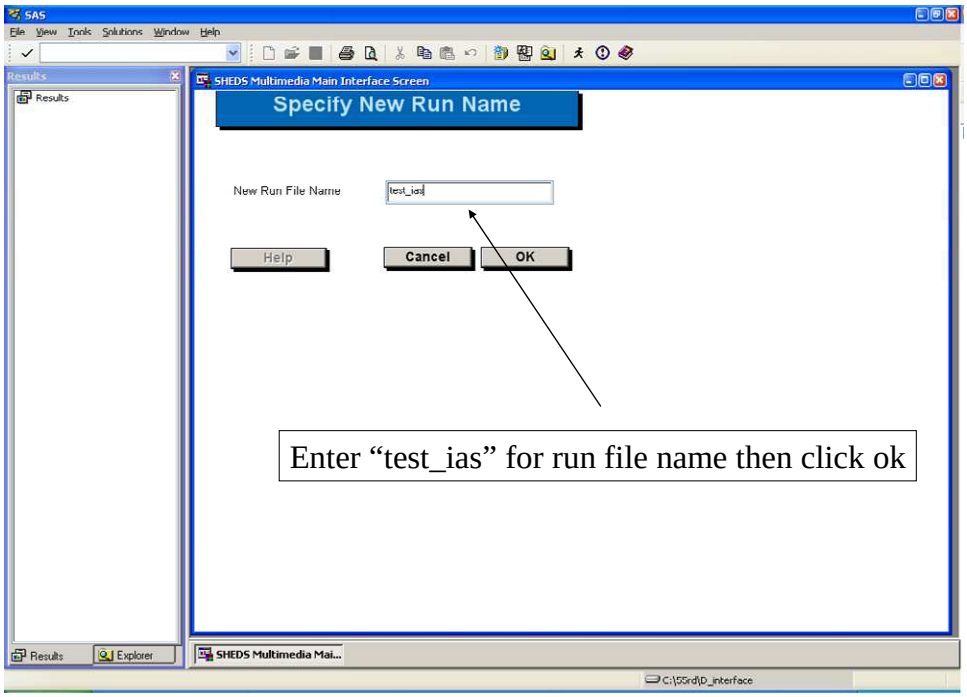


5) Select <Specify Run File>,<Create New Run File> to initiate the creation of a new run for arsenic.



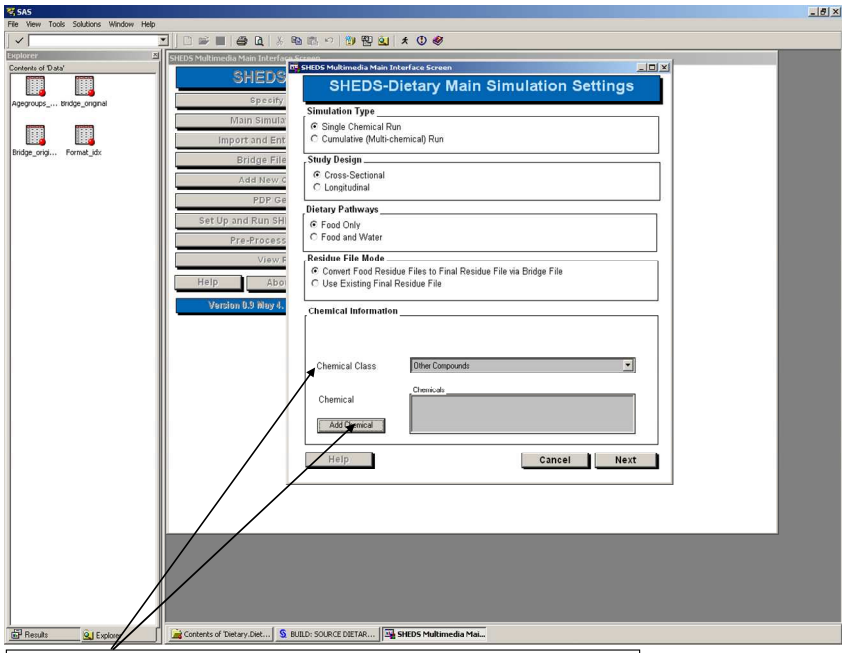


6) Enter the name of the new run as “test_ias” when prompted.

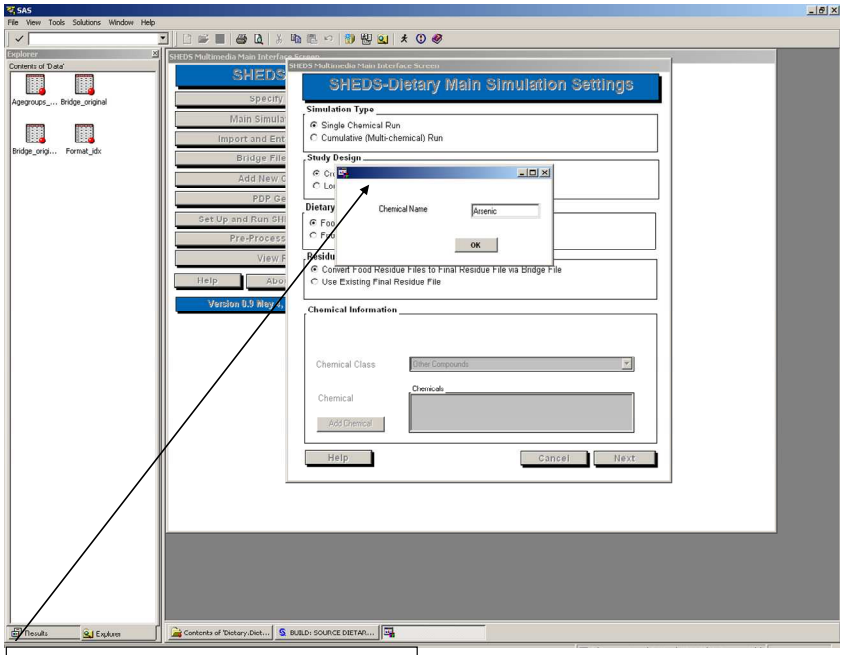


7) The Main Simulation Settings button will now be enabled. Select it and the Main Simulation Settings screen will appear. Select “Other Compounds” for the Chemical Class in the

Chemical Information box. Click the “Add Chemical” button. Enter “arsenic”. Click OK. Keep all other default settings and select <Next>. This will define a single chemical, cross-sectional simulation of food exposure. In this run, food residue files will be linked via a Bridge File to individual food commodities.

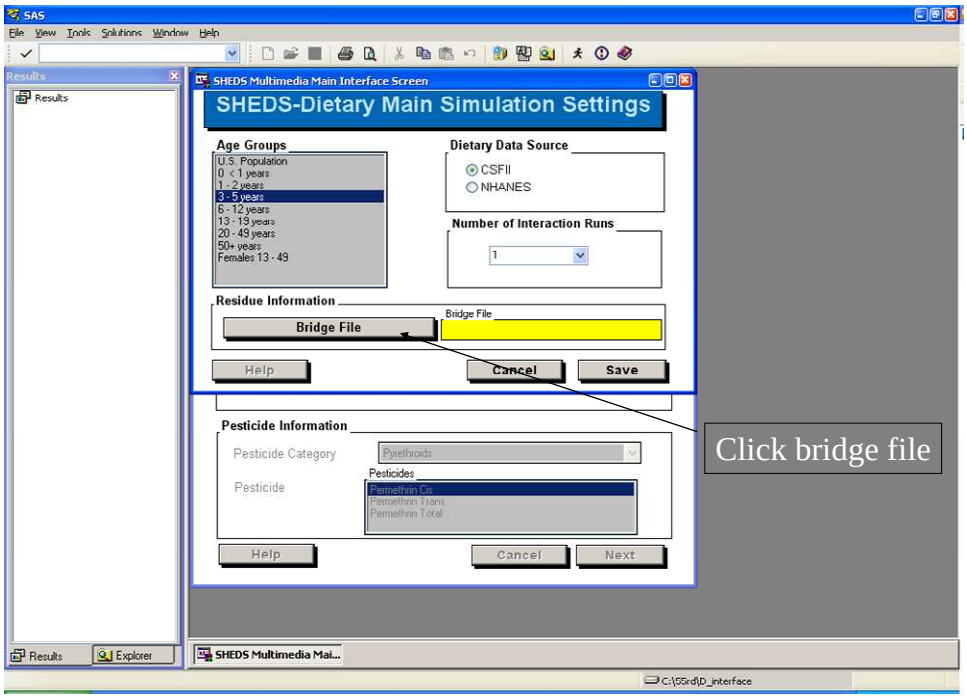


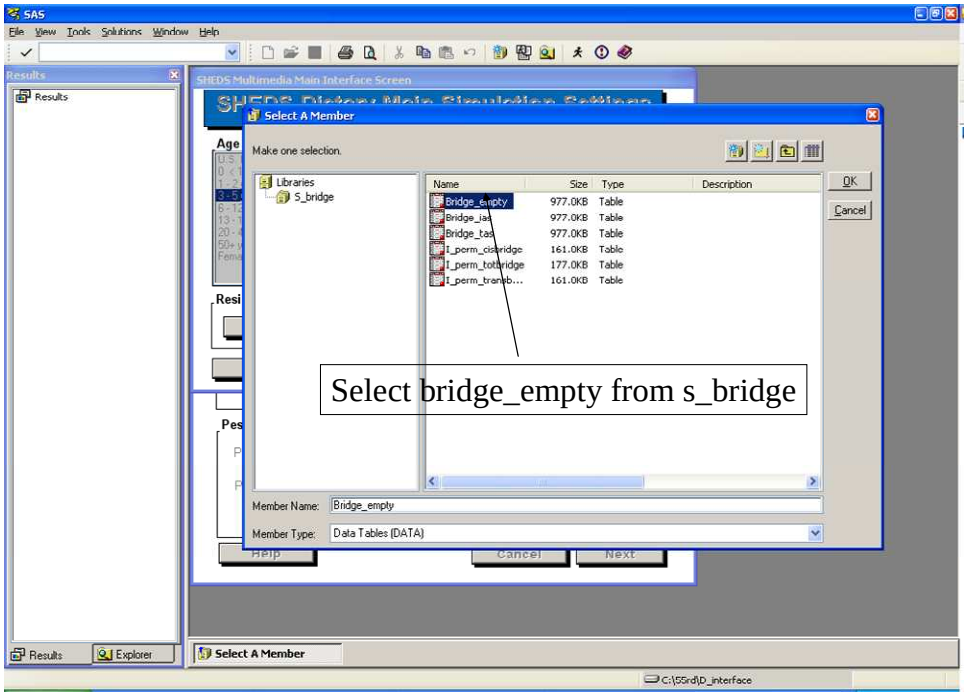
Select “Other Compounds” then click <Add Chemical>



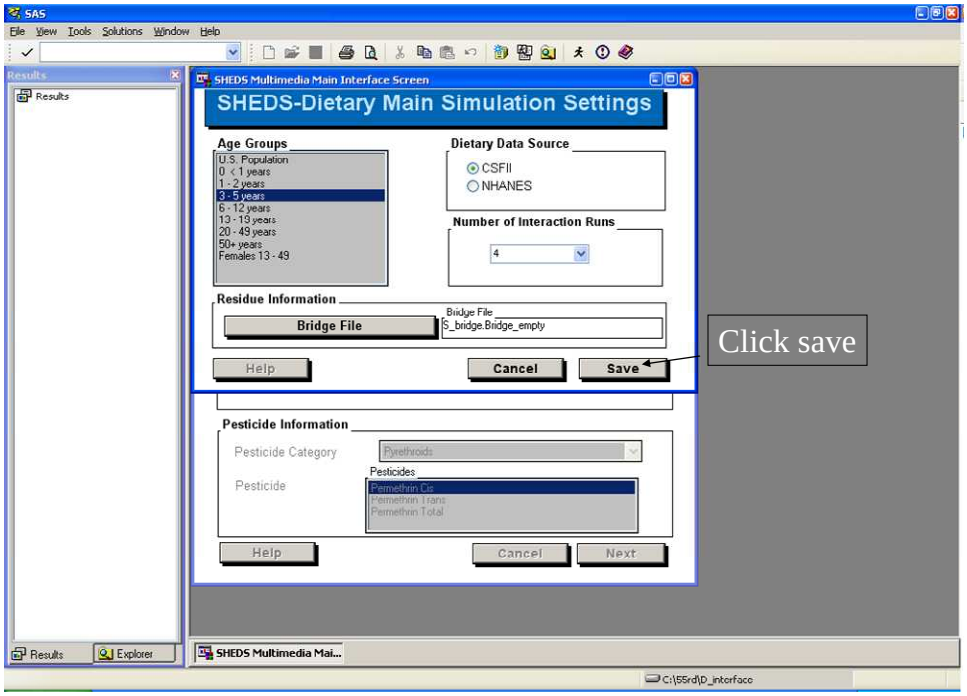
Enter “Arsenic” then click <OK>

8) The second Main Simulation Settings screen appears. Click the Bridge File button to select a Bridge File for the run. Selecting bridge_empty will assign a blank Bridge File to the run.

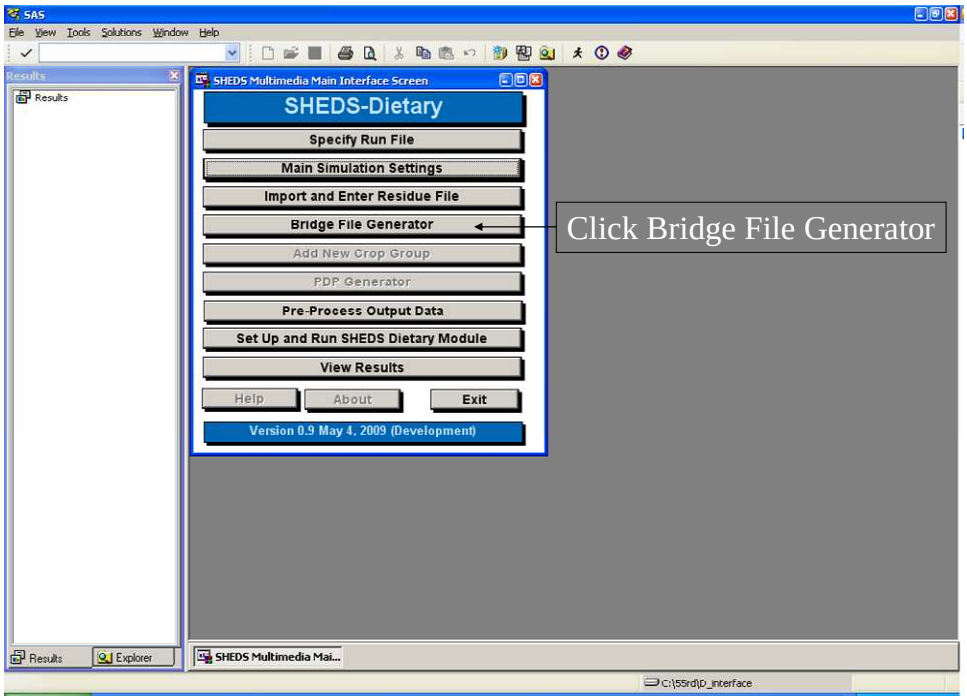


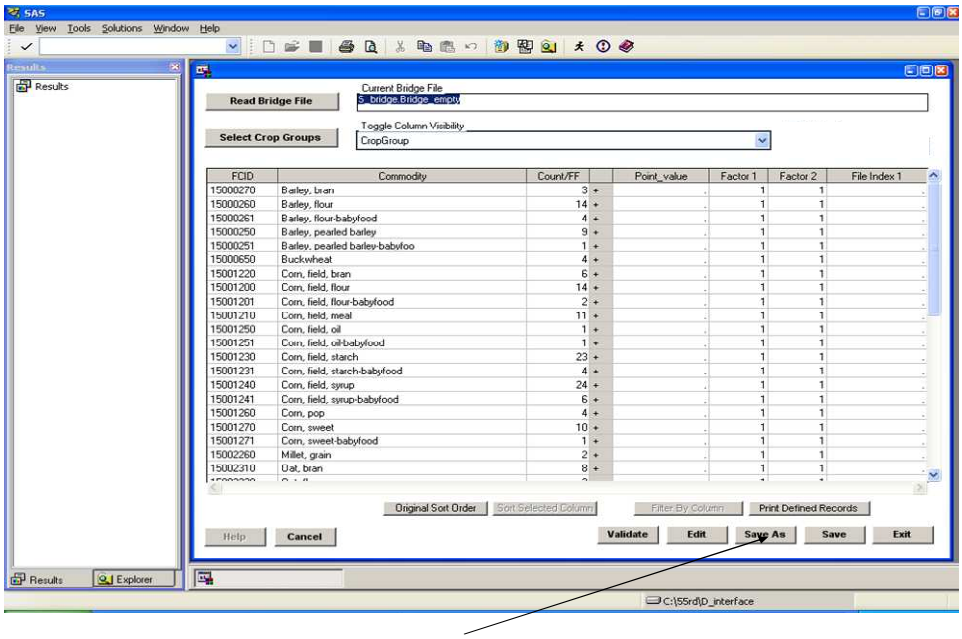


9) Once the Bridge File is selected, return to the settings screen and select 4 as the number of interaction runs and click <Save>.

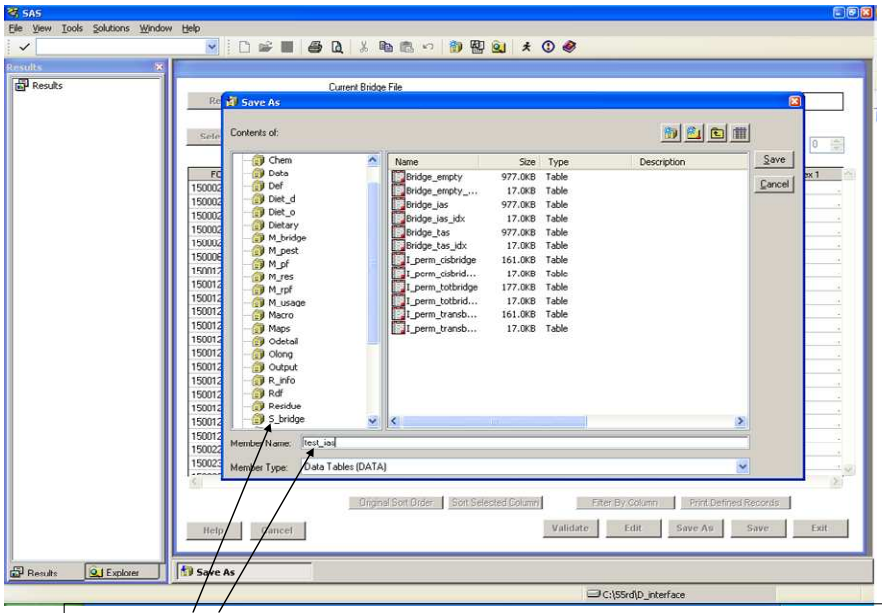


10) When SHEDS returns to the Main Screen, click the Bridge File Generator button. This will open the Bridge File Generator screen, which provides tools for assigning residue files to food commodities. As soon as the Generator screen opens, click <Save As> to save a unique Bridge File for arsenic, called “test_ias” in the S_bridge library. All Bridge Files for single chemicals runs must be saved in this directory.



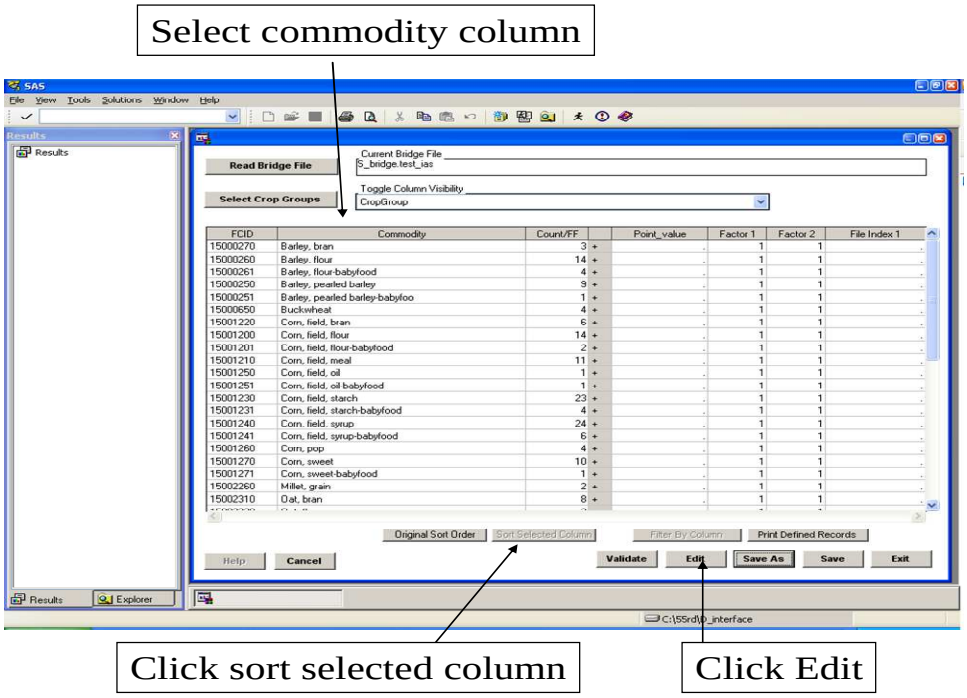


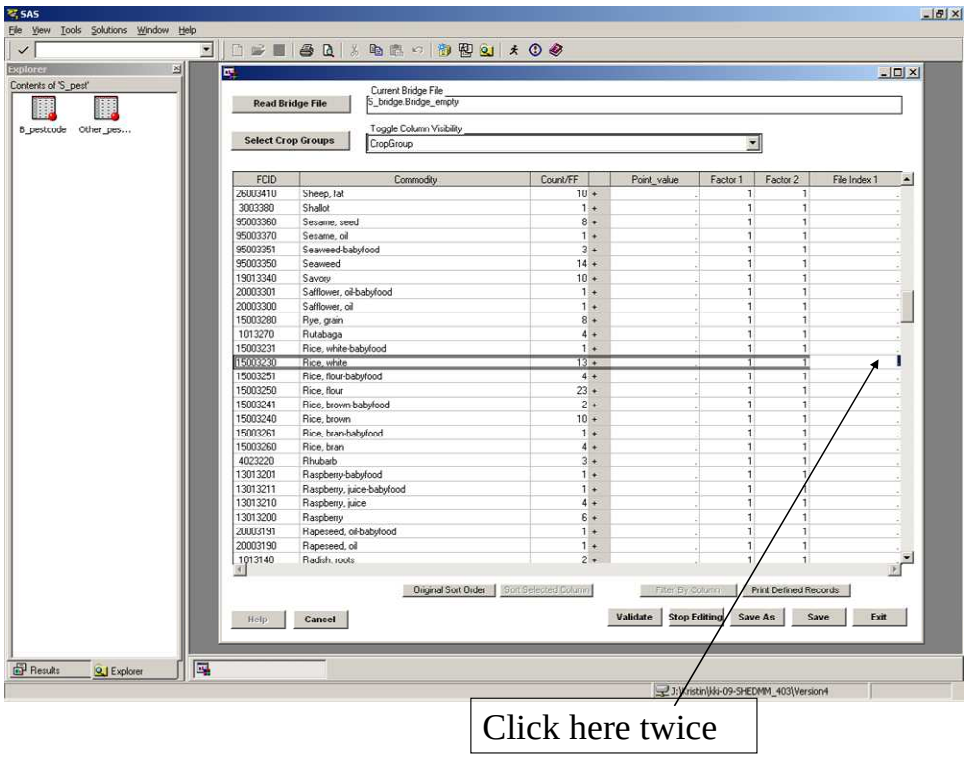
Click Save as



Find library s_bridge and enter “test_ias” in “Member Name”. Then click Save.

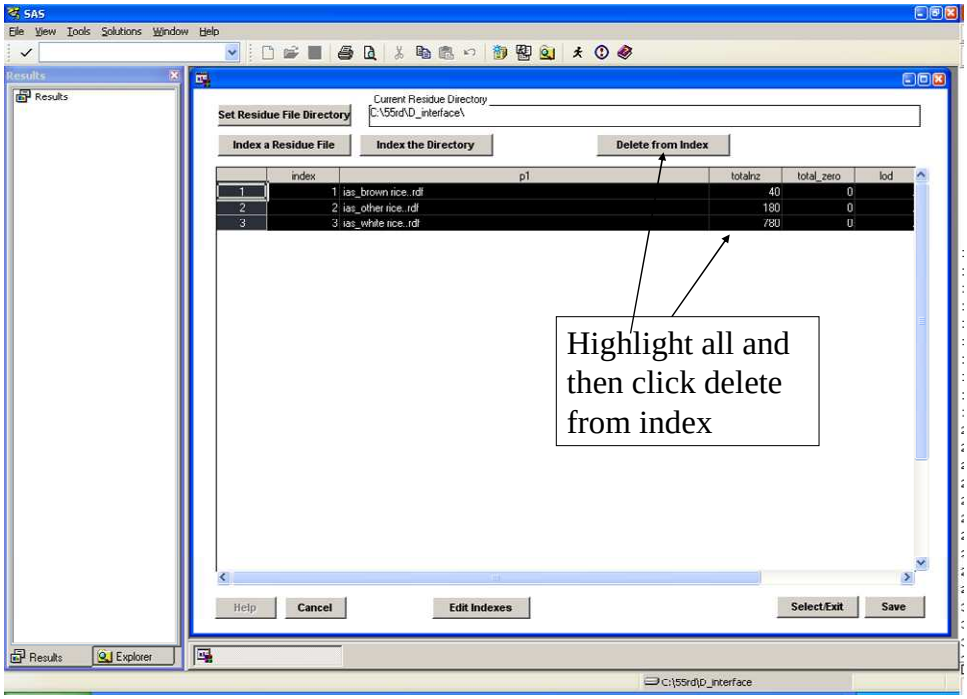
11) Once the Bridge File is saved, the user can begin the process of assigning residue files to commodities. In this case, the rice residue files referenced in 1) will be assigned to various rice food commodities. Select the Commodity column of the Bridge File, and click <Sort Selected Column>. This will bring up the rice commodities near the top of the file for easy editing (you may need to scroll down to see them). Click the Edit Button at the bottom of the screen to allow editing of the Bridge file. Double-click in the File Index 1 column for white rice, which will bring up the Residue File Index screen.



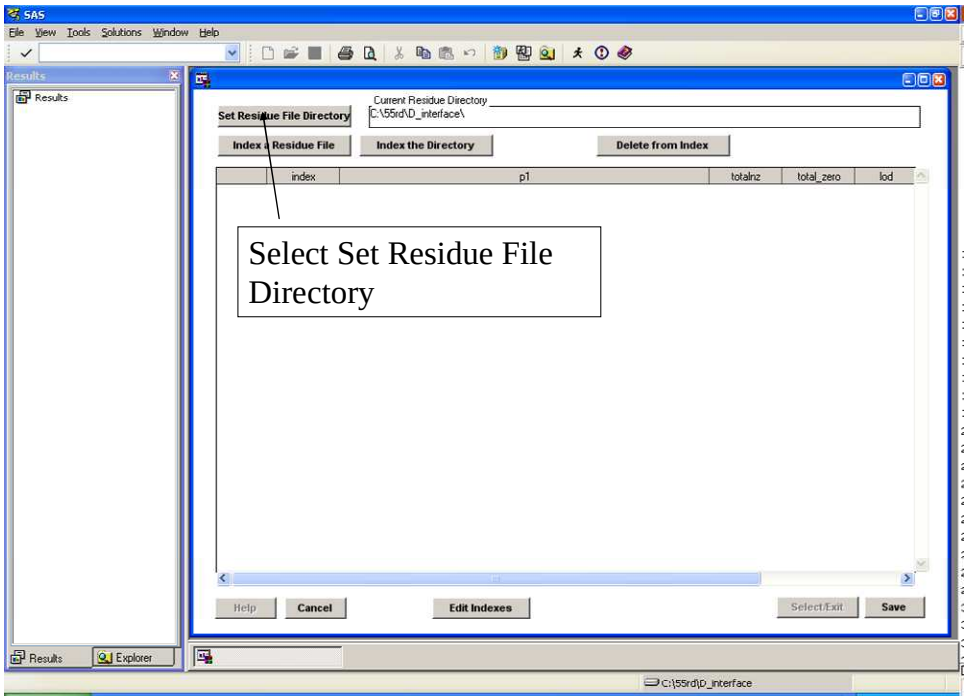


12) The index file should be empty, since the run was started with an empty Bridge File. However, if any residue files are already in the index, they can be deleted by highlighting

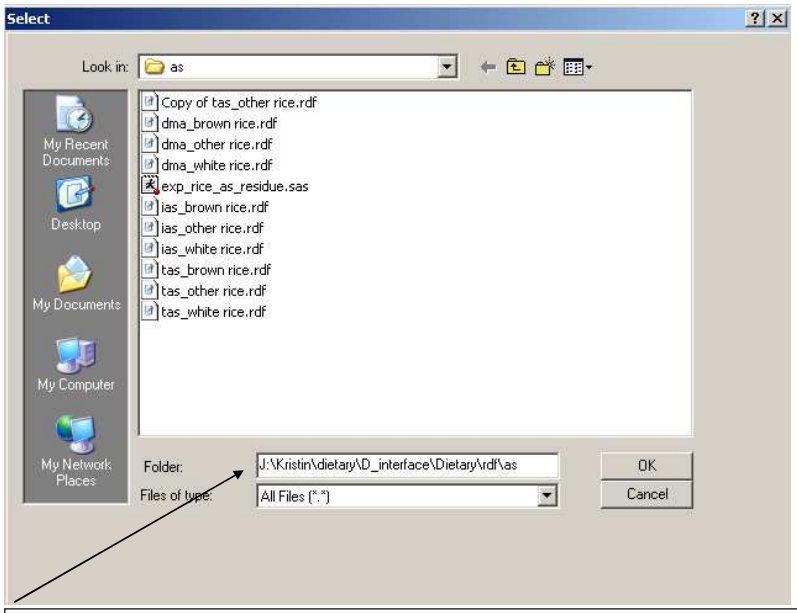
them and selecting <Delete from Index>. This allows the user to index only the residue files they wish to assign to commodities.



13) Select the directory where the arsenic residue files are located by clicking the <Set Residue File Directory> button. The files are located in <install>/Dietary/rdf/as, as defined in Step 1 (the folder name will be different than the one shown in the figure below, since different user's installation folder names may differ).

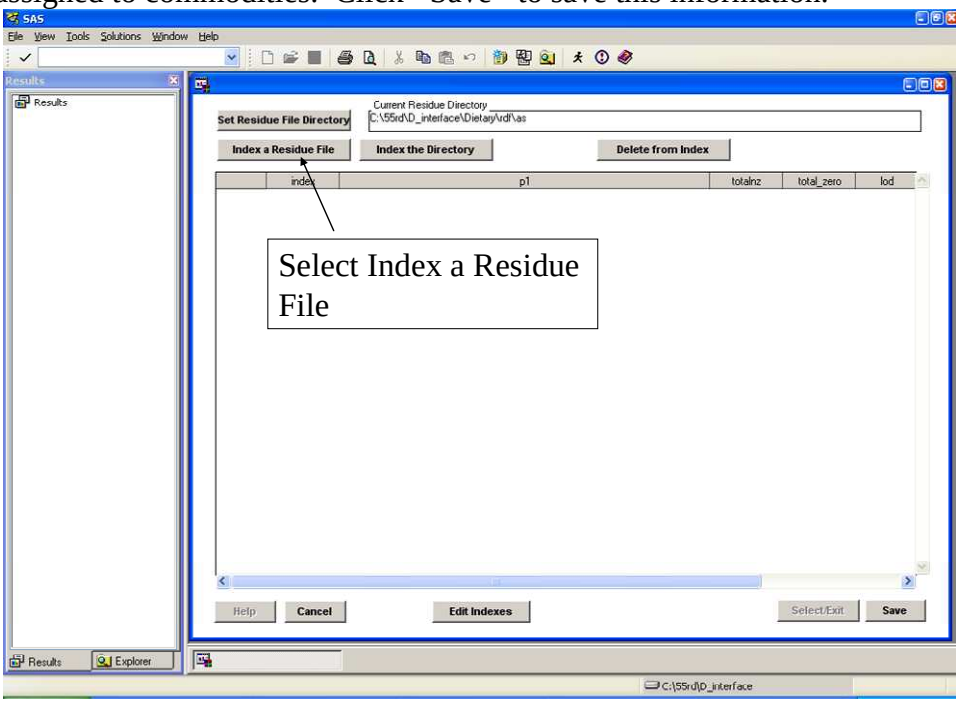


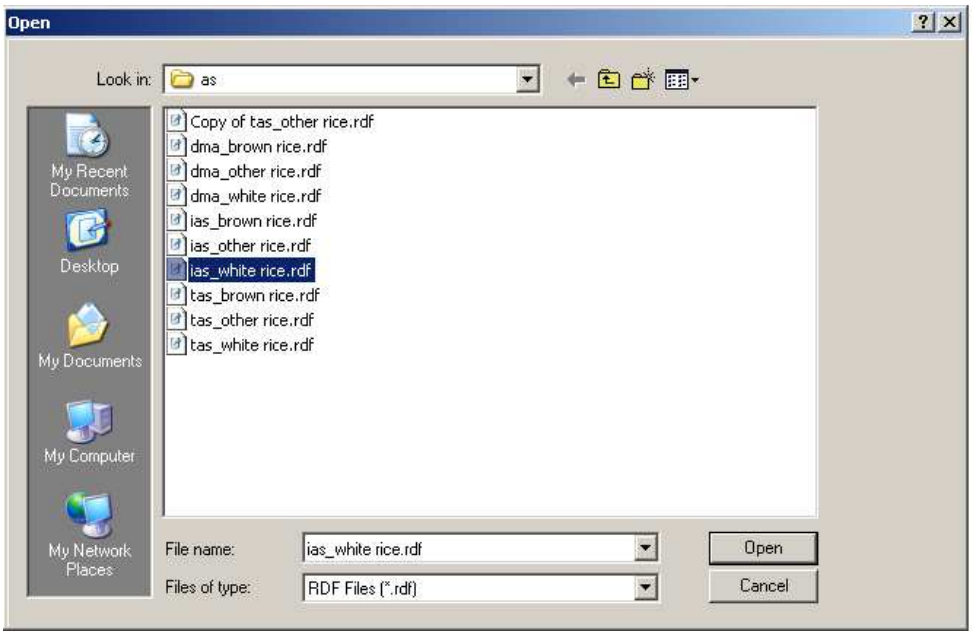
Select Set Residue File Directory

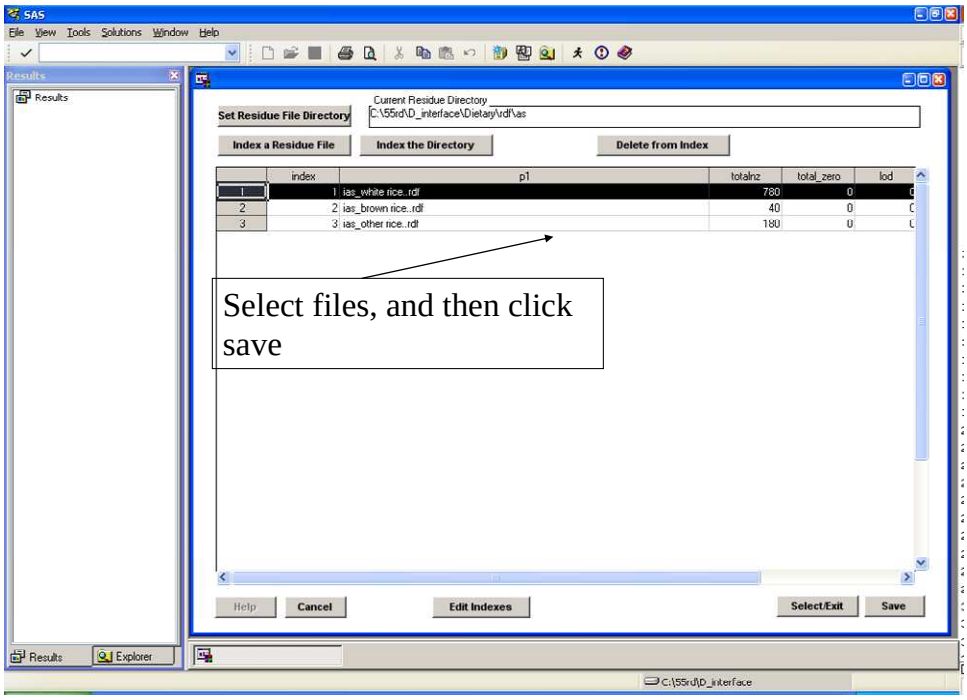


Select the directory .\D_interface\Dietary\rdf\as where "." indicates the SHEDS installation directory.

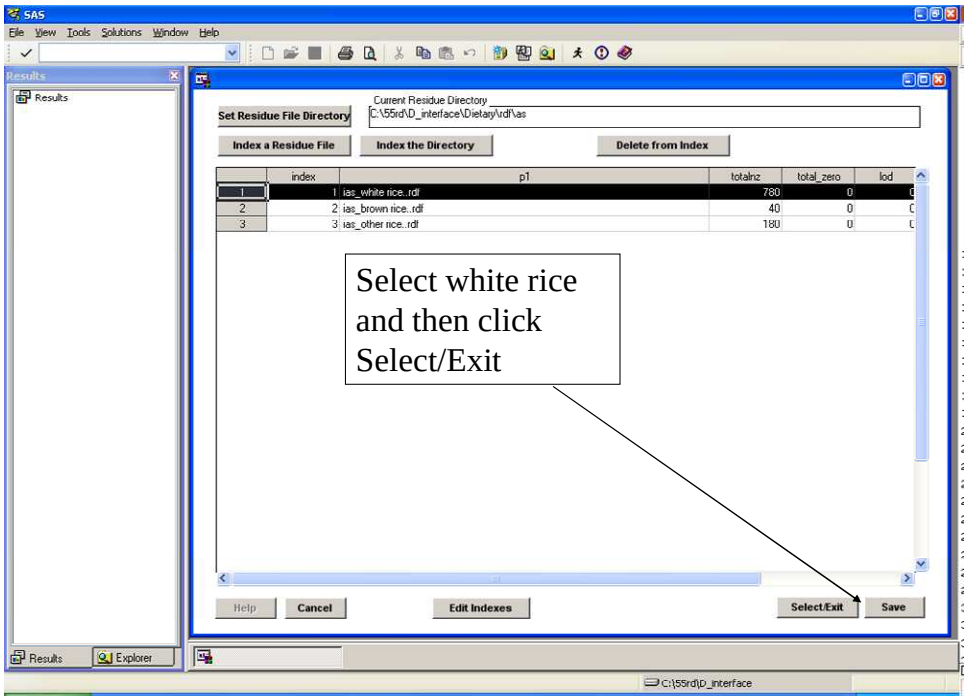
14) Assign residue files to the index so that they can be linked to the food commodities. Select <Index a Residue File> and choose ias_brown_rice.rdf from the dialog selection box. This will add this file as file #1 in the index. Repeat this procedure with ias_white_rice.rdf and ias_other_rice.rdf. Once the files have been indexed, they will remain in the index file and can be assigned to commodities. Click <Save> to save this information.



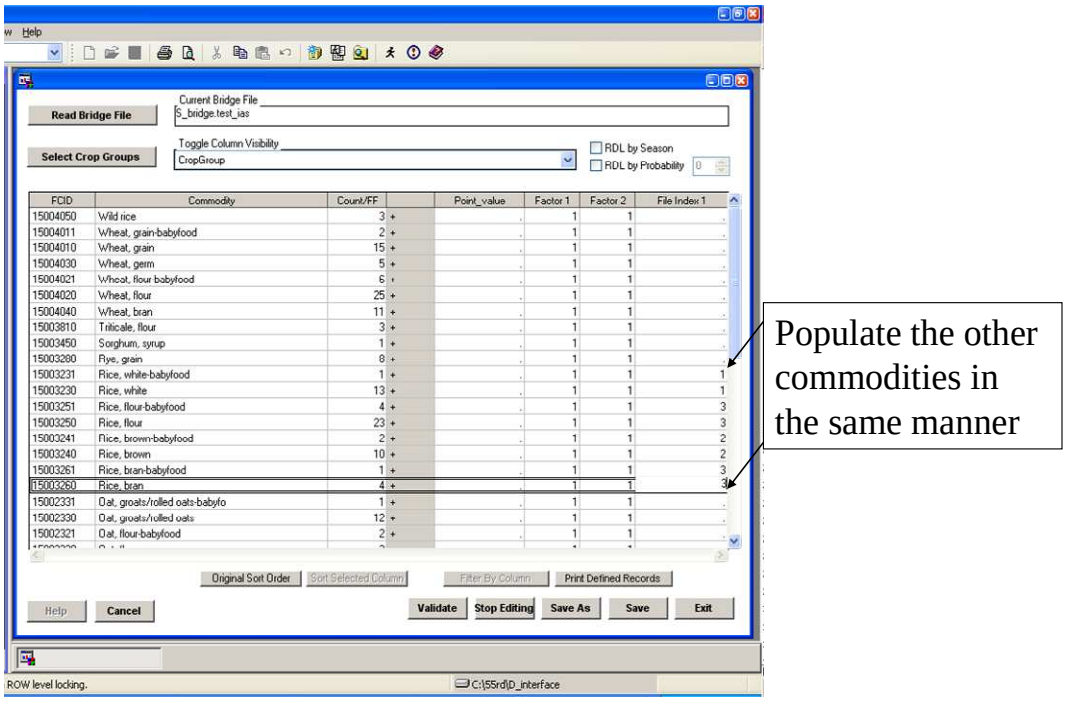




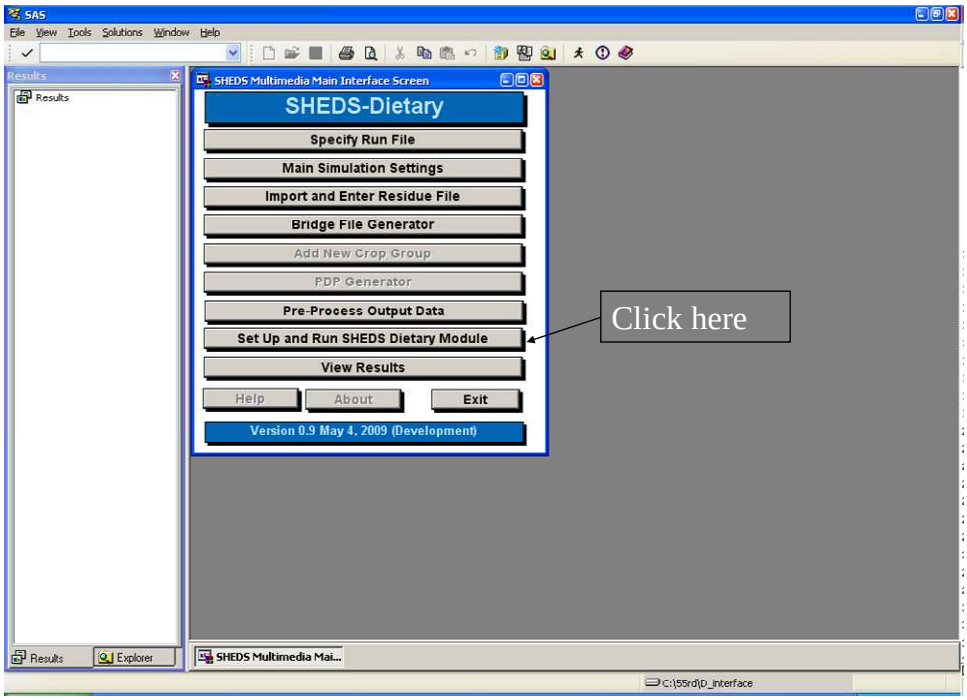
15) Select the white rice residue file by highlighting it. Then select <Select and Exit> to return to the Bridge File. Note that file index 1 (white rice) is now assigned to the selected rice food commodity.

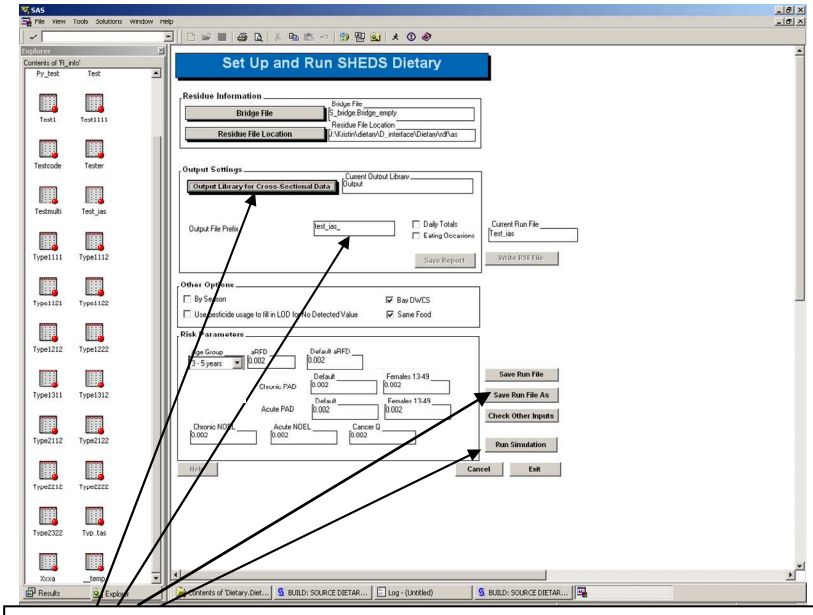


16) If desired, populate the other rice commodities with the appropriate indexes. Do this by double clicking on the File Index 1 column, and selecting an appropriate rdf file from the index (they will now be available for selection since they were added to the index in step 14), and clicking <Select and Exit>. When complete, select <Save> to save the changes to the Bridge File, then select Exit.



17) Select the <Set Up and Run SHEDS-Dietary> button from the Main SHEDS screen. This screen finalizes the settings for the run. Select the library where the model output is to be located, and provide a prefix for the run (“test_ias_”). Enter the desired risk (toxicological) parameters (or use the ones provided in the example), and then click <Save Run File> to save the Run File. The simulation is then run by selecting <Run Simulation>.

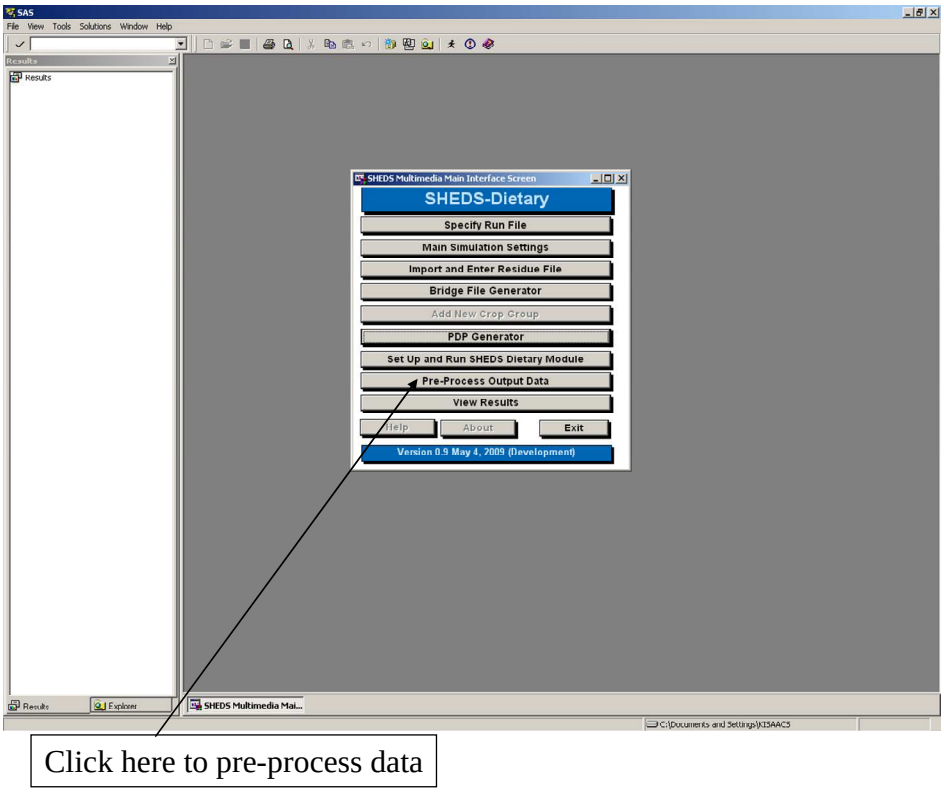




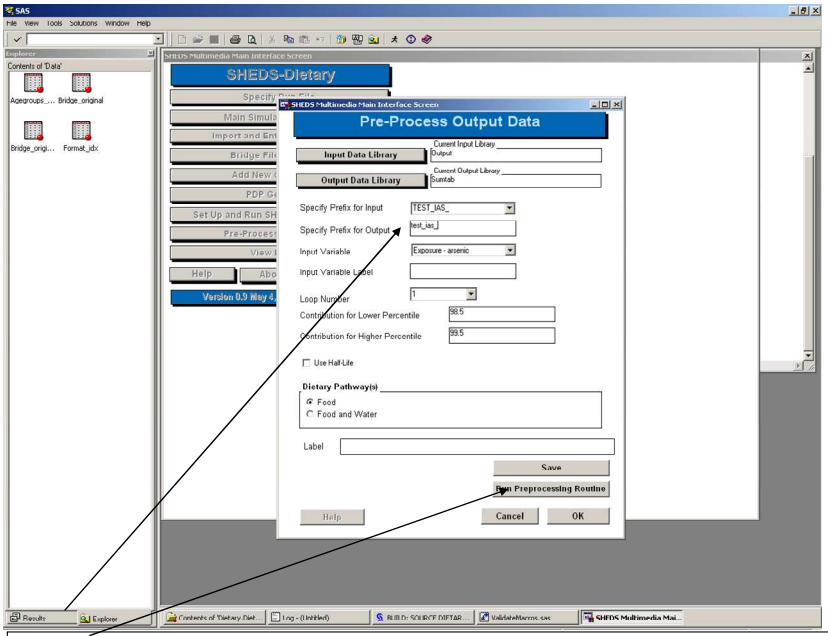
Enter Output library (output) and prefix (test_ias_) Click <Save Run File> and then click <Run Simulation> and then click <Exit> when simulation complete.

18) Now preprocess the raw model output data to generate summary tables and percentiles that can be visualized. Select <Preprocess Output Data> from the Main SHEDS screen. Select

the prefix of the run to be preprocessed (test_ias_), the location where the output summary data are to be stored (Output Data Library=sumtab), and a prefix for the summary data (also test_ias_). (Everything except the prefix should be the default). Also select which interaction run should be processed and the contribution percentiles. Then, click the Run Preprocessing Routine button, and then the OK button.

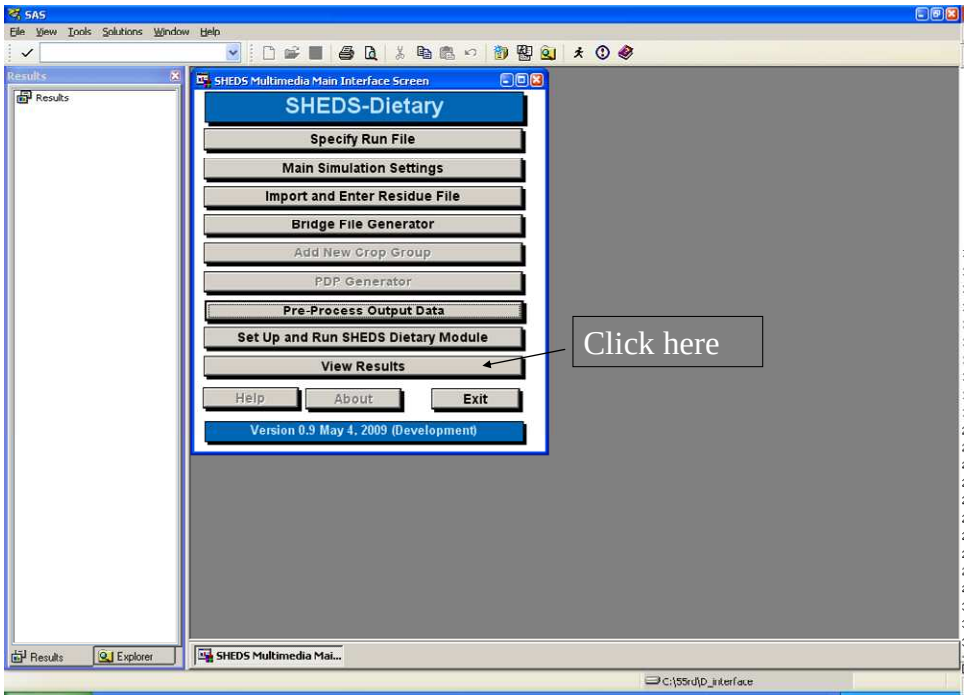


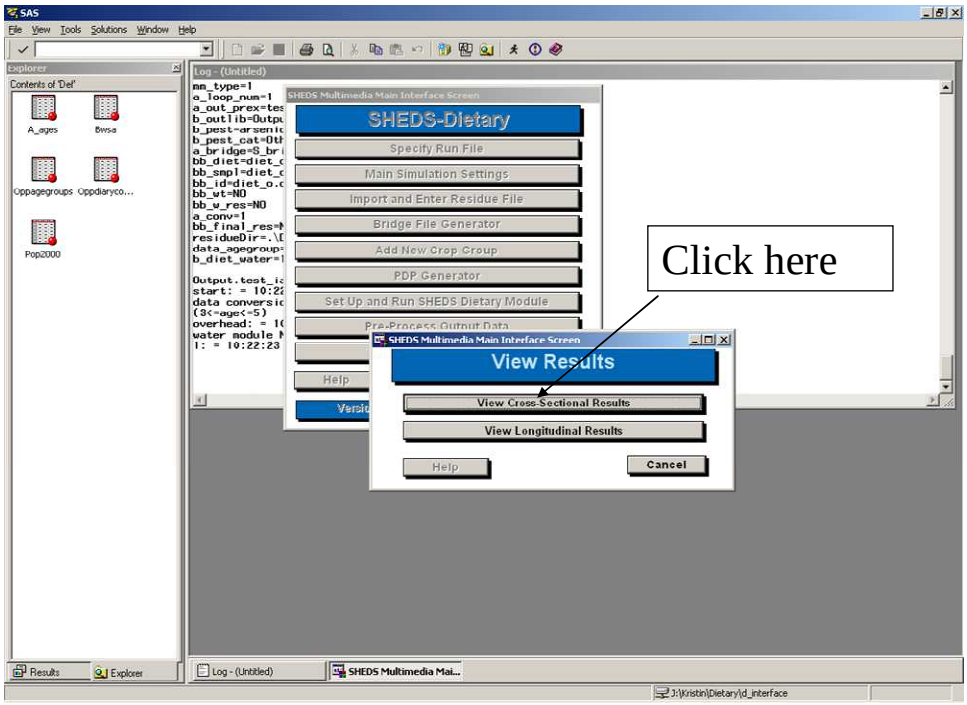
Click here to pre-process data



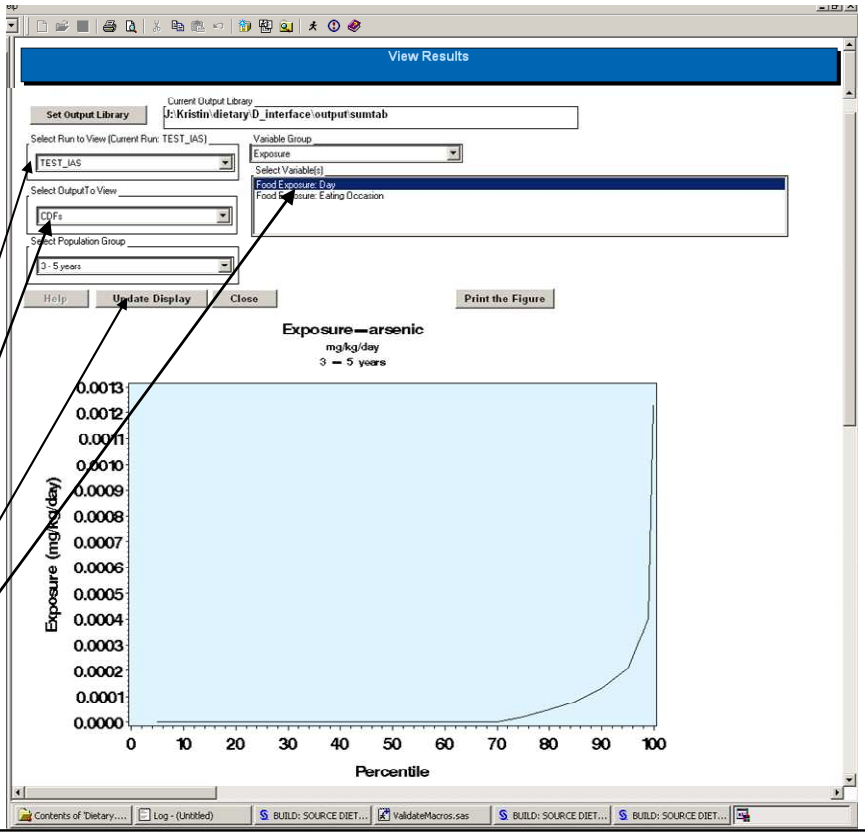
Enter a prefix for the summary data (test_ias_) and click <Run Preprocessing Routine>.

19) Click on the <View Results> button to display the View Results selection screen. Select <View Cross-Sectional Data>.



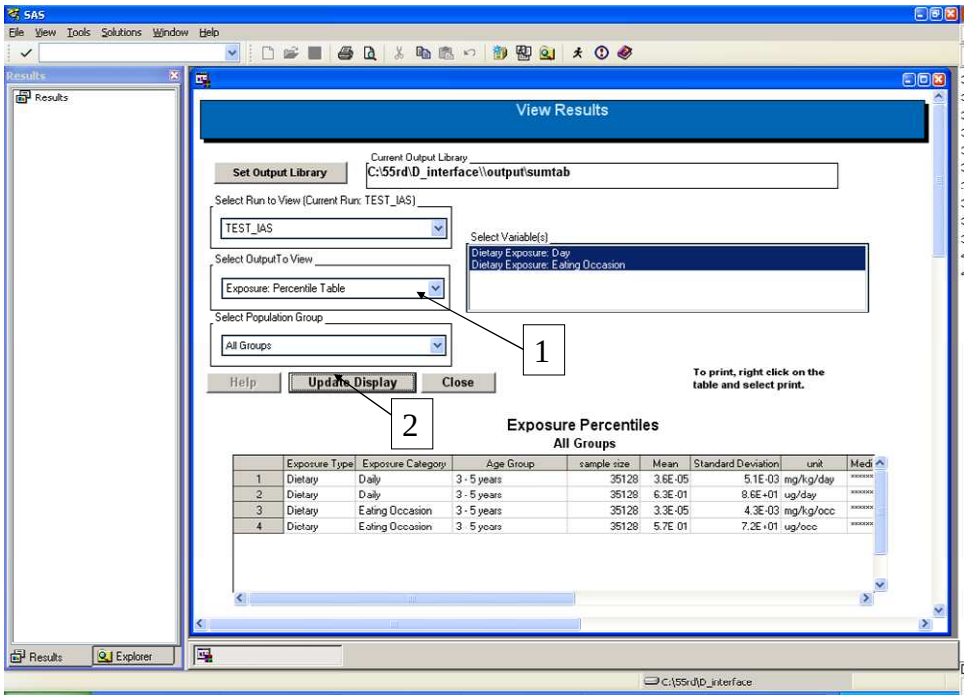


20) The main View Cross-Sectional Results screen will now appear. Select the run of interest (TEST_IAS) from the run selection list (the name will appear without the trailing underscore). Select “CDFs” as the output to view, and highlight the variable Food Exposure:Day. Selecting <Update Display> will update the figure with the selected options. In this way, different output tables and graphs can be generated.

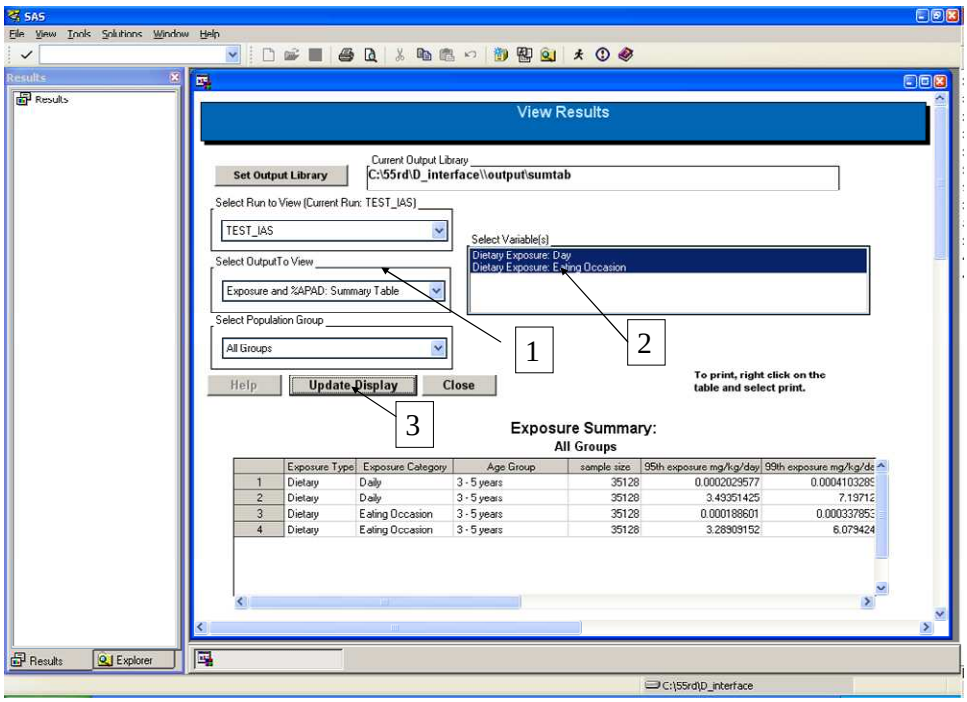


Select the run "test_ias", "CDFs" as output to view, "Food Exposure: Day" as variable, and click <Update Display>

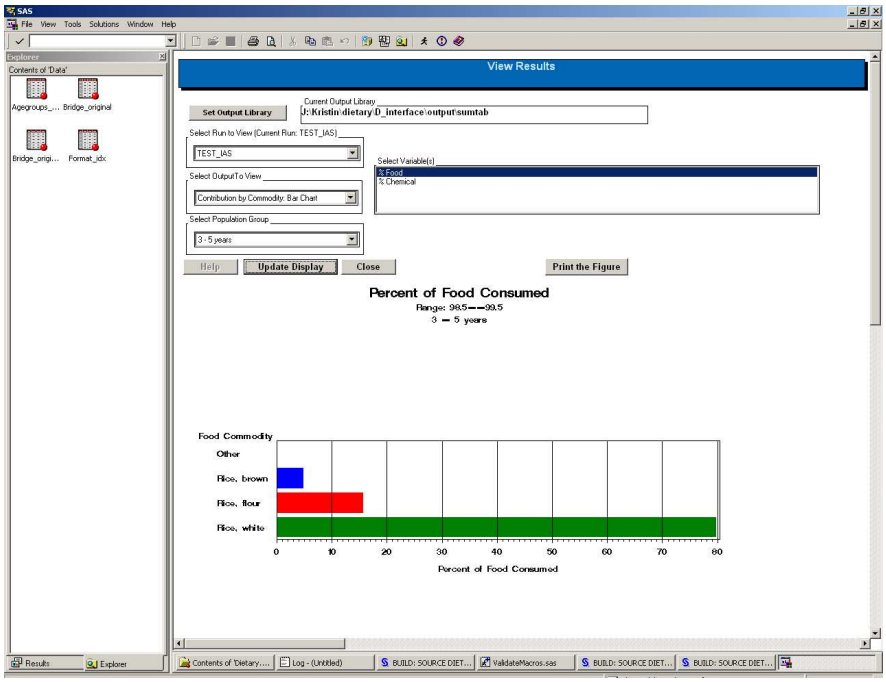
21) Select "Exposure Percentile Table" as the output to view, highlight both available variables, and click <Update Display>. This will generate the requested table for the selected variables.



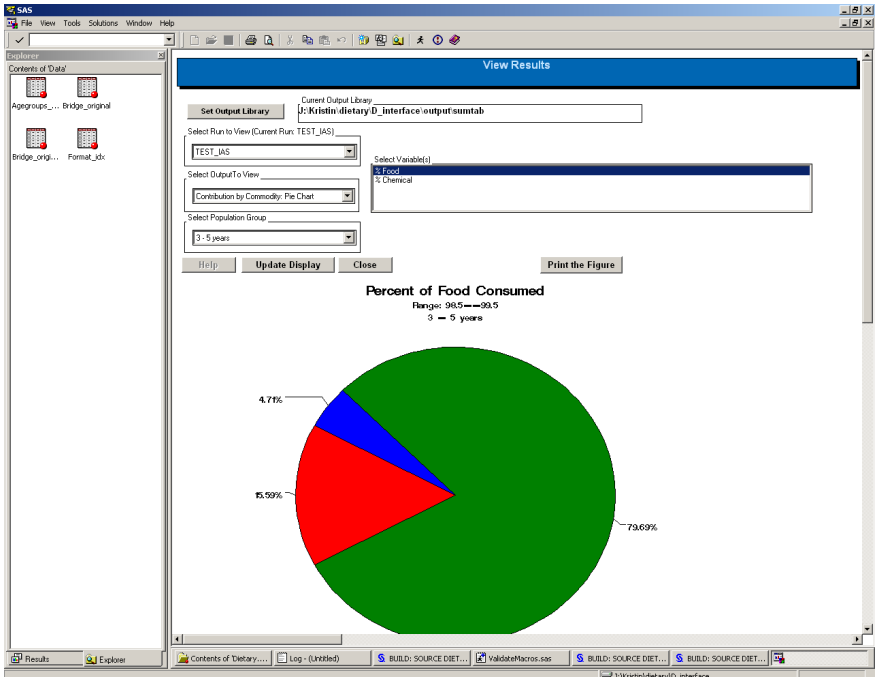
22) Repeat this process by selecting "Exposure and %APAD: Summary Table," selecting the two available variables, and again updating the display.



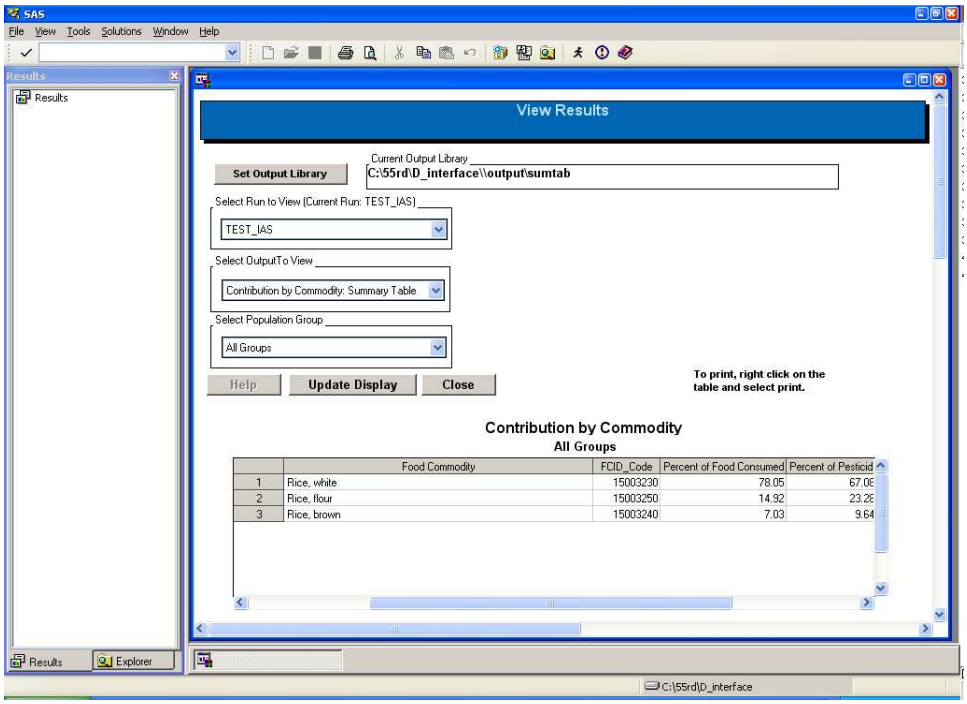
23) Selecting “Contribution by Commodity: Bar Chart” as output to view and % Food as the variable produces a bar chart of % food consumed by commodity. A plot of the contribution of food types to total chemical exposure can also be generated by selecting % Chemical as the variable.



24) Analogous Pie charts can also be displayed by selecting “Contribution by Commodity: Pie Chart.”



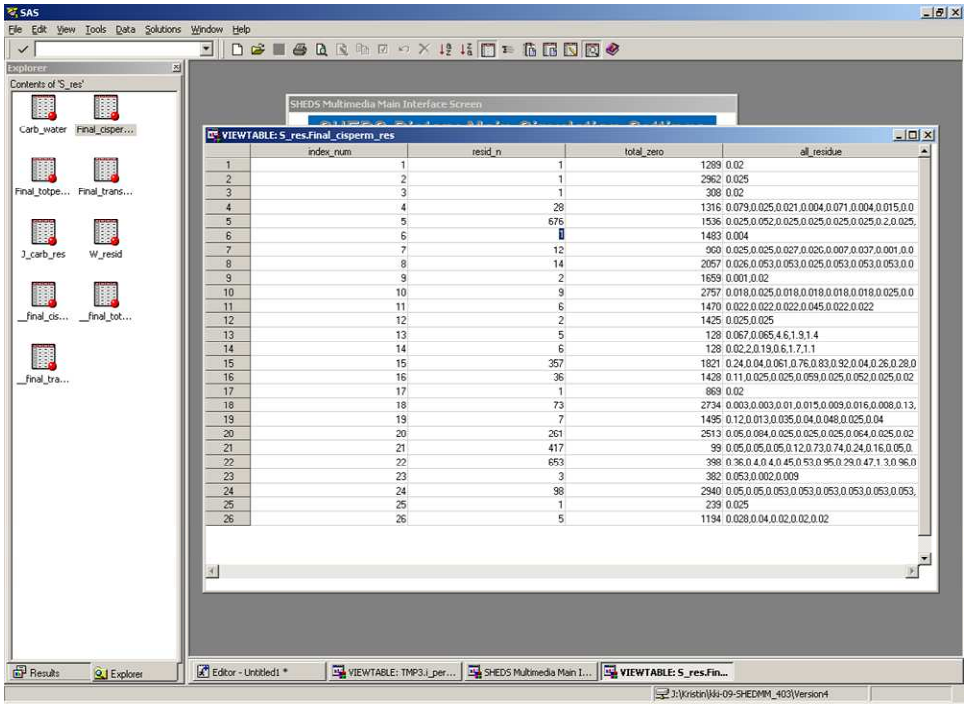
25) Finally, a contribution table can be created by selecting "Contribution by Commodity: Summary Table" as the output to view.



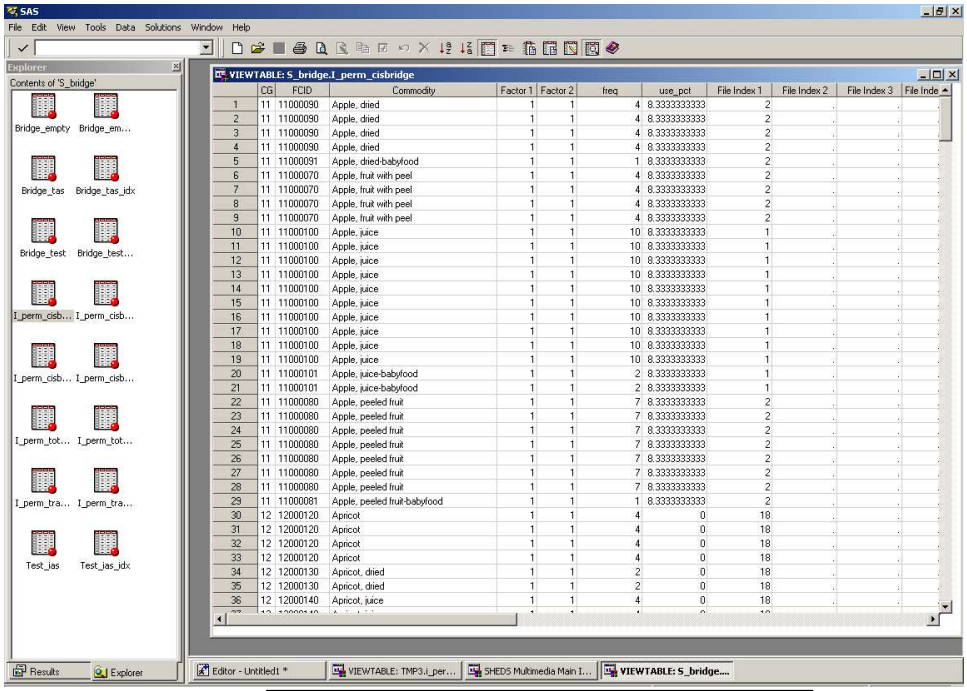
7.2 Case Study 2: Cis-Permethrin, Cross-Sectional Run

This case study is a single-chemical example for simulation of food exposure to cis-permethrin. This is also a cross-sectional simulation. This run uses a final residue file, rather than importing data from RDF files.

1) Create the Bridge File and final residue files for the chemical. This method is best used by persons familiar with the creation or editing of SAS datasets. The format of these files is described in the Appendix. In addition, the SHEDS installation provides several examples of these files that can be used as templates. A final residue file final_cisperm_res and Bridge File I_perm_cisbridge were generated. These files are included in the SHEDS-Dietary installation; they will be available for selection as the user steps through this case study.



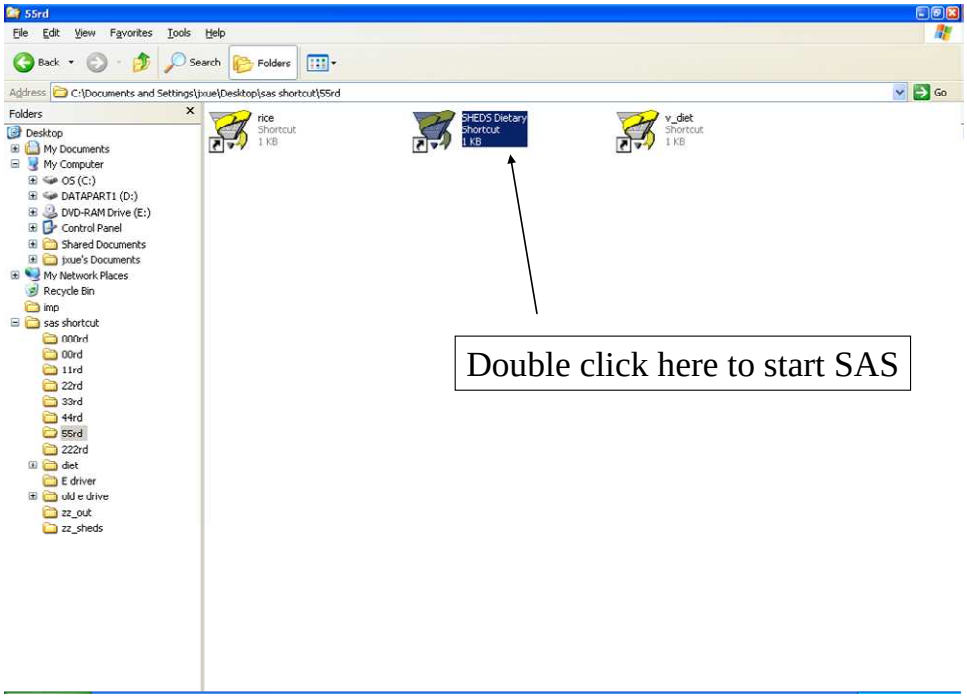
Final (processed) residue file, final_cisperm_res



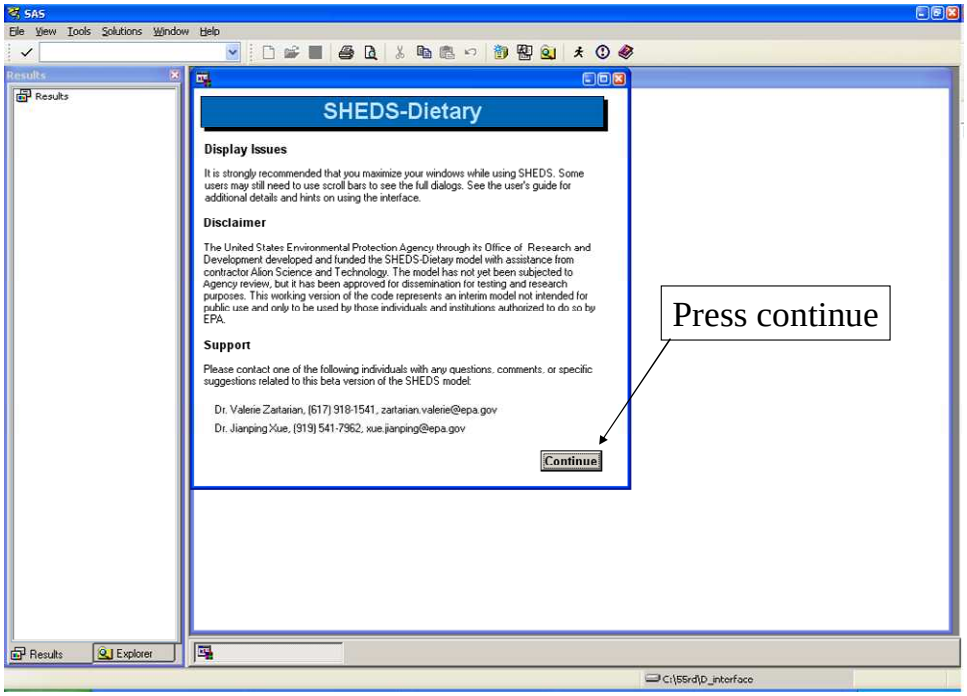
	CG	FCID	Commodity	Factor 1	Factor 2	freq	use_pct	File Index 1	File Index 2	File Index 3	File Inde
1	11	11000090	Apple, dried	1	1	4	8.3333333333	2	.	.	.
2	11	11000090	Apple, dried	1	1	4	8.3333333333	2	.	.	.
3	11	11000090	Apple, dried	1	1	4	8.3333333333	2	.	.	.
4	11	11000090	Apple, dried	1	1	4	8.3333333333	2	.	.	.
5	11	11000091	Apple, dried-babyfood	1	1	1	8.3333333333	2	.	.	.
6	11	11000070	Apple, fruit with peel	1	1	4	8.3333333333	2	.	.	.
7	11	11000070	Apple, fruit with peel	1	1	4	8.3333333333	2	.	.	.
8	11	11000070	Apple, fruit with peel	1	1	4	8.3333333333	2	.	.	.
9	11	11000070	Apple, fruit with peel	1	1	4	8.3333333333	2	.	.	.
10	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
11	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
12	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
13	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
14	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
15	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
16	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
17	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
18	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
19	11	11000100	Apple, juice	1	1	10	8.3333333333	1	.	.	.
20	11	11000101	Apple, juice-babyfood	1	1	2	8.3333333333	1	.	.	.
21	11	11000101	Apple, juice-babyfood	1	1	2	8.3333333333	1	.	.	.
22	11	11000080	Apple, peeled fruit	1	1	7	8.3333333333	2	.	.	.
23	11	11000080	Apple, peeled fruit	1	1	7	8.3333333333	2	.	.	.
24	11	11000080	Apple, peeled fruit	1	1	7	8.3333333333	2	.	.	.
25	11	11000080	Apple, peeled fruit	1	1	7	8.3333333333	2	.	.	.
26	11	11000080	Apple, peeled fruit	1	1	7	8.3333333333	2	.	.	.
27	11	11000080	Apple, peeled fruit	1	1	7	8.3333333333	2	.	.	.
28	11	11000080	Apple, peeled fruit	1	1	7	8.3333333333	2	.	.	.
29	11	11000081	Apple, peeled fruit-babyfood	1	1	1	8.3333333333	2	.	.	.
30	12	12000120	Apricot	1	1	4	0	18	.	.	.
31	12	12000120	Apricot	1	1	4	0	18	.	.	.
32	12	12000120	Apricot	1	1	4	0	18	.	.	.
33	12	12000120	Apricot	1	1	4	0	18	.	.	.
34	12	12000130	Apricot, dried	1	1	2	0	18	.	.	.
35	12	12000130	Apricot, dried	1	1	2	0	18	.	.	.
36	12	12000140	Apricot, juice	1	1	4	0	18	.	.	.

Bridge file, I_perm_cisbridge

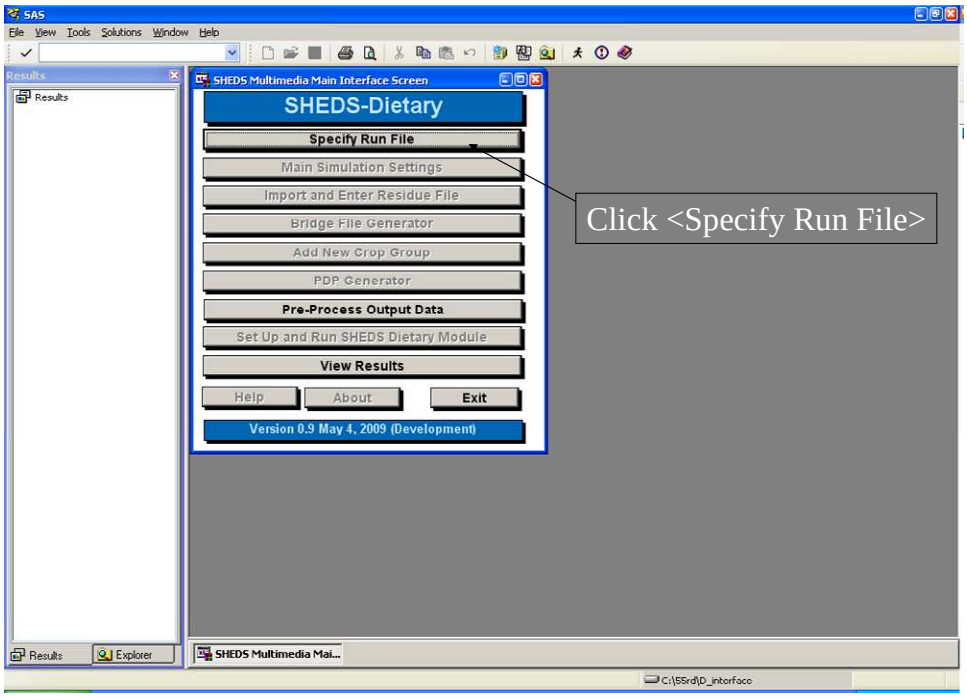
2) Initiate a SHEDS-Dietary session by double-clicking the SAS icon.

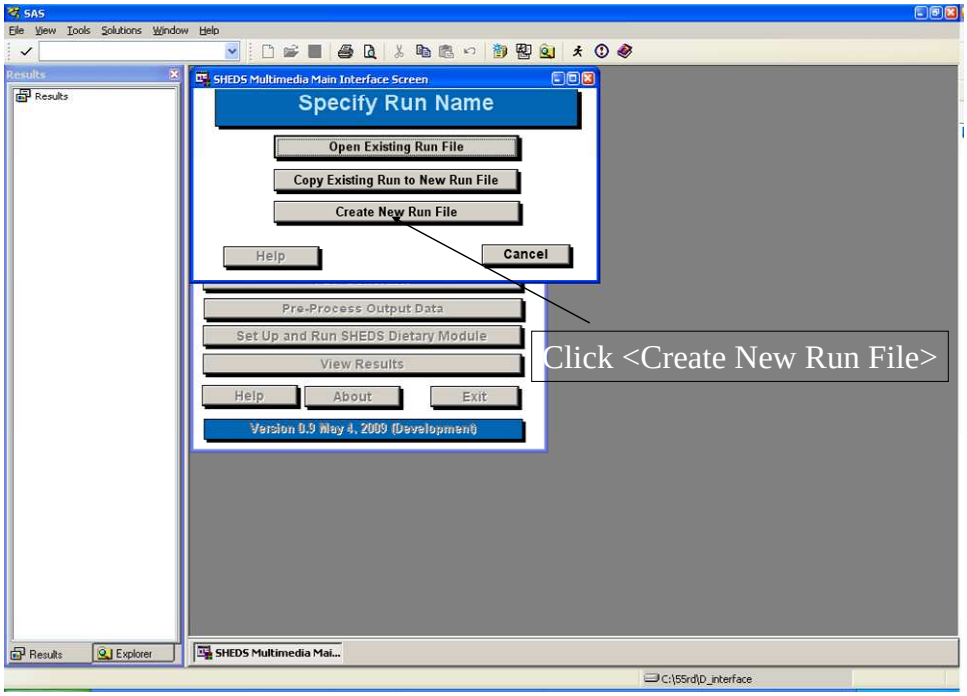


3) The SHEDS disclaimer screen appears first; select <Continue> to proceed to the main SHEDS screen.

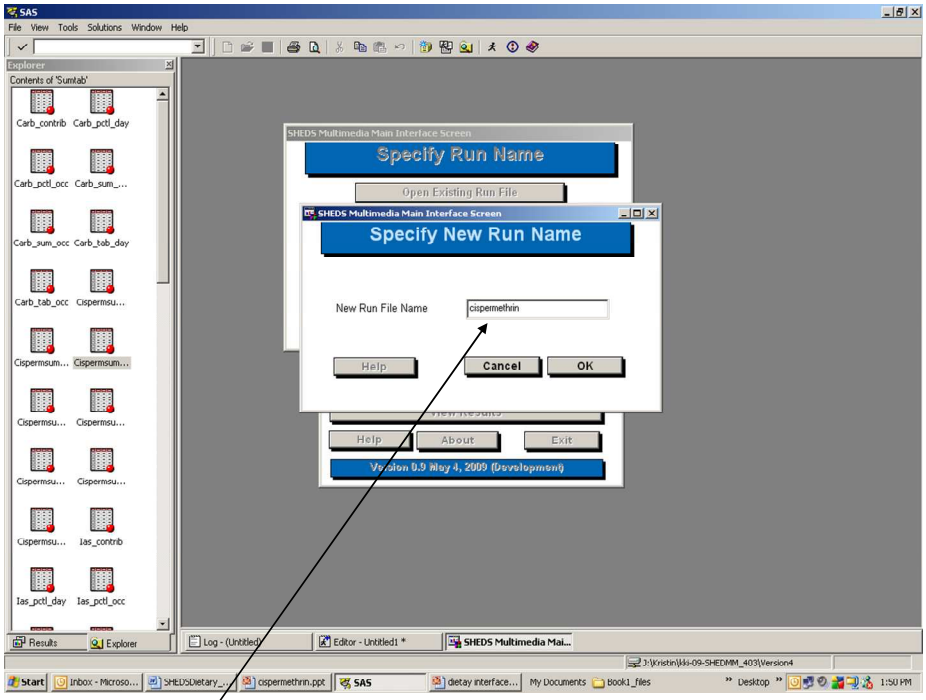


4) Select <Specify Run File>-><Create New Run File> to initiate the creation of a new run for cis-permethrin.


SAS
File View Tools Solutions Window Help
Results
SHEDS Multimedia Main Interface Screen
SHEDS-Dietary
Specify Run File
Main Simulation Settings
Import and Enter Residue File
Bridge File Generator
Add New Crop Group
PDP Generator
Pre-Process Output Data
Set Up and Run SHEDS Dietary Module
View Results
Help
About
Exit
Version 0.9 May 4, 2009 (Development)
Click <Specify Run File>
Results
Explorer
SHEDS Multimedia Mai...
C:\SSrd\D_interface

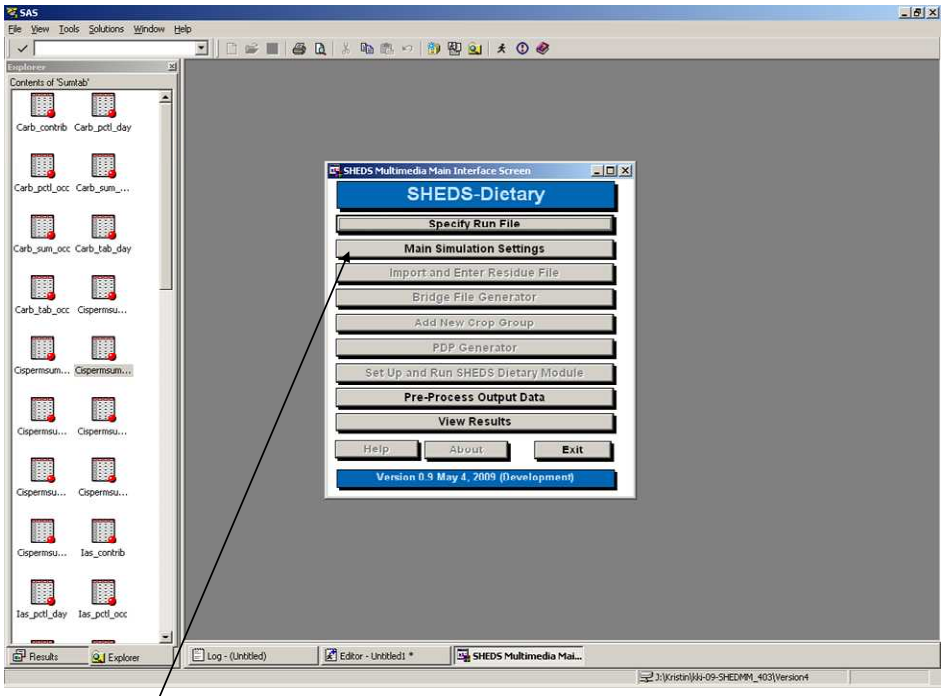

SAS
File View Tools Solutions Window Help
Results
SHEDS Multimedia Main Interface Screen
Specify Run Name
Open Existing Run File
Copy Existing Run to New Run File
Create New Run File
Help
Cancel
Pre-Process Output Data
Set Up and Run SHEDS Dietary Module
View Results
Help
About
Exit
Version 0.9 May 4, 2009 (Development)
Click <Create New Run File>
Results
Explorer
SHEDS Multimedia Mai...
C:\SSrd\D_interface

5) Enter the name of the new run as “cispermethrin” when prompted and select <OK>.

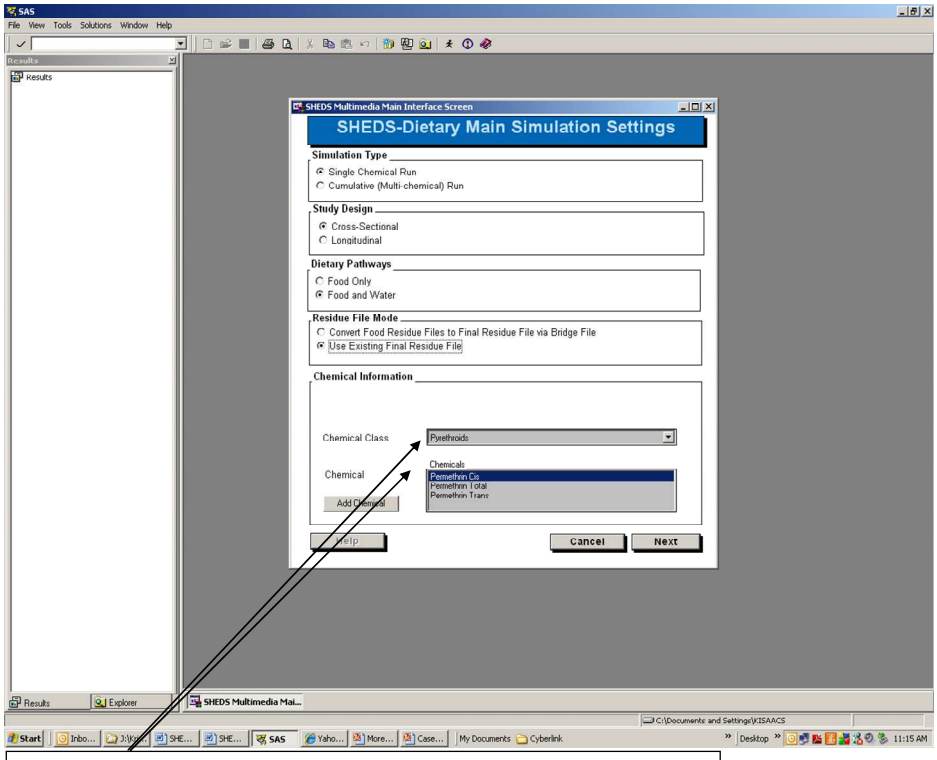


Enter name for new run, “cispermethrin”

6) The Main Simulation Settings button will now be enabled. Select it and the Main Simulation Settings screen will appear. Select “Pyrethroids” for Chemical Class in the Chemical Information box and Permethrin Cis for pesticide. Select “Use Existing Final Residue File” in the Residue File Mode box (note that this option is different from that used in Case Study #1), then hit the Next button.

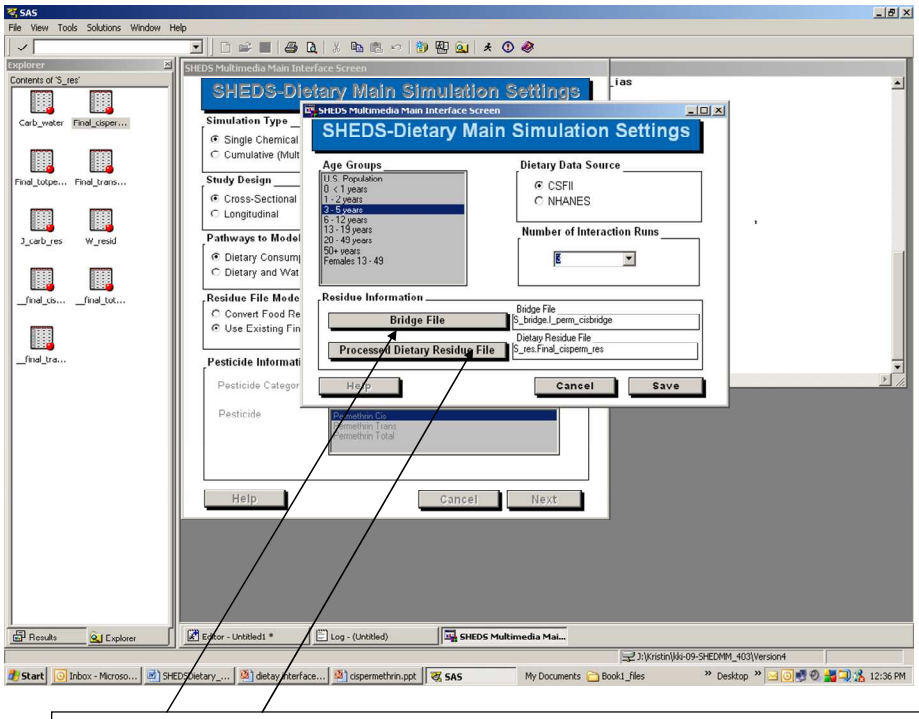


Select <Main Simulation Settings>



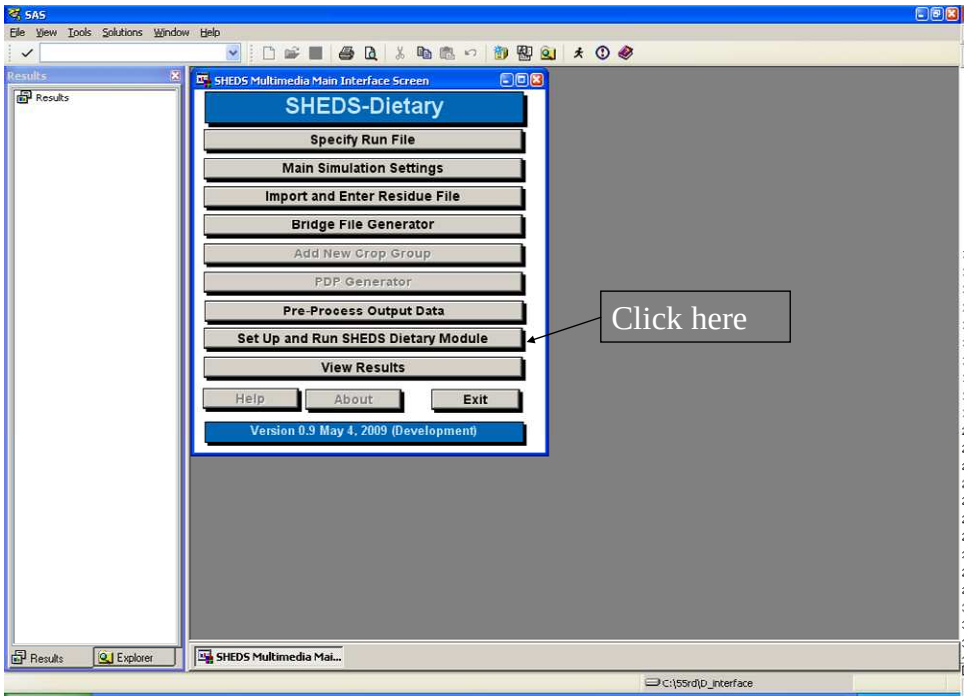
Select Pyrethroids, Permethrin Cis, then click <Next>

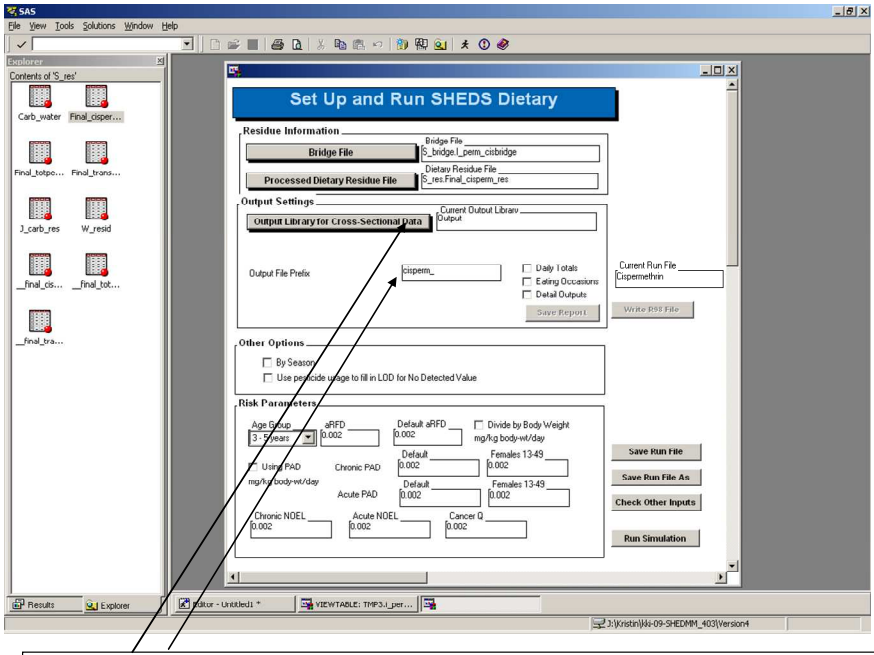
7) The second Main Simulation Settings screen appears. Click the Bridge File button to select a Bridge File for the run. Select I_perm_cisbridge from the file selection dialog, then hit OK. The dialog widget will be filled in with the full name of the dataset (including the SAS library). For the Processed Food Residue File, select the file Final_cisperm_res from the selection dialog. Then select 3 as the number of interaction runs and click <Save>.



Select bridge file and final residue files, click <Save>

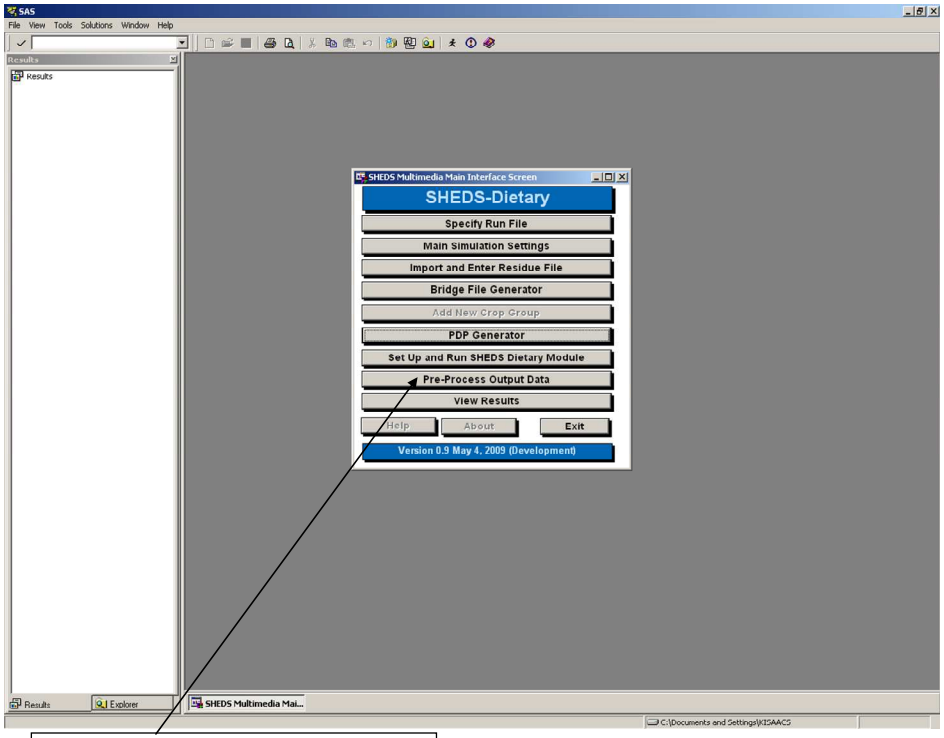
8) Select the <Set Up and Run SHEDS-Dietary> button from the Main SHEDS screen. This screen finalizes the settings for the run. Specify the Output Library where the model output is to be located ("output"), and provide an Output File Prefix for the run ("cisperm_"). Edit any desired risk (toxicological) parameters (or use the ones provided in the example). The simulation is then run by selecting <Run Simulation>, then hit <Exit>.



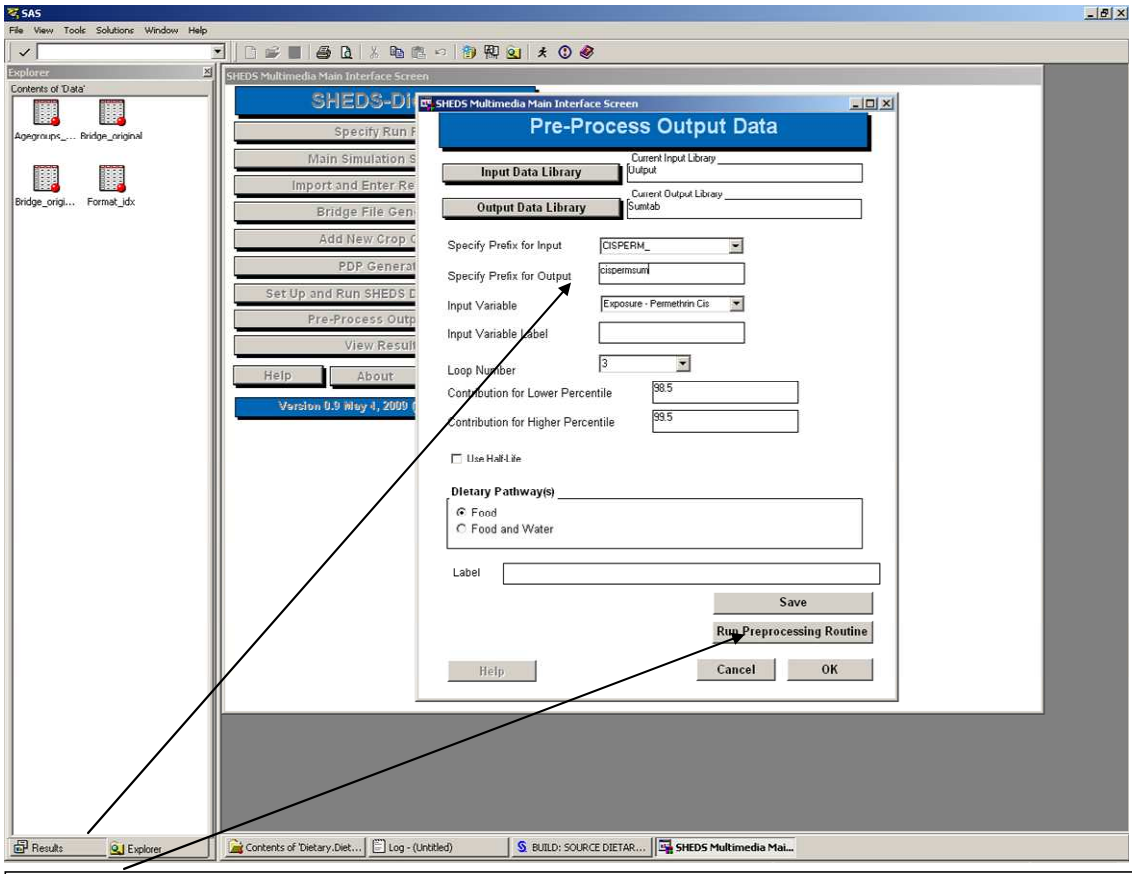


Enter Output directory and prefix, then <Run Simulation>

9) Now preprocess the raw model output data to generate summary tables and percentiles that can be visualized. Select <Pre-Process Output Data> from the Main SHEDS screen. Select the prefix of the run to be preprocessed ("cisperm_"), the location where the output summary data are to be stored (the "sumtab" library, the default), and a prefix for the summary data ("cispermsum"). Select the variable to process. Since this is a single chemical run, the only available variable is Exposure: Permethrin Cis. Also select how many interaction runs should be processed and the contribution percentiles. Click <Run Preprocessing Routine>, then <OK>.

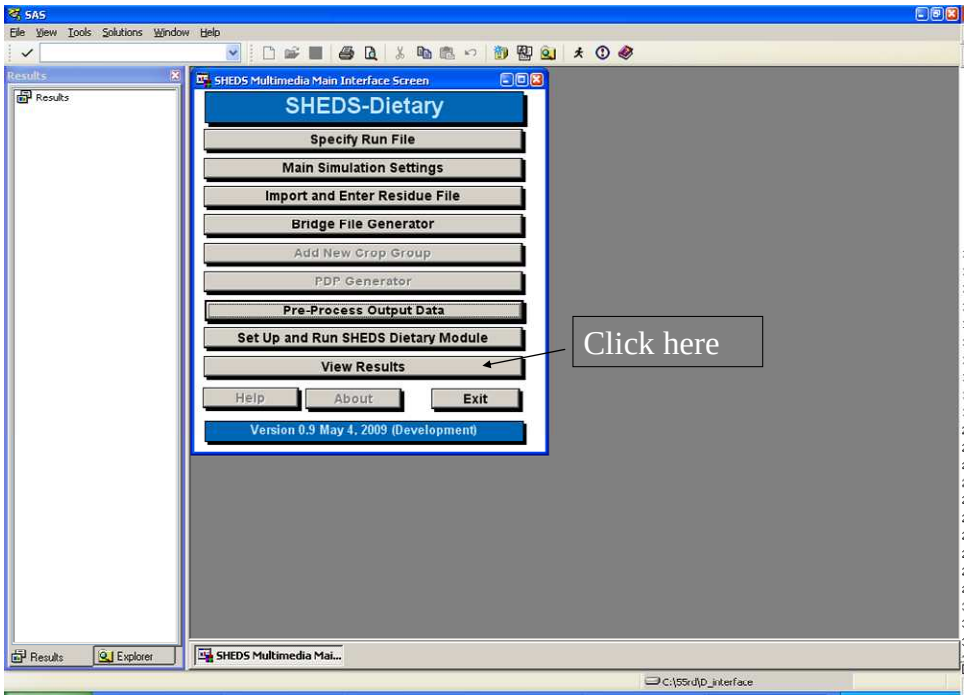


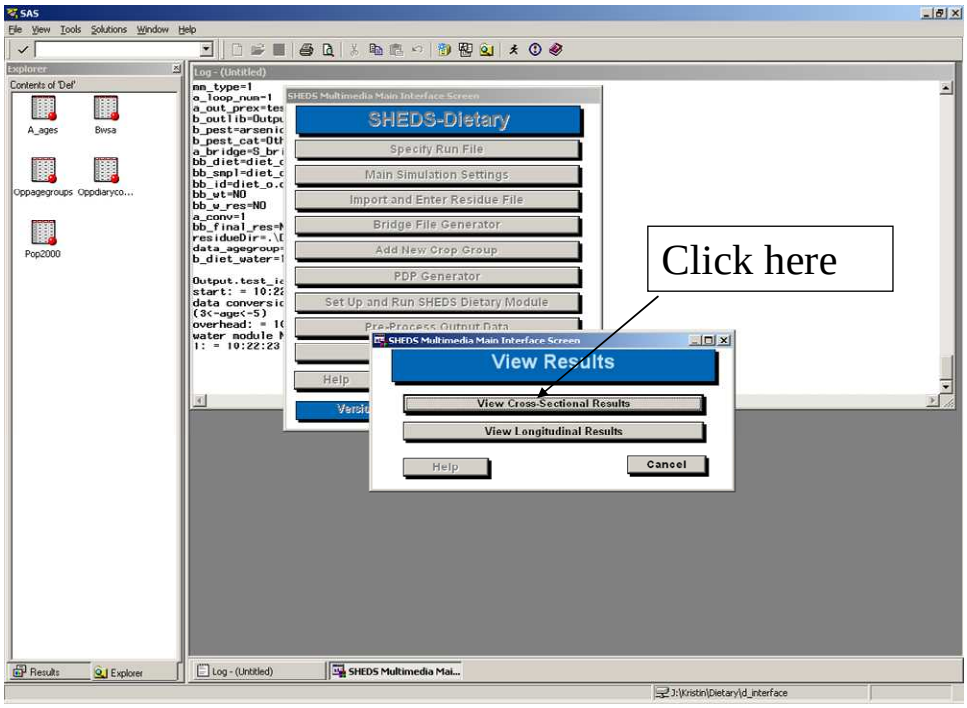
Click here to pre-process data



Enter a prefix for the summary data ("cispermsum") and click <Run Preprocessing Routine>.

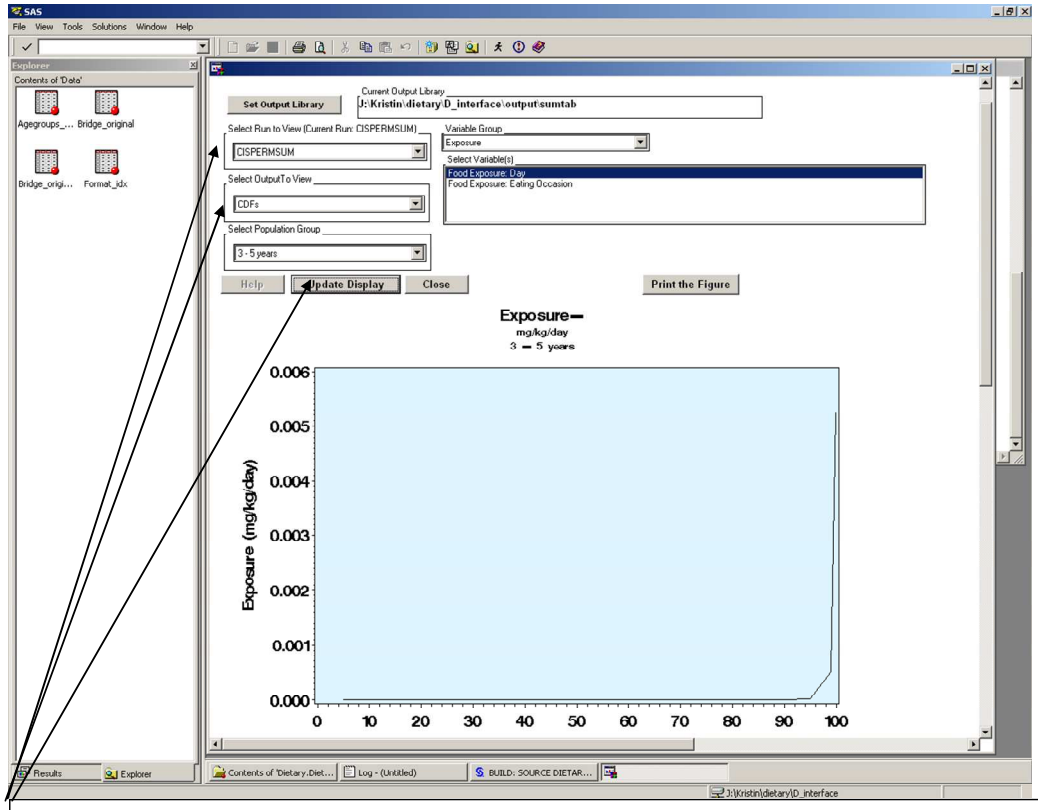
10) Click on the <View Results> button to display the View Results selection screen. Select <View Cross-Sectional Results>.





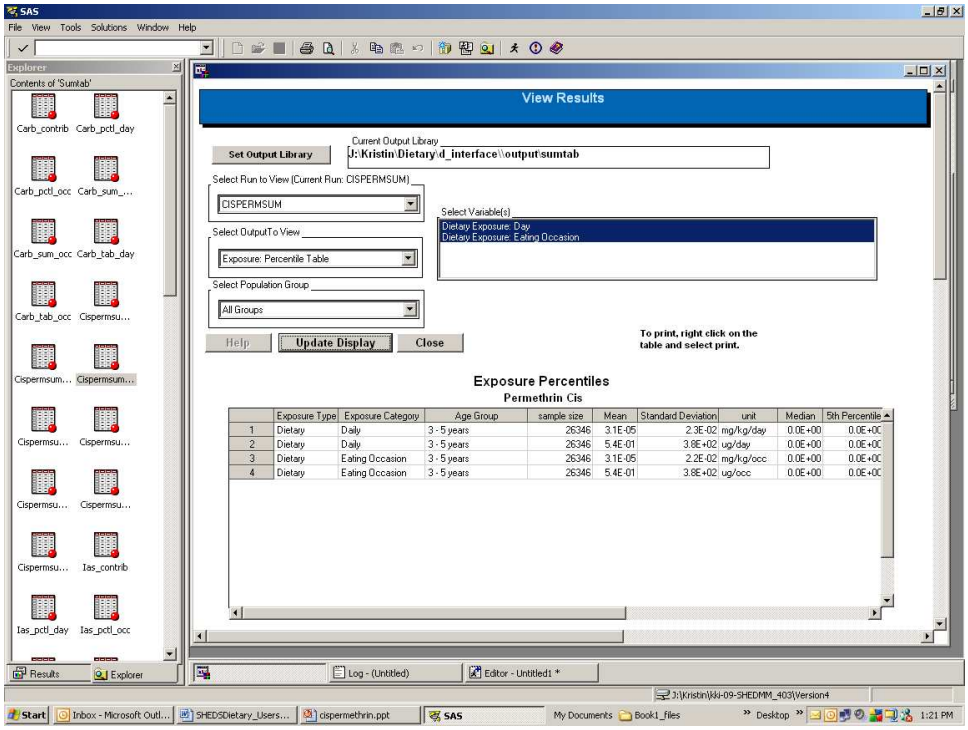
11) The main View Cross-Sectional Results screen will now appear. Select the run of interest from the run selection list, by selecting the prefix that was entered in the Pre-process screen (cispermsum, in this case). Select "CDFs" as the output to view, and highlight one of the two available variables (daily or eating occasion food exposure). Selecting <Update Display>

will update the figure with the selected options. In this way, different output tables and graphs can be generated.

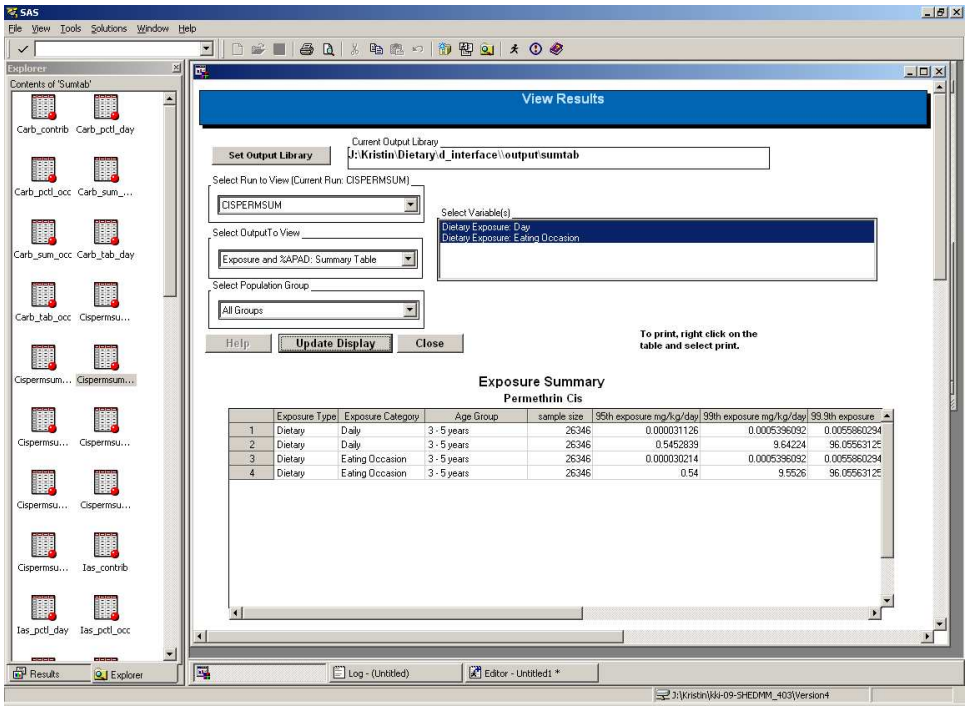


Select the run “cispermsum”, “CDFs” as output to view, and <Update Display>

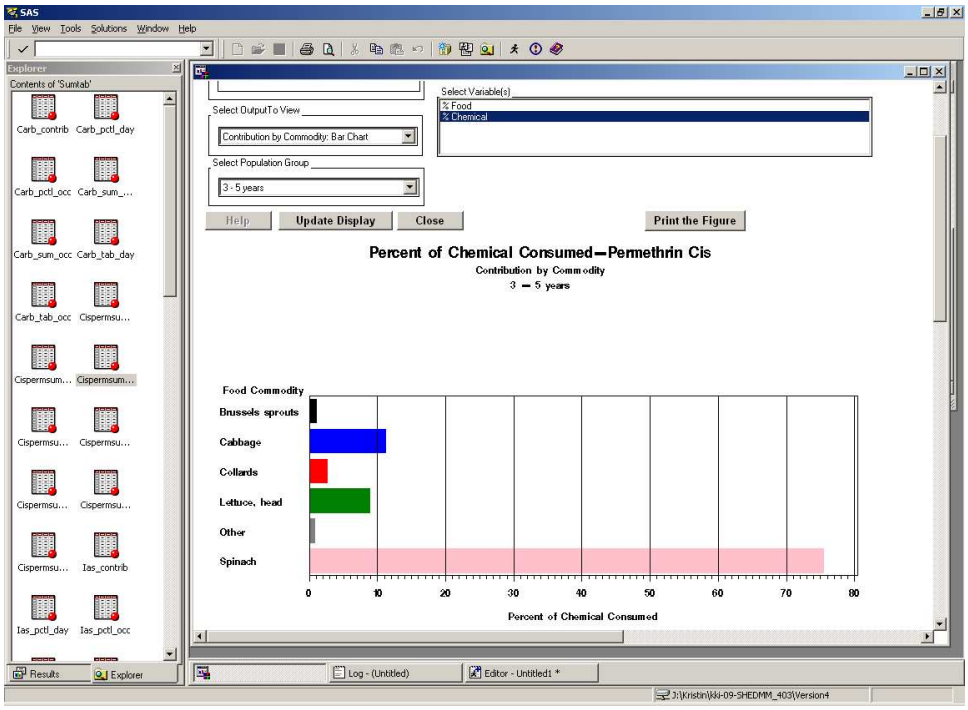
12) Select “Exposure Percentile Table” as the output to view, select the two available variables, and click <Update Display>. This will generate the requested table for the selected variables.



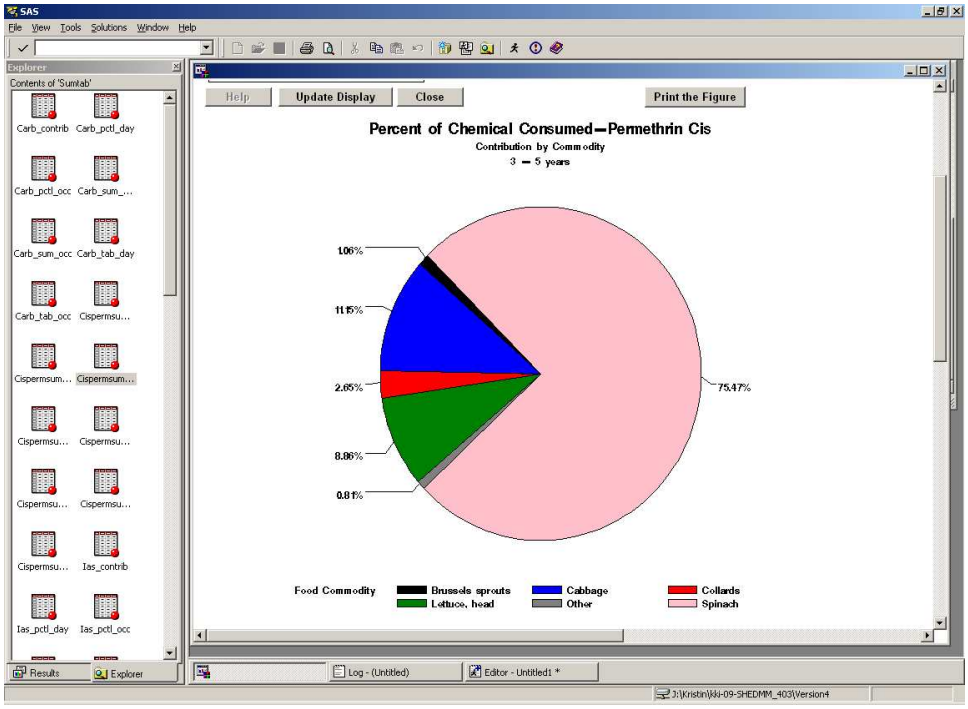
13) Repeat this process by selecting “Exposure and %APAD: Summary Table” and again updating the display.



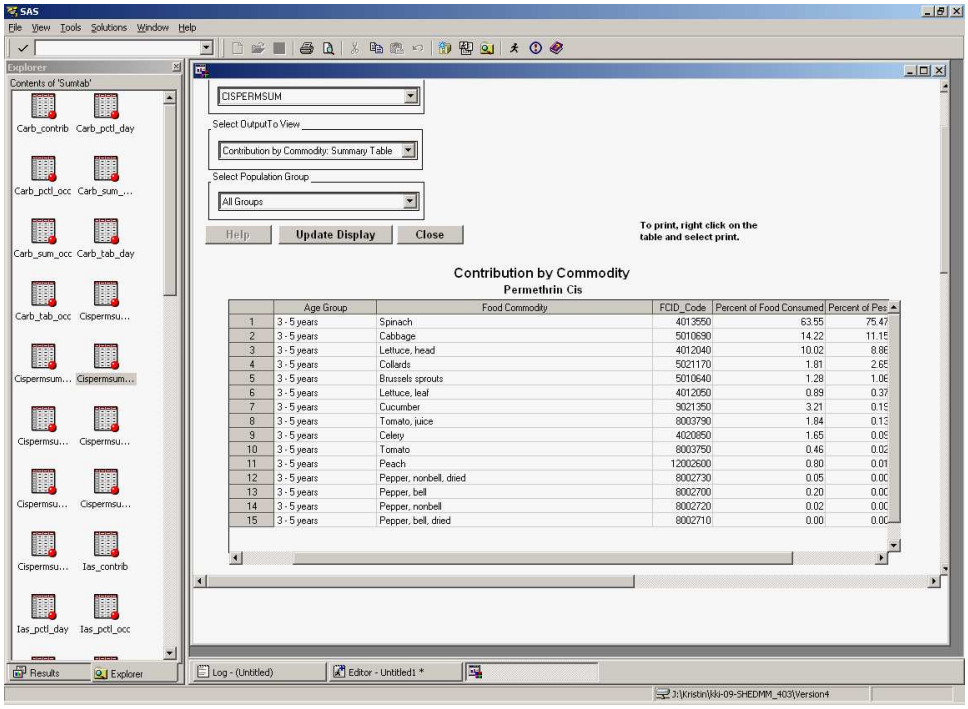
14) Selecting “Contribution by Commodity: Bar Chart” as output to view and %Chemical as the variable produces a bar chart of the contribution of food types to total chemical exposure.



15) An analogous Pie chart can also be displayed by selecting “Contribution by Commodity: Pie Chart.”



16) Finally, a contribution table can be created by selecting "Contribution by Commodity: Summary Table" as the output to view.



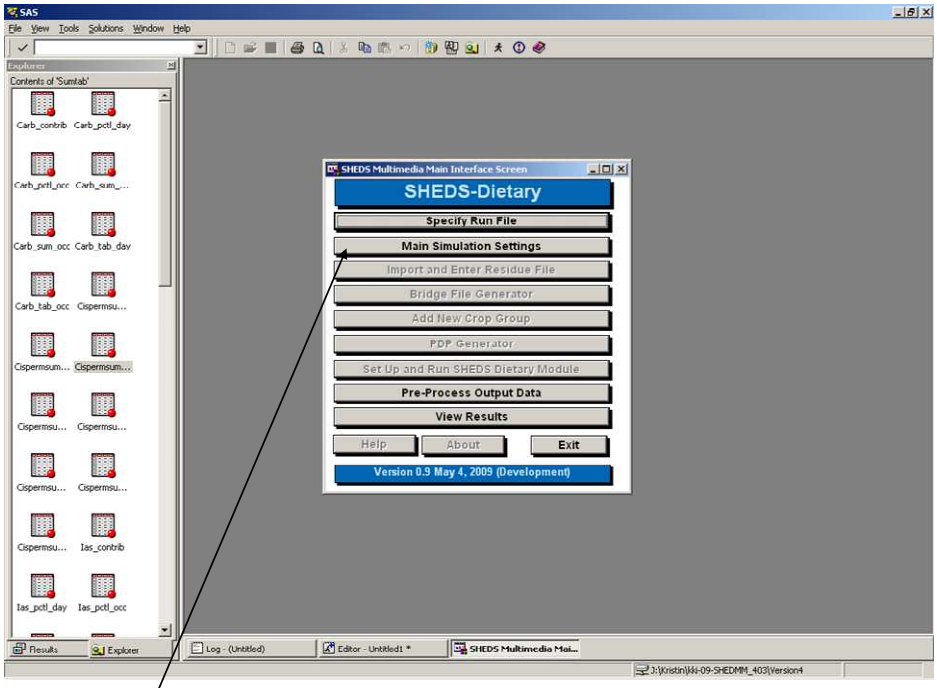
	Age Group	Food Commodity	FCID_Code	Percent of Food Consumed	Percent of Pes
1	3 - 5 years	Spinach	4013550	63.55	75.47
2	3 - 5 years	Cabbage	5010630	14.22	11.15
3	3 - 5 years	Lettuce, head	4012040	10.02	8.86
4	3 - 5 years	Collards	5021170	1.81	2.65
5	3 - 5 years	Brussels sprouts	5010640	1.28	1.06
6	3 - 5 years	Lettuce, leaf	4012050	0.89	0.37
7	3 - 5 years	Cucumber	9021350	3.21	0.15
8	3 - 5 years	Tomato, juice	8003790	1.84	0.13
9	3 - 5 years	Celery	4020850	1.65	0.09
10	3 - 5 years	Tomato	8003750	0.46	0.02
11	3 - 5 years	Peach	12002600	0.80	0.01
12	3 - 5 years	Pepper, nonbell, dried	8002730	0.05	0.00
13	3 - 5 years	Pepper, bell	8002700	0.20	0.00
14	3 - 5 years	Pepper, nonbell	8002720	0.02	0.00
15	3 - 5 years	Pepper, bell, dried	8002710	0.00	0.00

7.3 Case Study 3: Cis-Permethrin, Longitudinal Run

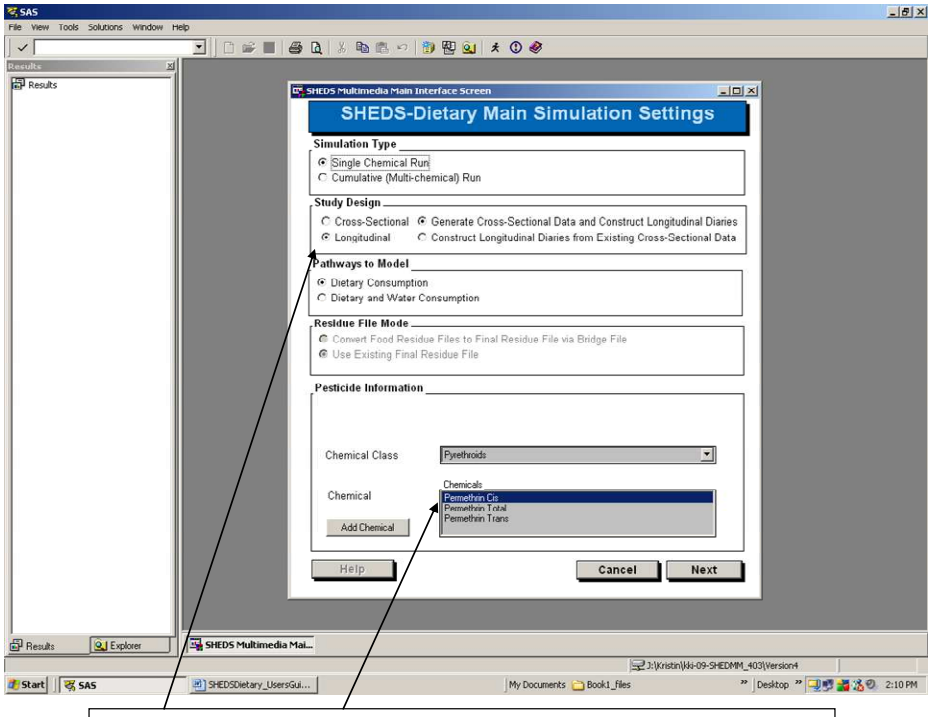
This case study is a single-chemical example for simulation of food exposure to cis-permethrin. This is a longitudinal, rather than cross-sectional, simulation. This run also uses a final residue file, rather than converting food residue files.

Steps 1)-5). Repeat Steps 1-5 of Case Study 2, giving the run the name “Cisperm”.

6) The Main Simulation Settings button will now be enabled. Select it and the Main Simulation Settings screen will appear. Select “Pyrethroids” for chemical category and Permethrin Cis for chemical. Select “Longitudinal” under the Study Design box, then hit <Next>.

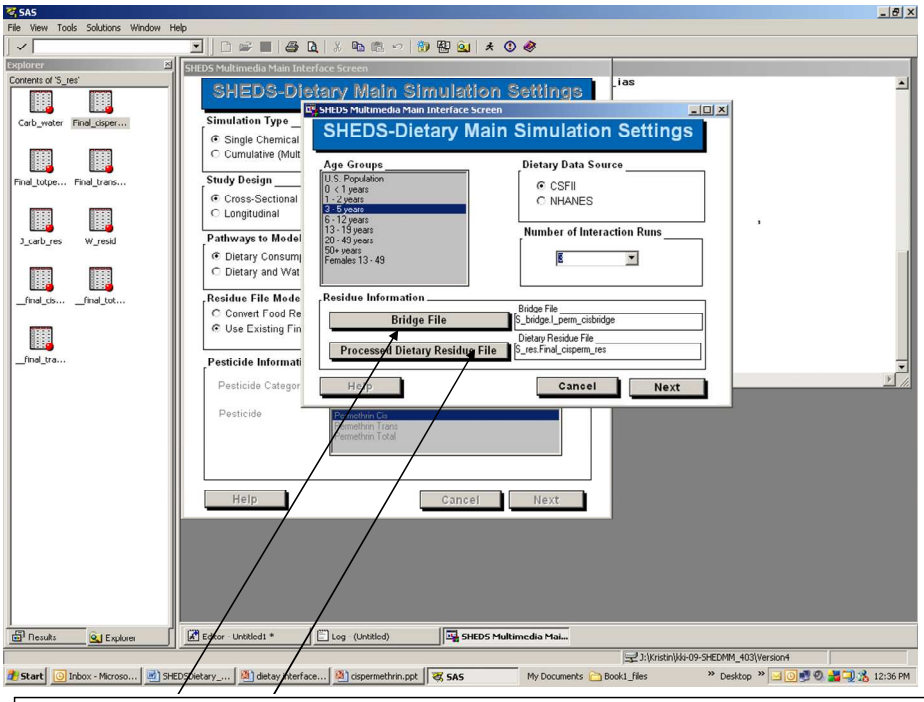


Select <Main Simulation Settings>



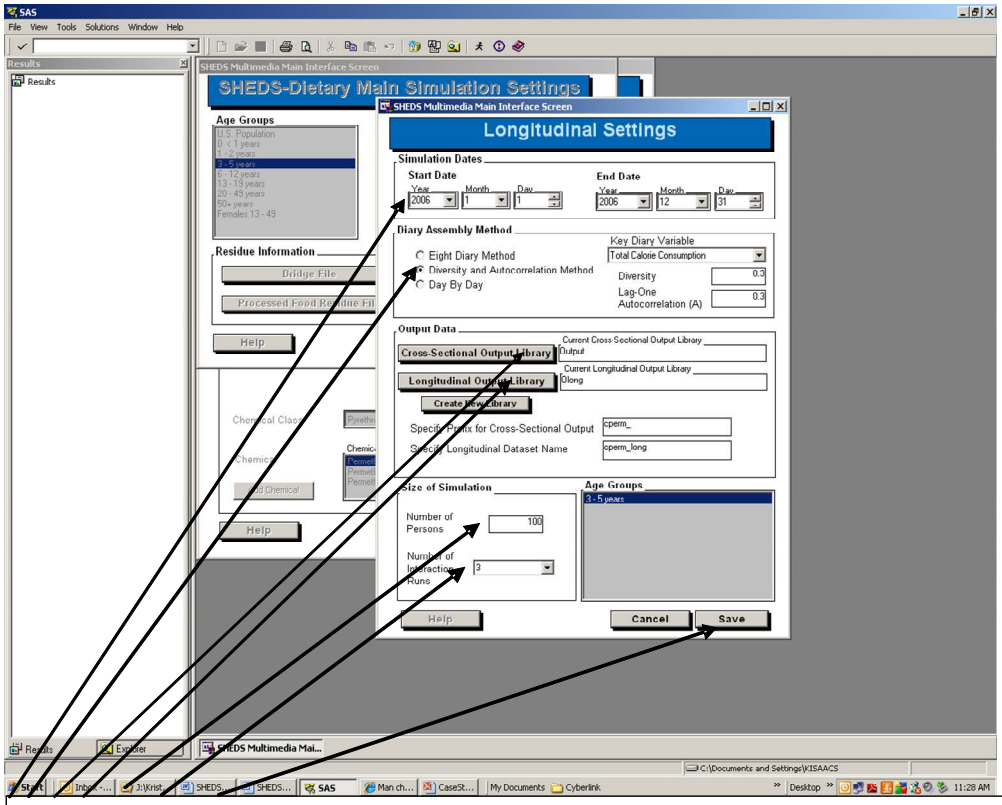
Select <Longitudinal> and <Permethrin Cis>

7) The second Main Simulation Settings screen appears. Click the Bridge File button to select a Bridge File for the run. Select I_perm_cisbridge from the file selection dialog, then <OK>. For Processed Food Residue file, select the file final_cisperm_res from the selection dialog. (The text field will be filled in automatically with the full name of the dataset, including the SAS library prefix). Then select 3 as the number of interaction runs and click <Next>.



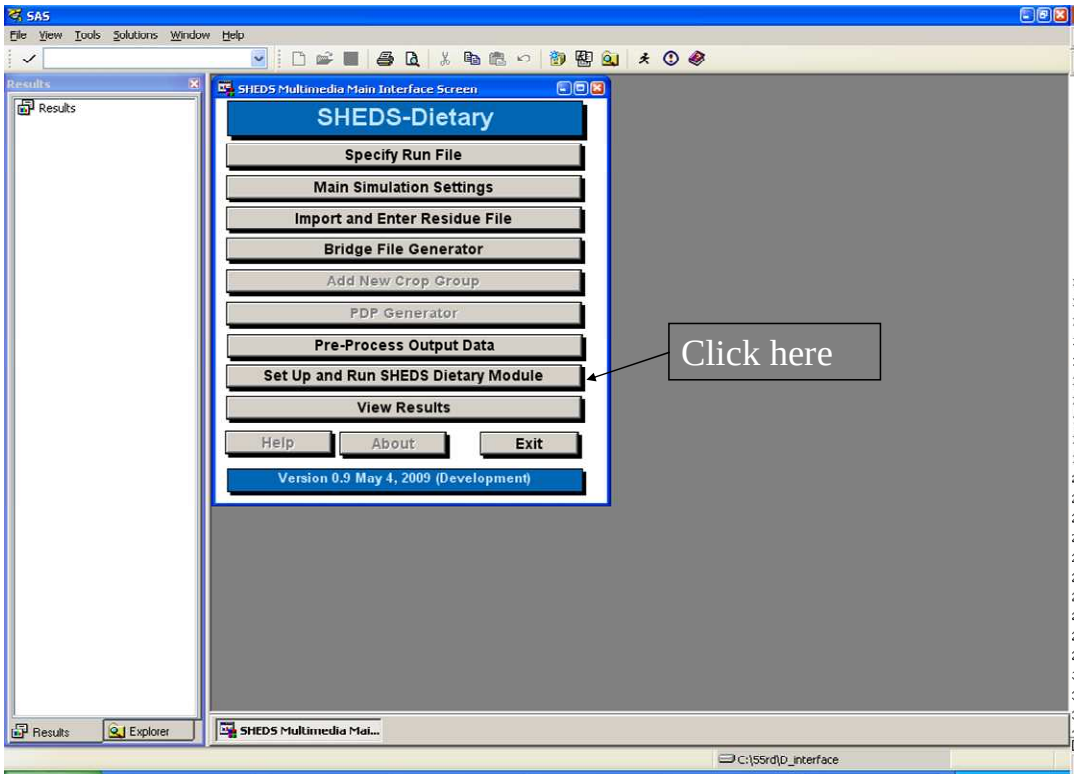
Select bridge file and final residue file, click next

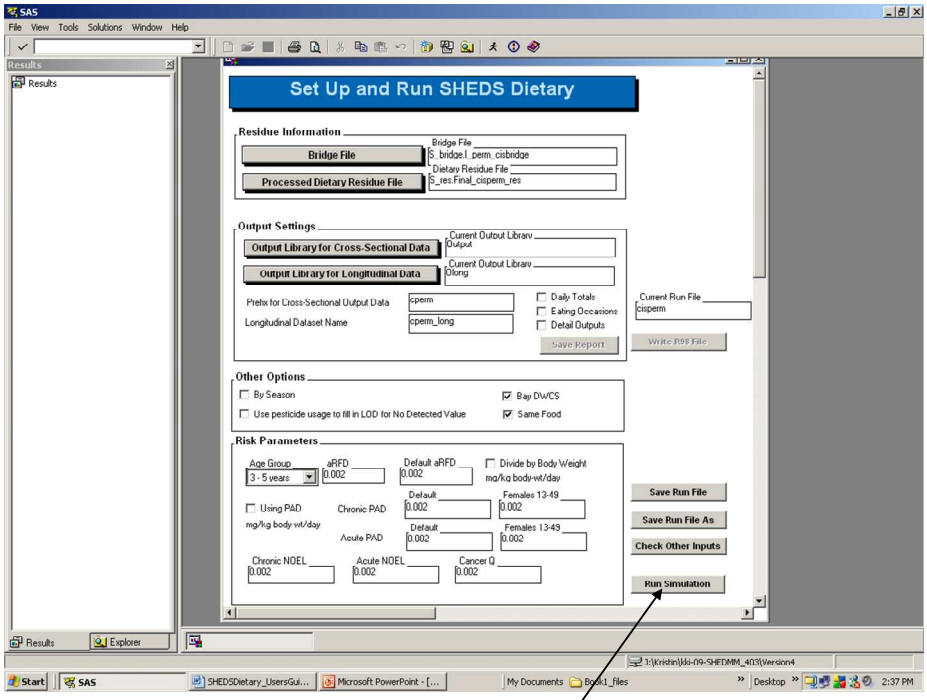
8) The Longitudinal dataset screen now opens. Select 1-1-2006 as the start date of the run and 12-31-2006 as the end date. The dates can be entered as text in the fields or selected using the arrow buttons. Select "Diversity and Autocorrelation" as the Diary Assembly Method. Enter 0.3 for both the Diversity and Autocorrelation values. Enter "cperm_" as the prefix for the cross-sectional output data, and "cperm_long" as the name of the longitudinal dataset file. Choose to simulate 100 people. Select 3 as the number of cross-sectional interaction runs to include when creating the longitudinal exposures, then hit <Save>.



Select <Diversity and Autocorrelation method. Enter diversity and autocorrelation values. Select run dates, names for output files, number of persons, number of interaction runs to use, and. Click <Save>.

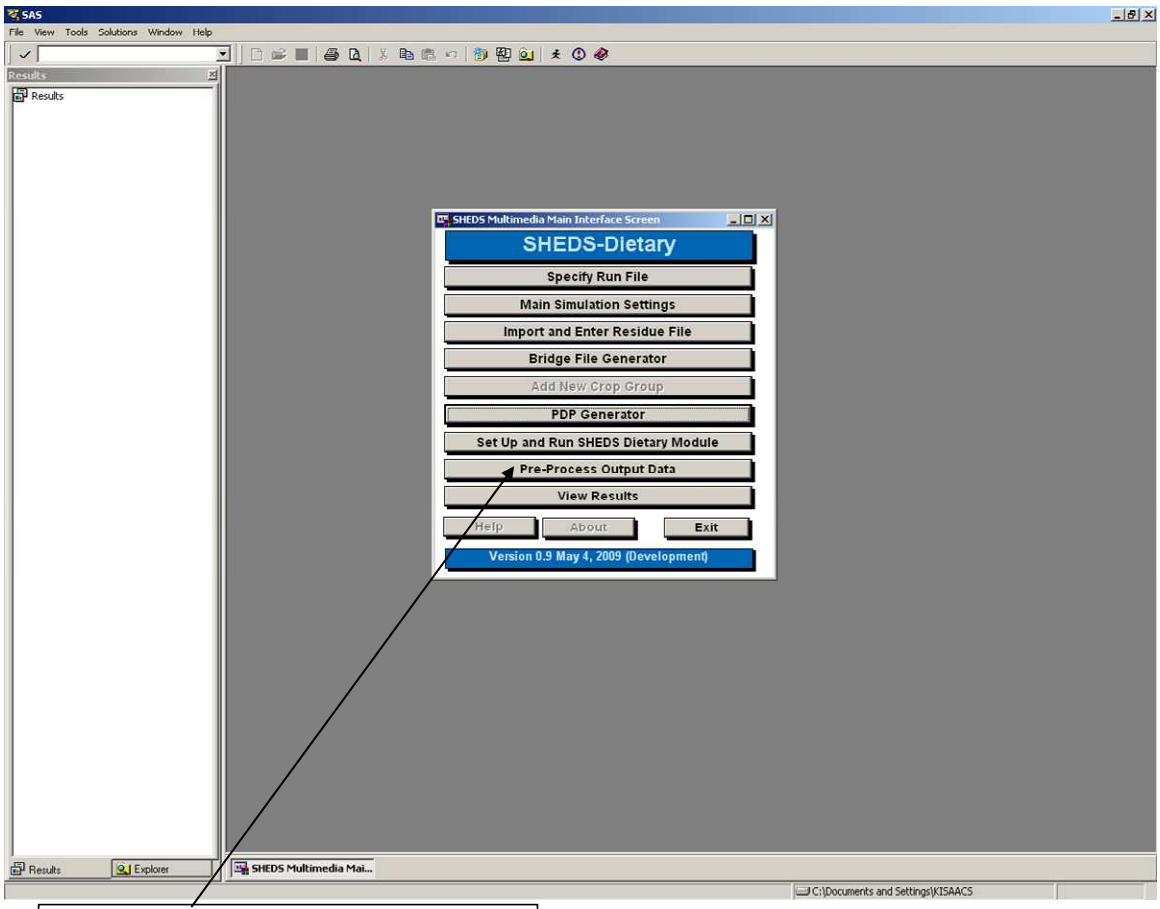
9) Select the <Set Up and Run SHEDS-Dietary> button from the Main SHEDS screen. This screen finalizes the settings for the run. Edit any of the example risk parameters as desired. The simulation is then run by selecting <Run Simulation>. Depending on computing resources, this may take more than several minutes. When completed, hit <Exit.>



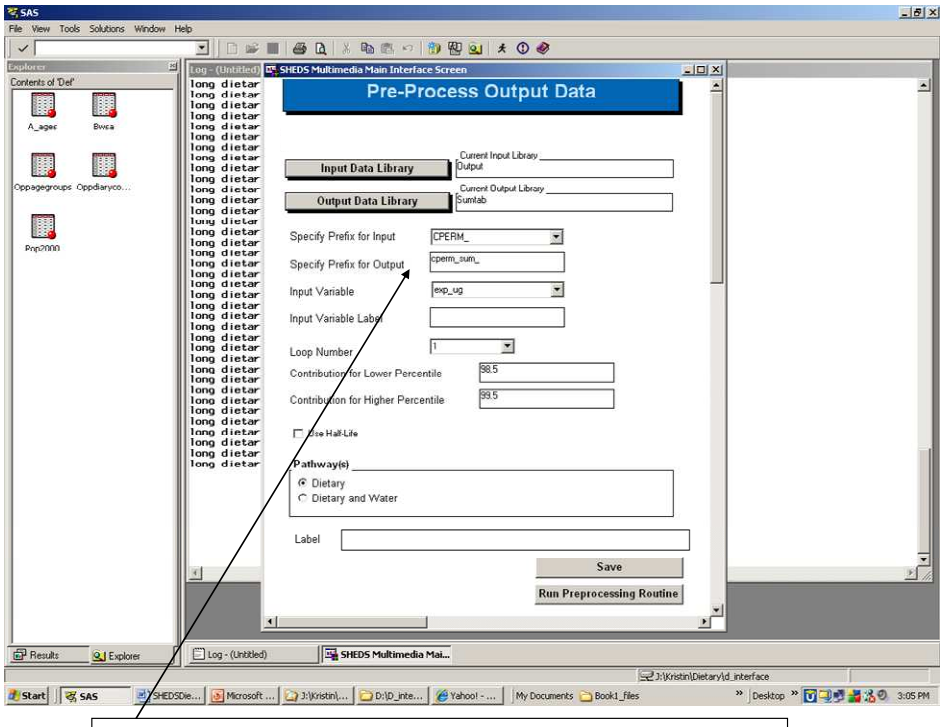


Accept defaults, and click <Run Simulation>

10) Now preprocess the raw model output data to generate summary tables and percentiles that can be visualized. Select <Pre-Process Output Data> from the Main SHEDS screen. Select the prefix of the run to be preprocessed (prefix for input =“cperm_”), the location where the output summary data are to be stored (the “sumtab” library), and a prefix for the summary data (“cperm_sum_”). Select the variable to process. Since this is a single chemical run, the only available variable is Exposure - Permethrin Cis. Also select how many interaction runs should be processed (loop number=1) and the contribution percentiles, then hit <Run Pre-Processing Routine>, then <OK>.



Click here to pre-process data



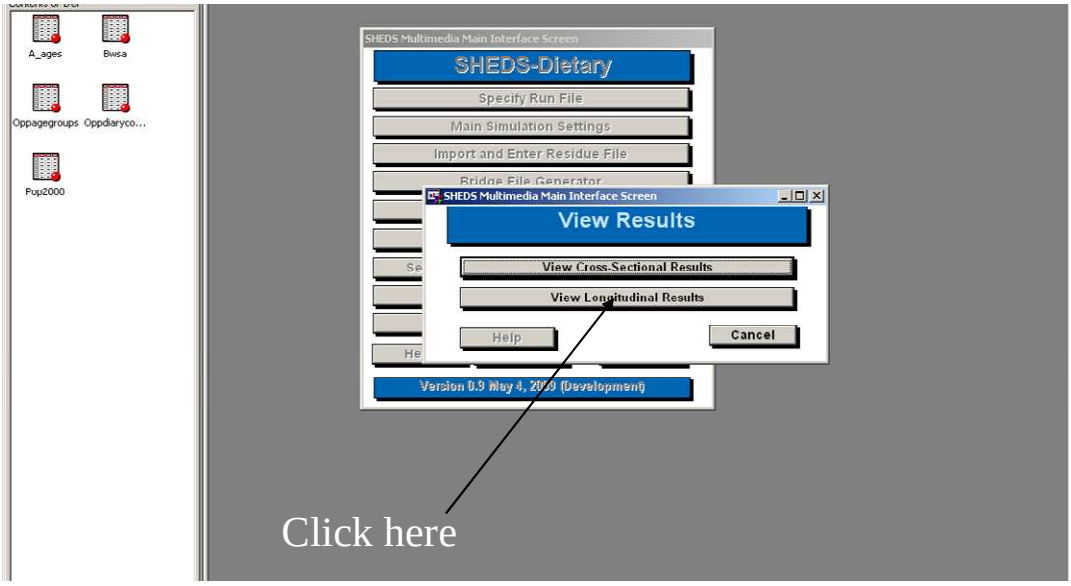
Choose a prefix for the summary output; click <save>

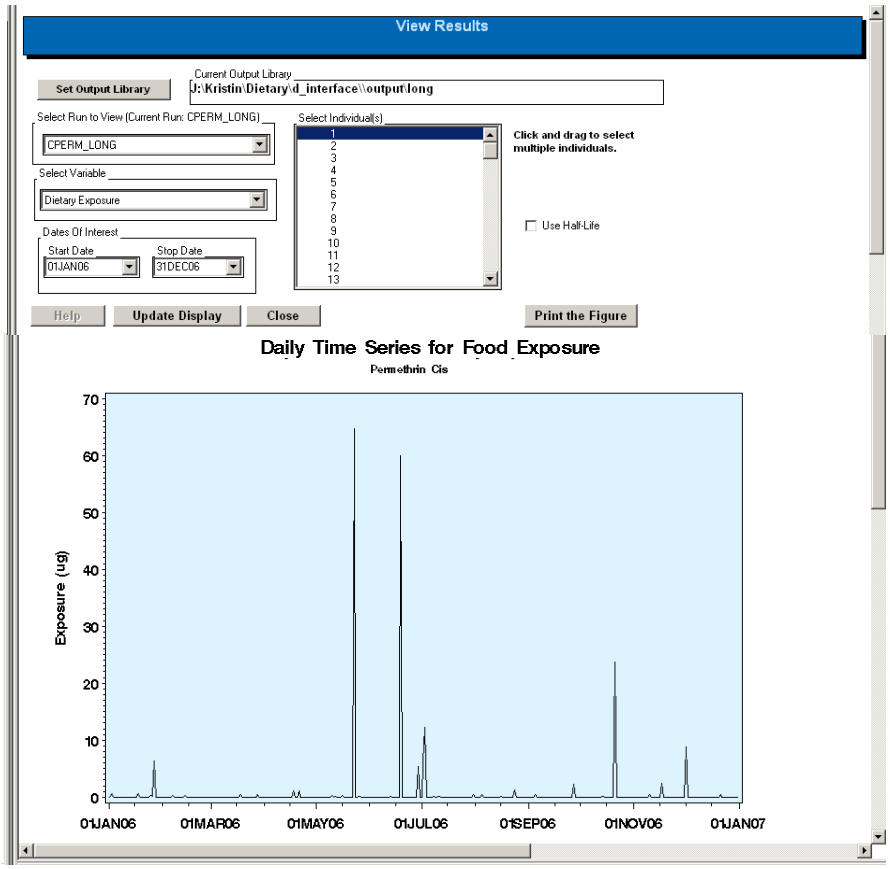
Steps 11)-17) Follow Steps 10-16 of Case Study 2 to visualize the summary Cross-Sectional data associated with this run.

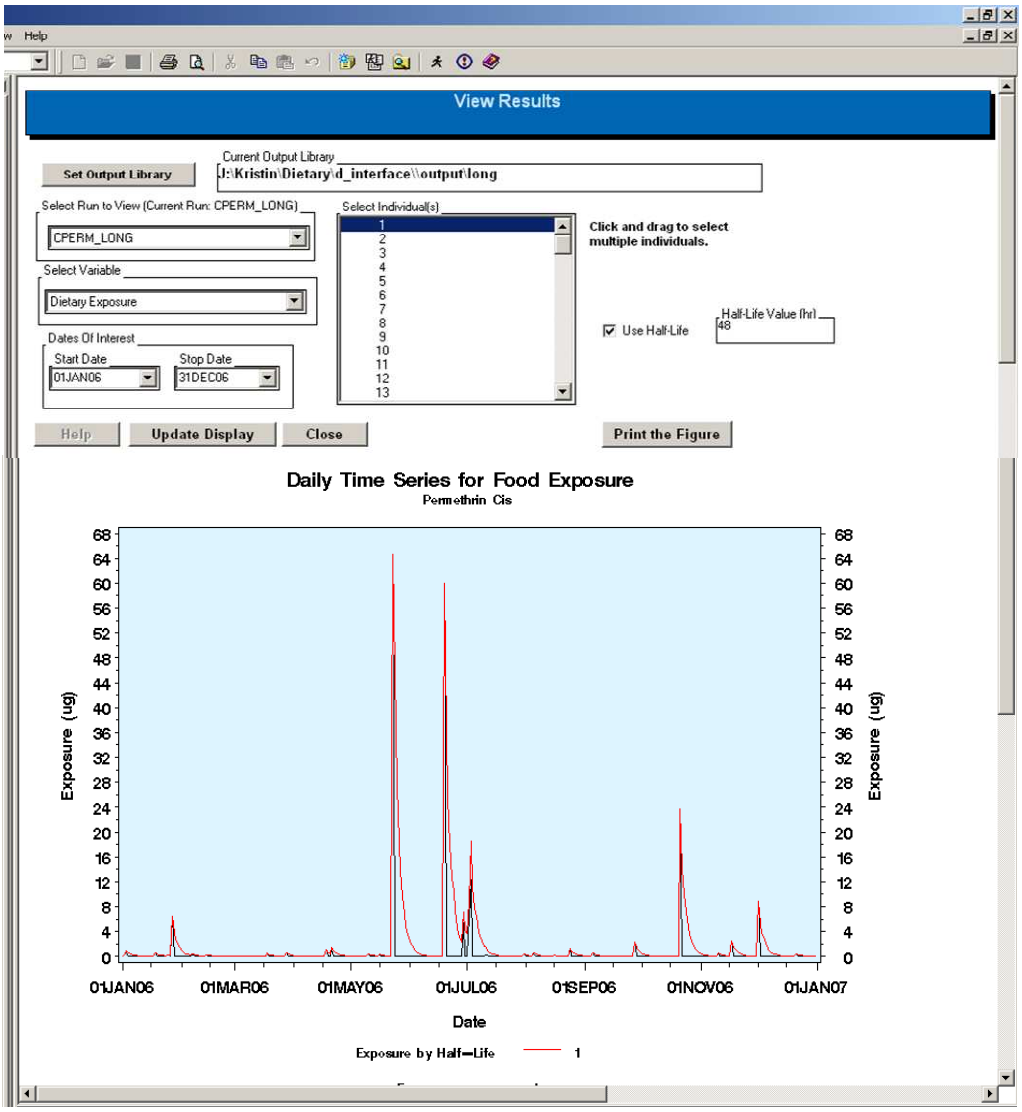
18) Select View Results from the Main Screen. Select View Longitudinal Results. The View Longitudinal Results screen will appear. Select the name of the output longitudinal dataset ("cperm_long"). The display will update to show the longitudinal exposure pattern for person number 1. Any person from the simulation can be viewed, by using the "Select Individuals" list box. Multiple persons can be visualized at once by clicking and dragging on the selection box to highlight multiple persons, and then clicking "Update Display."

The persistence of the chemical in the body can also be added to the plot, by checking "use-half life", entering a half-life value (hit the return button), and clicking "Update Display". The example below depicts the results of using a half-life of 48 hours.

NOTE: Time series may not look identical to that shown below due to the stochastic nature of the longitudinal diary assembly.


A_ages
Bwsa
Oppagegroups
Oppdiaryco...
Pop2000
SHEDS Multimedia Main Interface Screen
SHEDS-Dietary
Specify Run File
Main Simulation Settings
Import and Enter Residue File
Bridge File Generator
SHEDS Multimedia Main Interface Screen
View Results
View Cross-Sectional Results
View Longitudinal Results
Help
Cancel
Version 0.9 May 4, 2009 (Development)
Click here

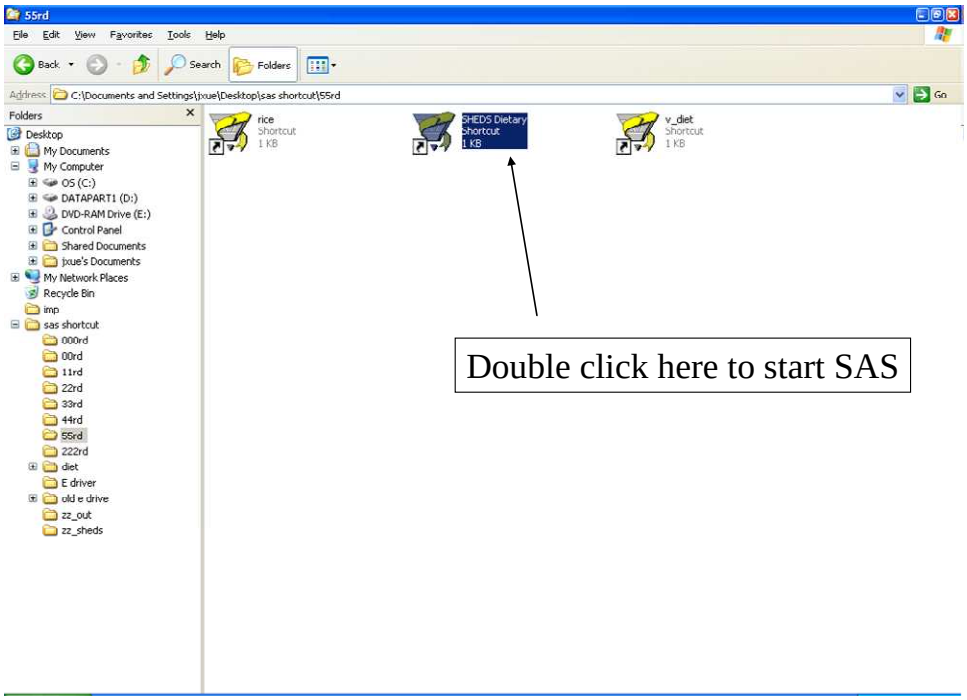

View Results
Set Output Library
Current Output Library
J:\Kristin\Dietary\d_interface\\output\long
Select Run to View (Current Run: CPERM_LONG)
CPERM_LONG
Select Variable
Dietary Exposure
Dates Of Interest
Start Date
01JAN06
Stop Date
31DEC06
Select Individual(s)
1
2
3
4
5
6
7
8
9
10
11
12
13
Click and drag to select multiple individuals.
Use Half-Life
Help
Update Display
Close
Print the Figure
Daily Time Series for Food Exposure
Permethrin Cis
Exposure (ug)
70
60
50
40
30
20
10
0
01JAN06
01MAR06
01MAY06
01JUL06
01SEP06
01NOV06
01JAN07


View Results
Set Output Library
Current Output Library
J:\Kristin\Dietary\d_interface\\output\long
Select Run to View (Current Run: CPERM_LONG)
CPERM_LONG
Select Variable
Dietary Exposure
Dates Of Interest
Start Date
01JAN06
Stop Date
31DEC06
Select Individual(s)
Click and drag to select multiple individuals.
Use Half-Life
Half-Life Value (hr)
48
Help
Update Display
Close
Print the Figure
Daily Time Series for Food Exposure
Permethrin Cis
Exposure (ug)
Date
01JAN06
01MAR06
01MAY06
01JUL06
01SEP06
01NOV06
01JAN07
Exposure by Half-Life
1

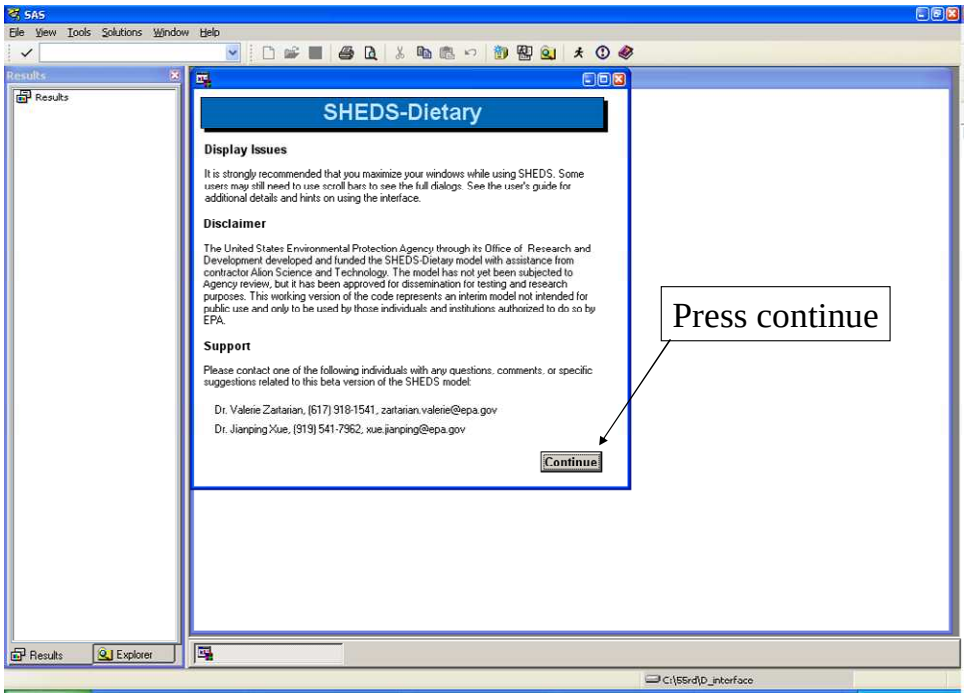
7.4 Case Study 4: Pyrethroids, Cross-Sectional Run

This case study is a cumulative (multi-chemical) example for simulation of food exposure. This is a cross-sectional simulation. This run uses files created by the PDP Generator.

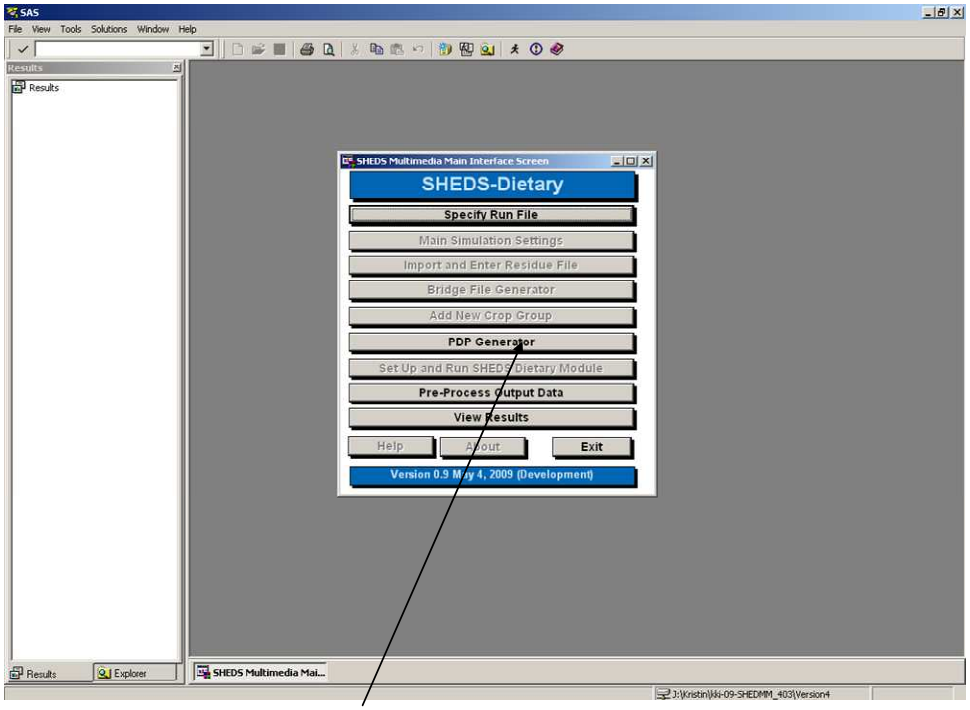
1) Initiate a SHEDS-Dietary session by double-clicking the SAS icon.



2) The SHEDS disclaimer screen appears first; select <Continue> to proceed to the main SHEDS screen.

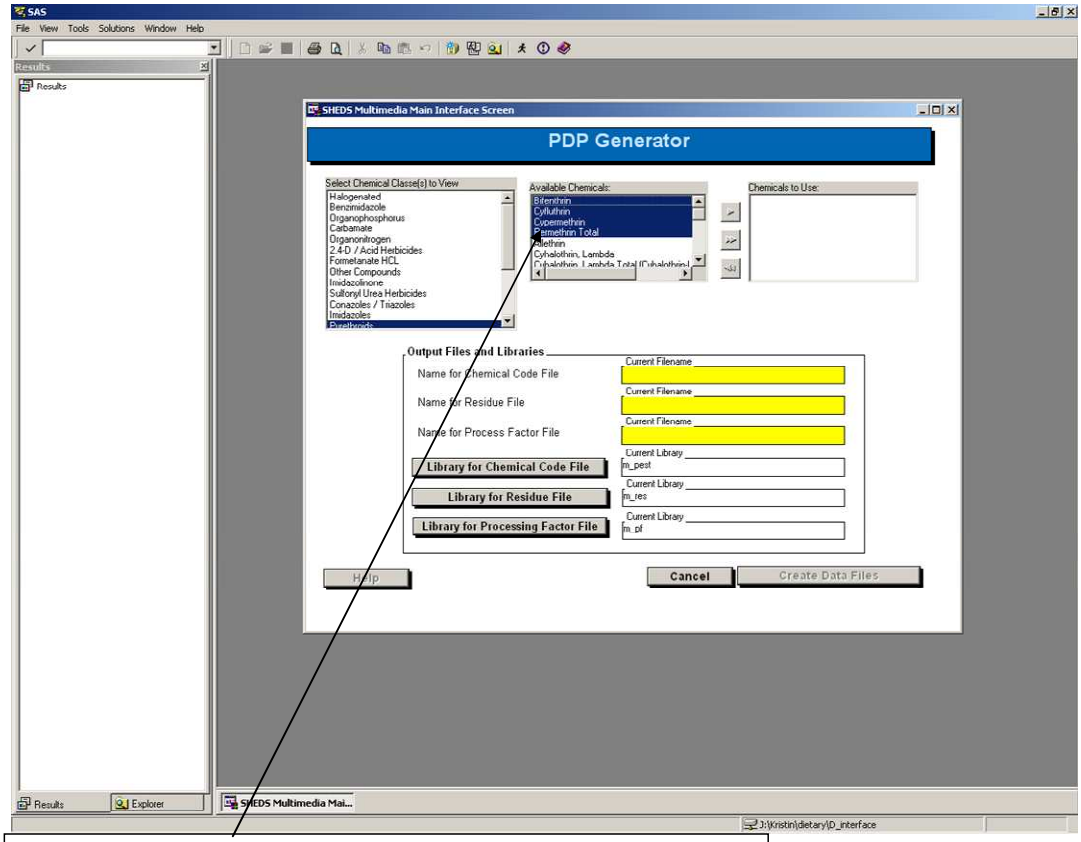


3) Select the PDP Generator.

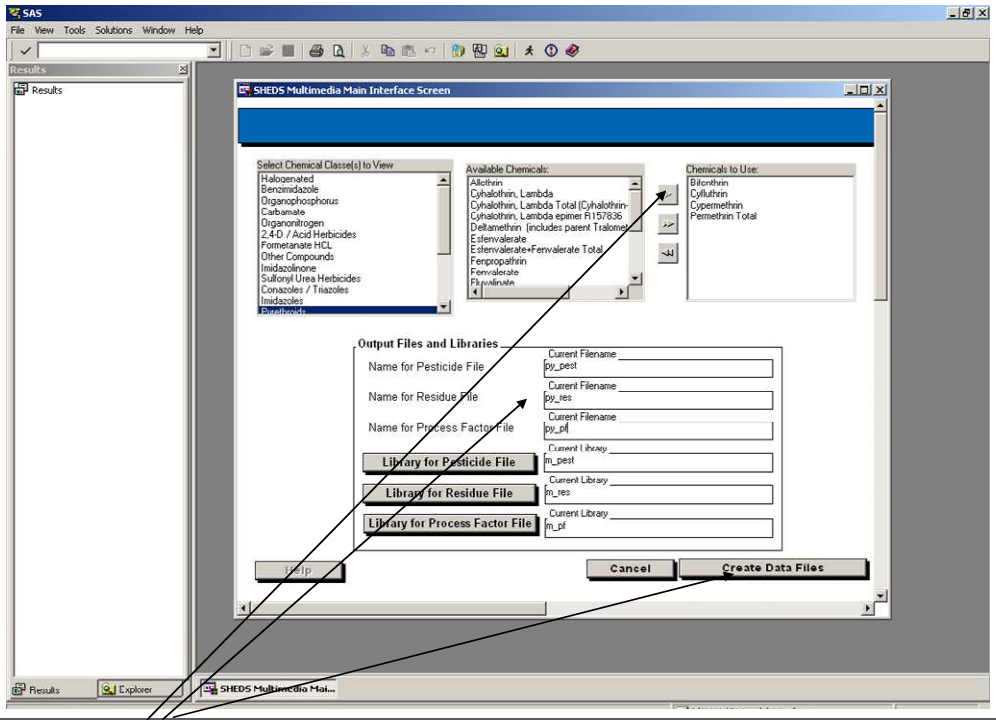


Click <PDP Generator>

4) Select the chemical class “Pyrethroids”. (Note that additional classes can also be viewed by clicking on the class name). For this example, click and drag in the Available Chemicals list box to highlight “Bifenthrin”, Cyfluthrin”, “Cypermethrin”, and “Permethrin Total.” Click the single arrow button to select these chemicals. They will move to the Chemicals to Use listbox. Enter names for the Chemical code file, the residue file, and the processing factor file: py_pest, py_res, and py_pf. Click “Create Data Files”. (This may take several minutes). When the screen closes, the file creation is complete.

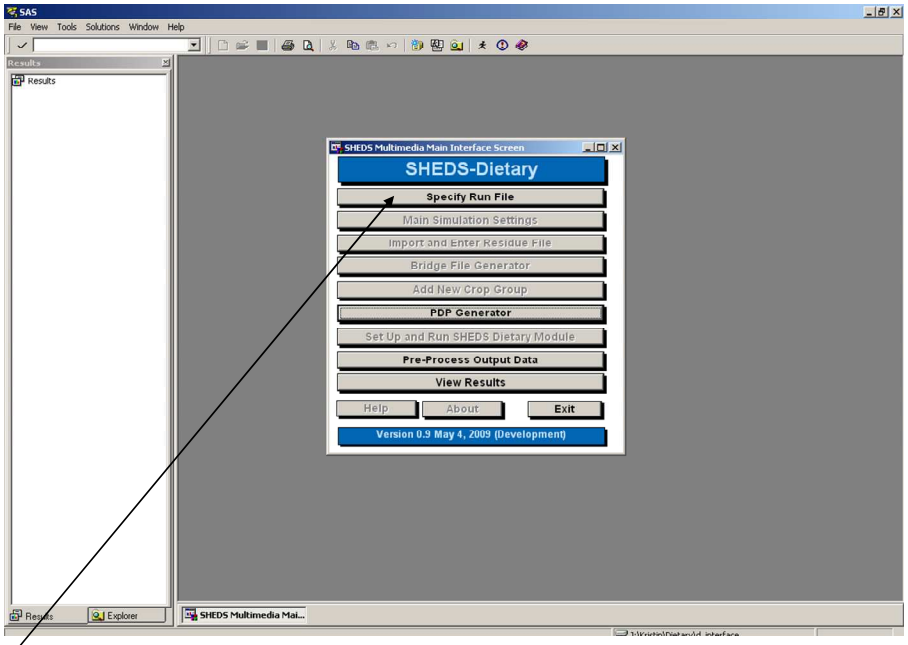


Click and drag to highlight the first four chemicals

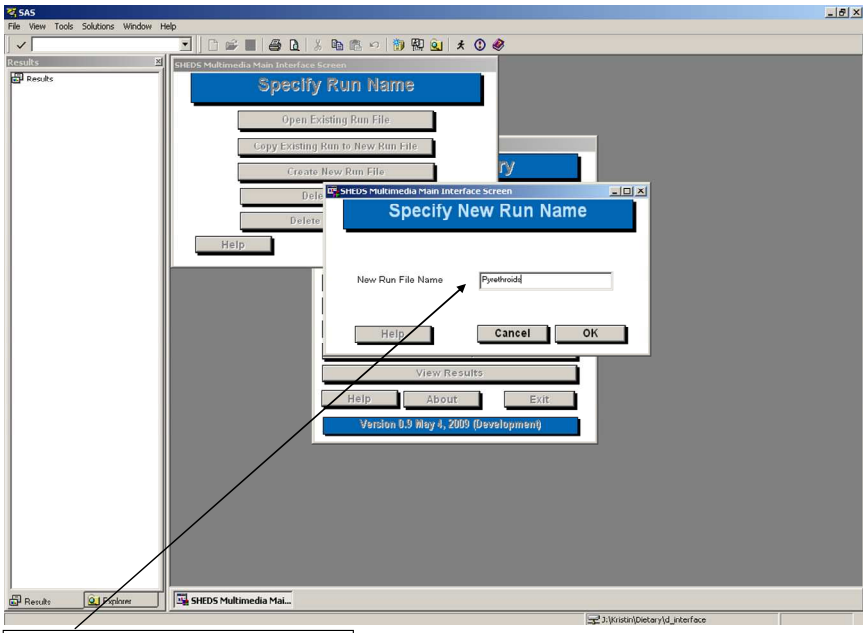


Click arrow key to select chemicals, enter filenames, and click <Create Data Files>

5) Select <Specify Run File>-><Create New Run File> to initiate the creation of a new run for Pyrethroids. Enter the name of the new run as “Pyrethroids” when prompted and select <OK>.



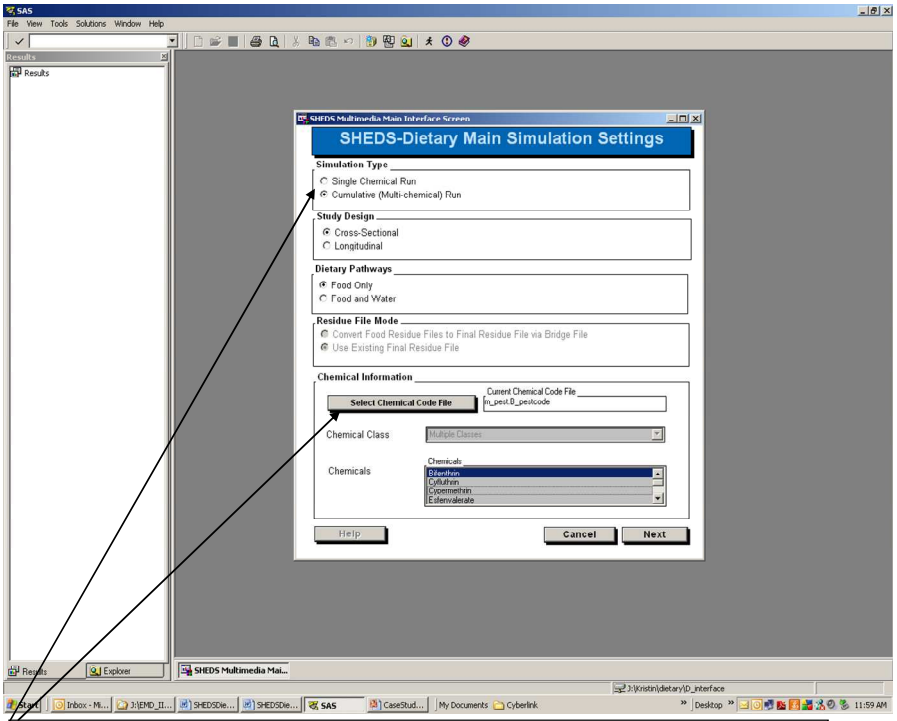
Click <Specify Run File>



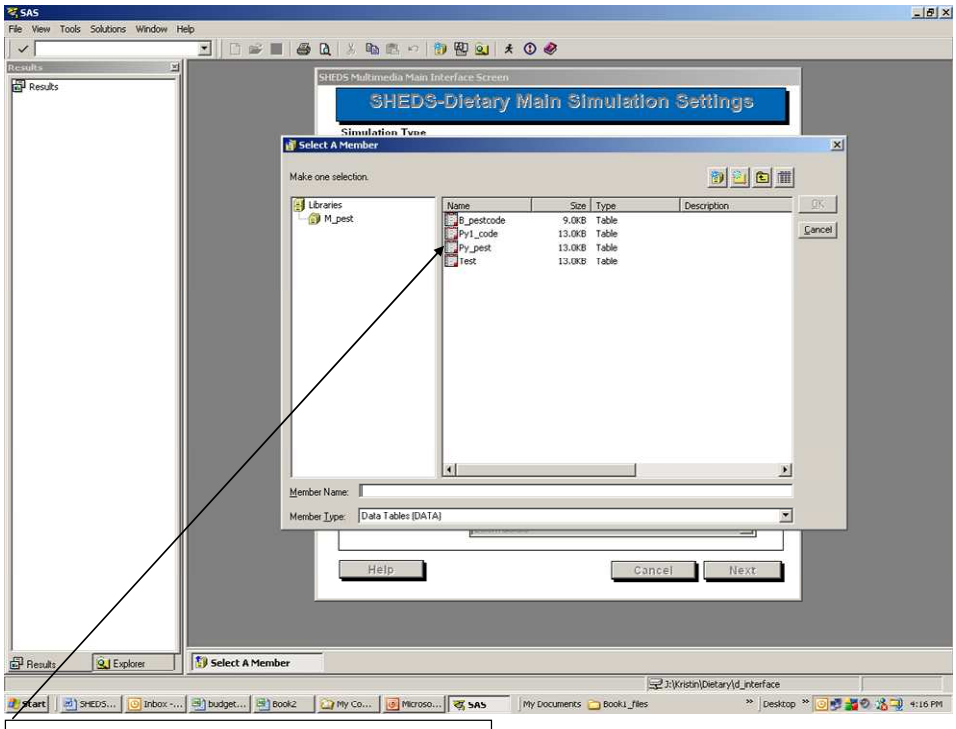
Enter run name, “Pyrethroids”

6) The Main Simulation Settings button will now be enabled. Select it and the Main Simulation Settings screen will appear. Select “Cumulative (Multi-Chemical) Run”. Click <Select Chemical Code File>. From the list, select “py_pest”, the pesticide code file you created using

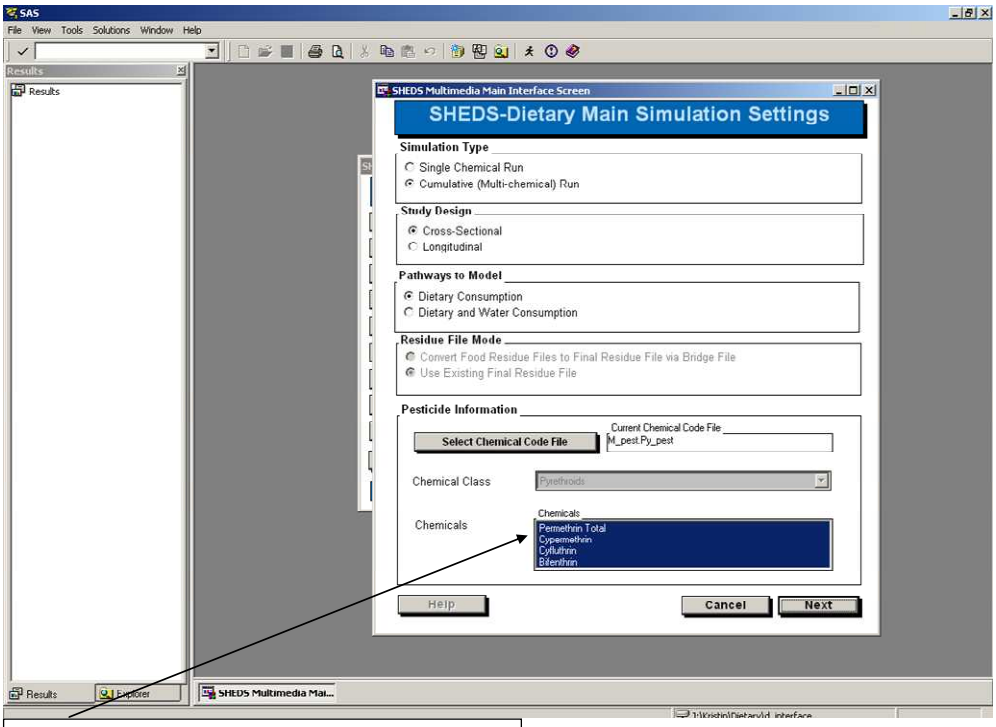
the PDP Generator. When you return to the Main Simulation screen, highlight all the available chemicals and click <Next>.



Select <Cumulative Run> and click <Select Chemical Code File>

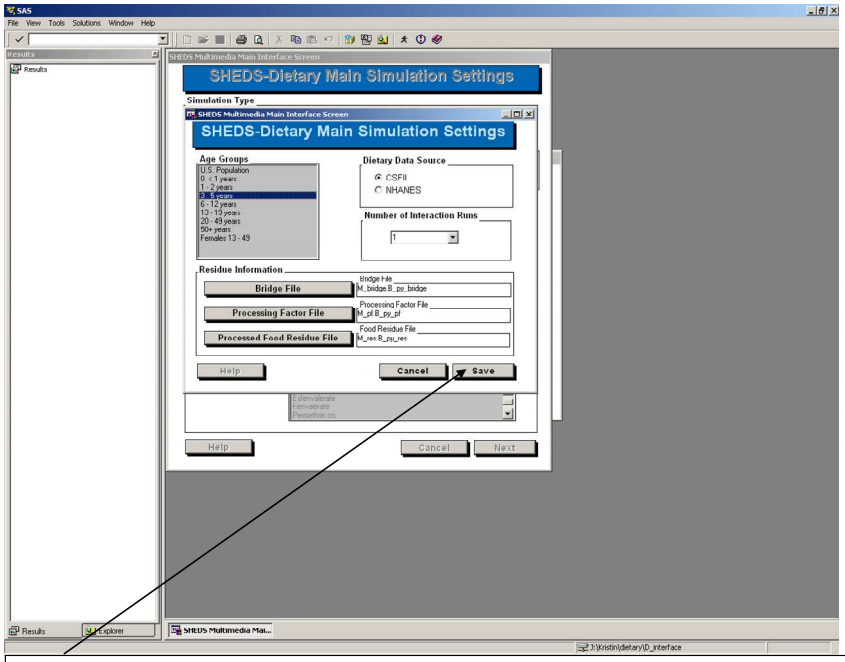


Select file “Py_pest” and click <OK>.



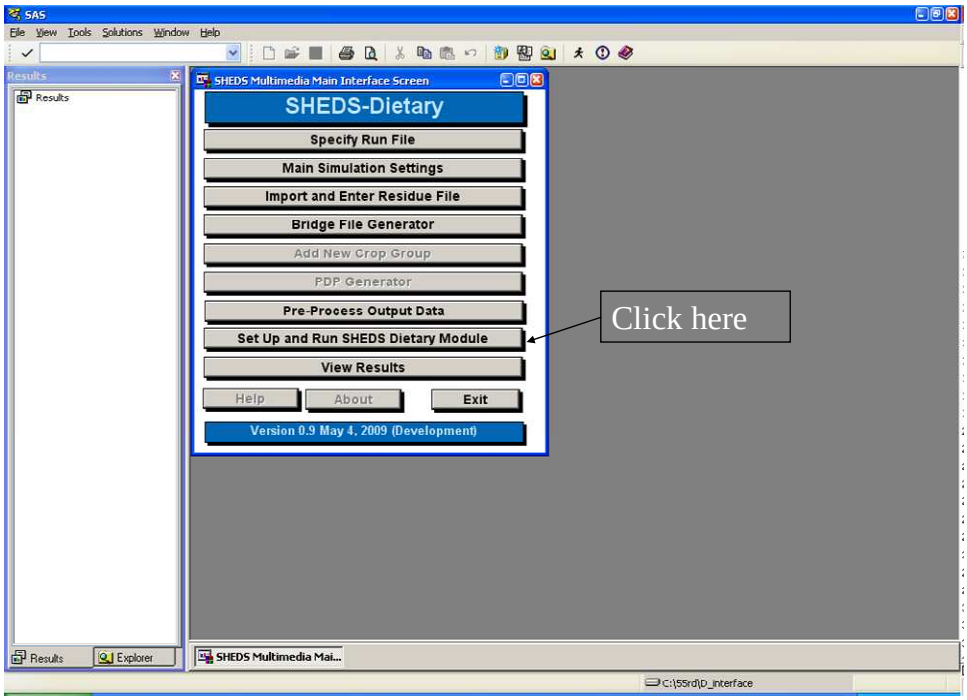
Select all four chemicals, click <Next>

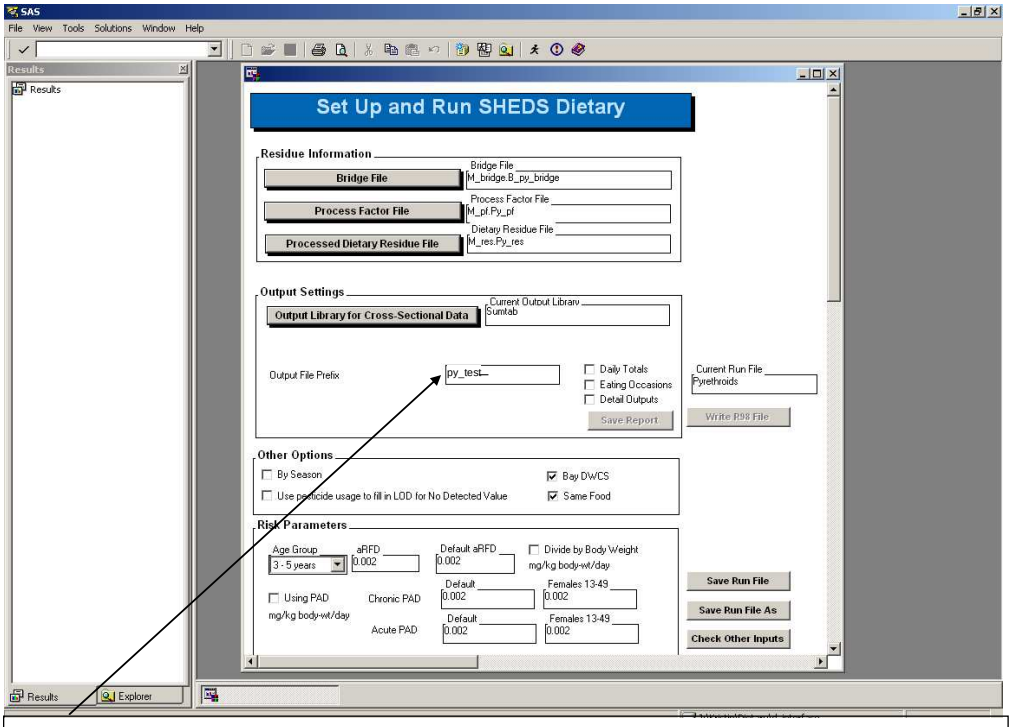
7) The second Main Simulation Settings screen appears. Click the Bridge File button to select a Bridge File for the run. Select B_py_Bridge from the file selection dialog. Repeat the process to select the processing factor and dietary residue files, selecting “py_pf” and “py_res” (text fields will fill in with the full dataset name, including the SAS library prefix) . Then select 1 as the number of interaction runs and click <Save>.



Click <Bridge File>, select “B_py_bridge’ from dialog. Repeat for Processing factor and Dietary residue files, selecting “py_pf” and “py_res,” respectively. Click <Save>.

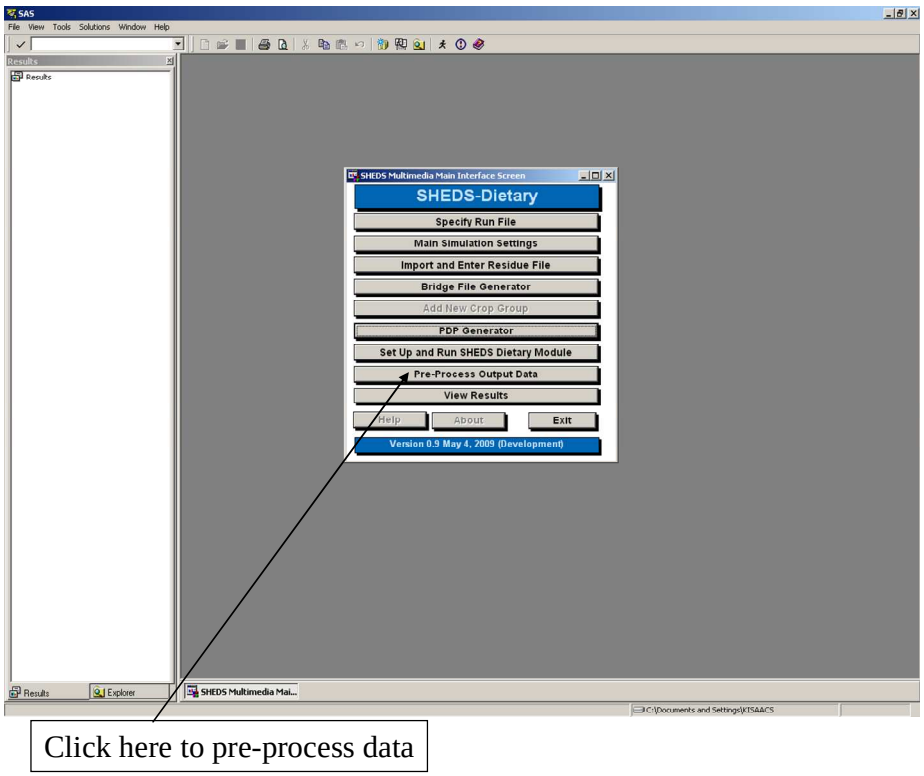
8) Select the <Set Up and Run SHEDS-Dietary> button from the Main SHEDS screen. This screen finalizes the settings for the run. Select the library where the model output is to be located (“sumtab”), and provide a prefix for the run (“py_test_”). Edit any desired risk (toxicological) parameters. The simulation is then run by selecting <Run Simulation>.

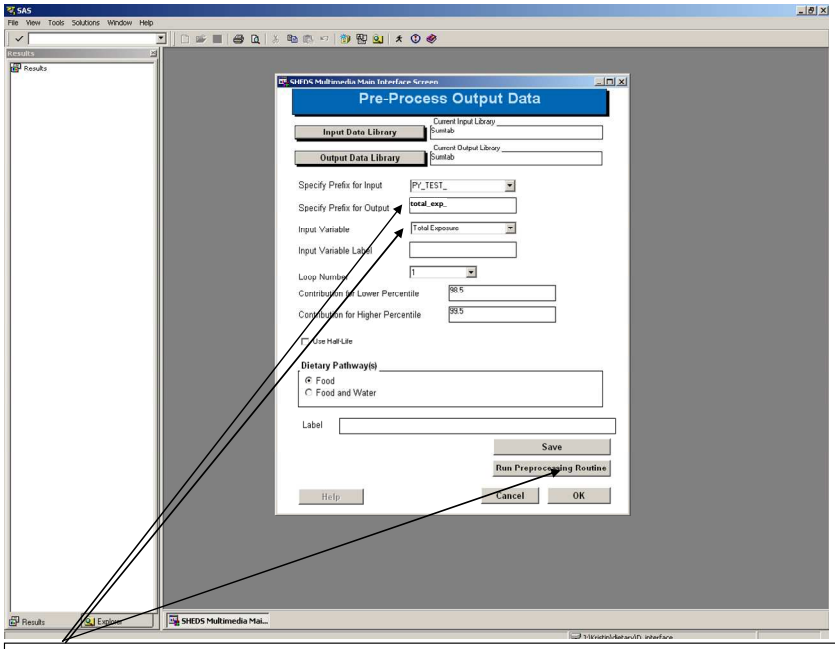




Enter prefix “py_test” for run ouput; click <Run Simulation>

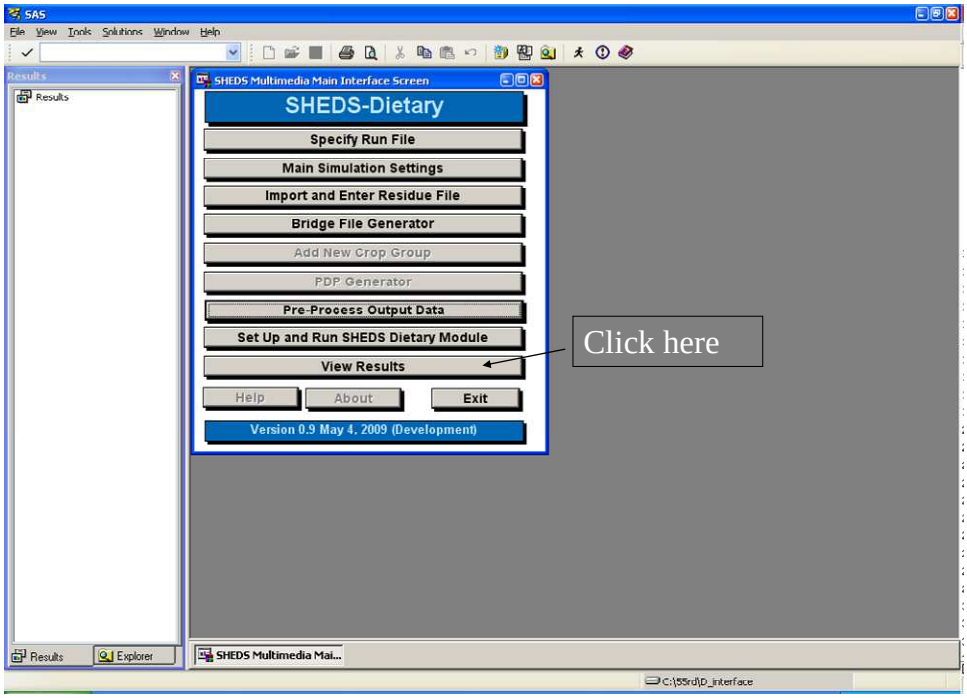
9) Now preprocess the raw model output data to generate summary tables and percentiles that can be visualized. Select <Preprocess Output Data> from the Main SHEDS screen. Select the prefix of the run to be preprocessed ("py_test_"), the location where the output summary data are to be stored (the "sumtab" library), and a prefix for the output ("total_exp_"). Select the variable to process. Since this is a multiple chemical run, exposure variables for many different chemicals are available. Select "Total Exposure", which the cumulative exposure due to the four selected chemicals for the run. Also select how many interaction runs should be processed and the contribution percentiles.

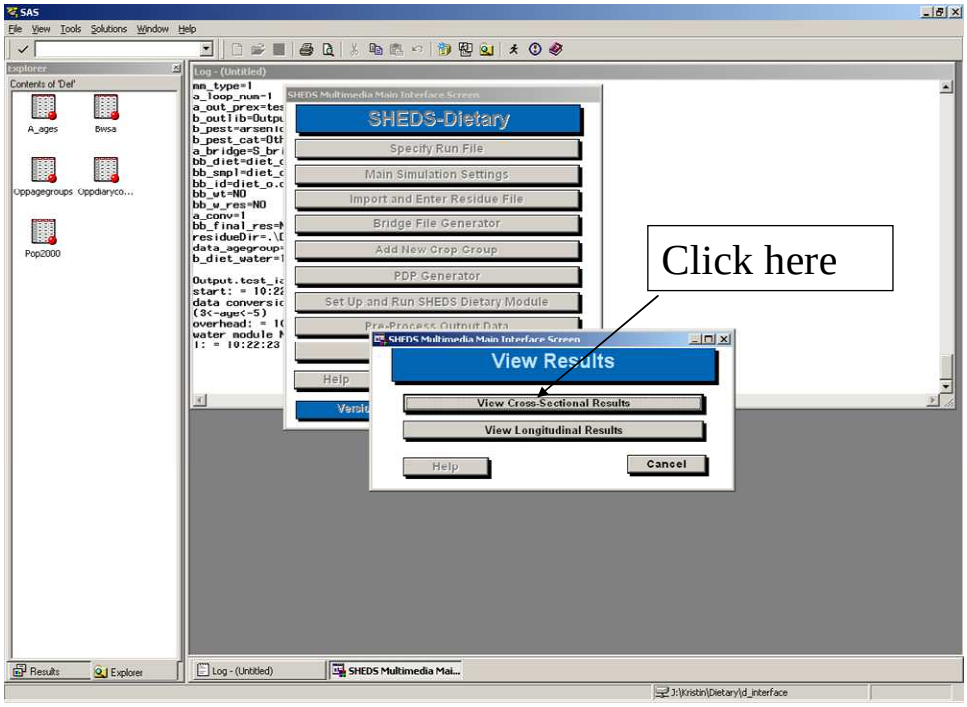




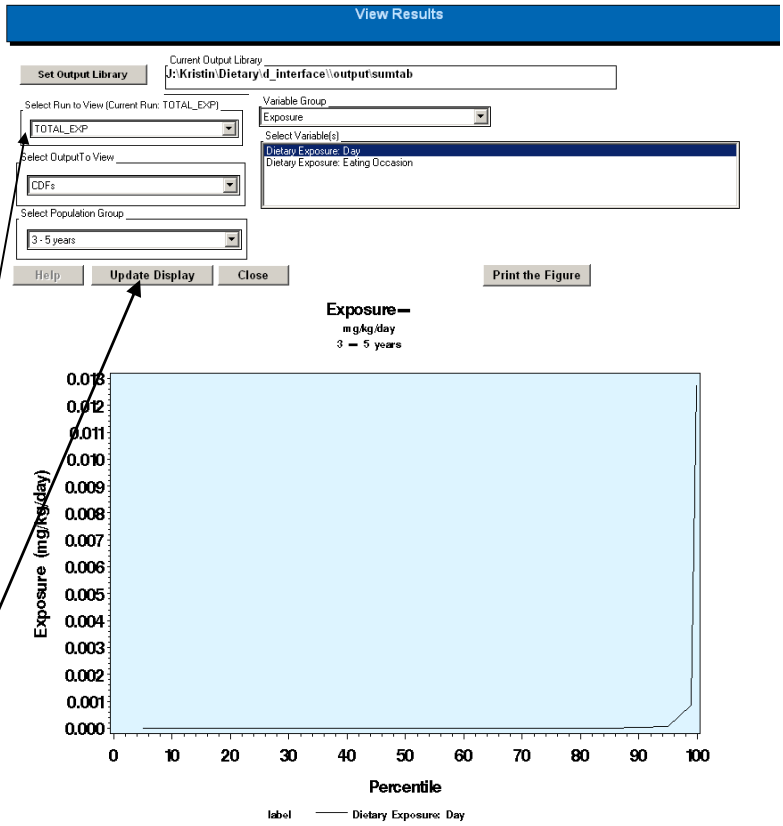
Enter "total_exp" for output Prefix. Select input variable "Total Exposure." Click <Run Preprocessing Routine>.

10) Click on the <View Results> button to display the View Results selection screen. Select <View Cross-Sectional Data>.



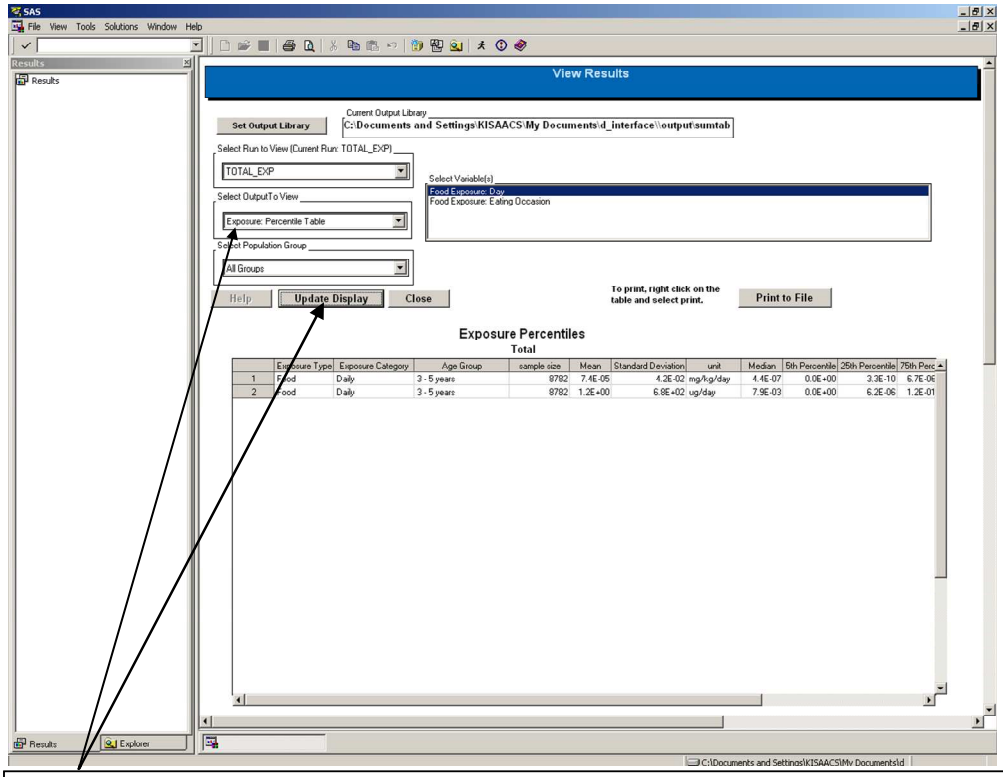


11) The main View Cross-Sectional Results screen will now appear. Select the run of interest from the run selection list, by selecting the prefix that was entered in the Pre-process screen ("total_exp", in this case). Select "CDFs" as the output to view, and highlight one of the two available variables (daily or eating occasion food exposure). Selecting <Update Display> will update the figure with the selected options. In this way, different output tables and graphs can be generated.



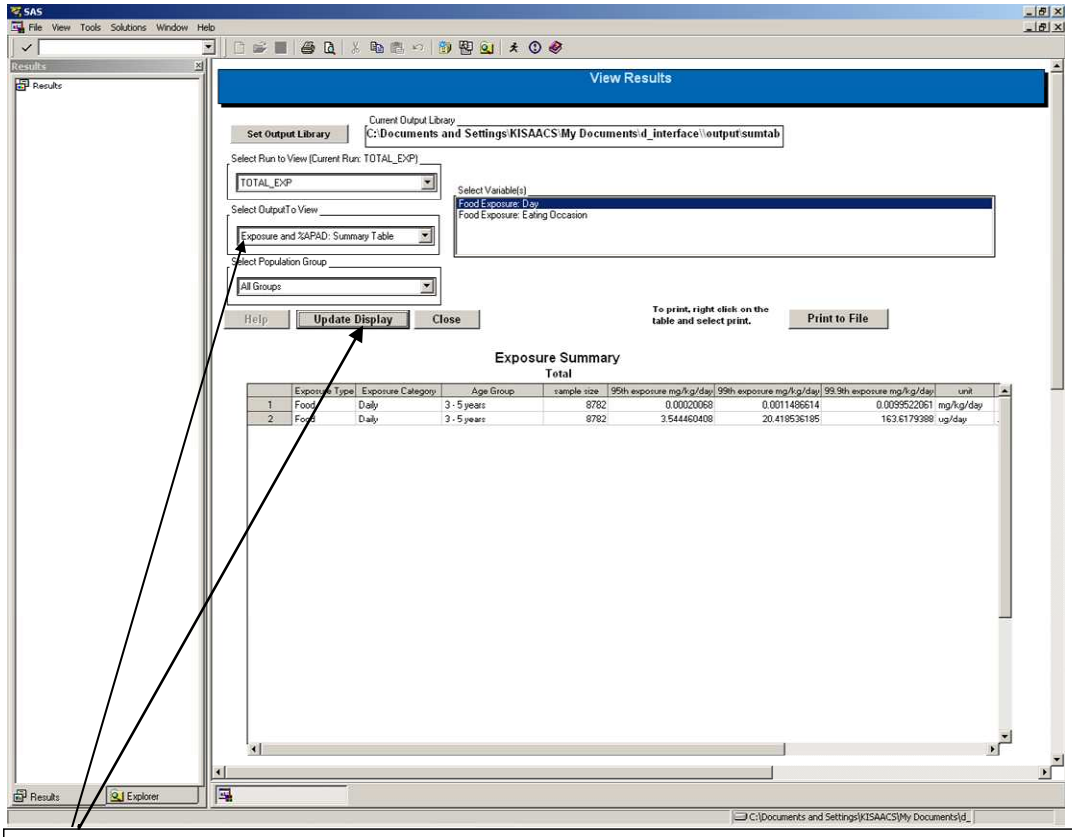
Select “TOTAL_EXP” from list. Click <Update Display>.

11) Select “Exposure Percentile Table” as the output to view, and click <Update Display>. This will generate the requested table for the selected variables.



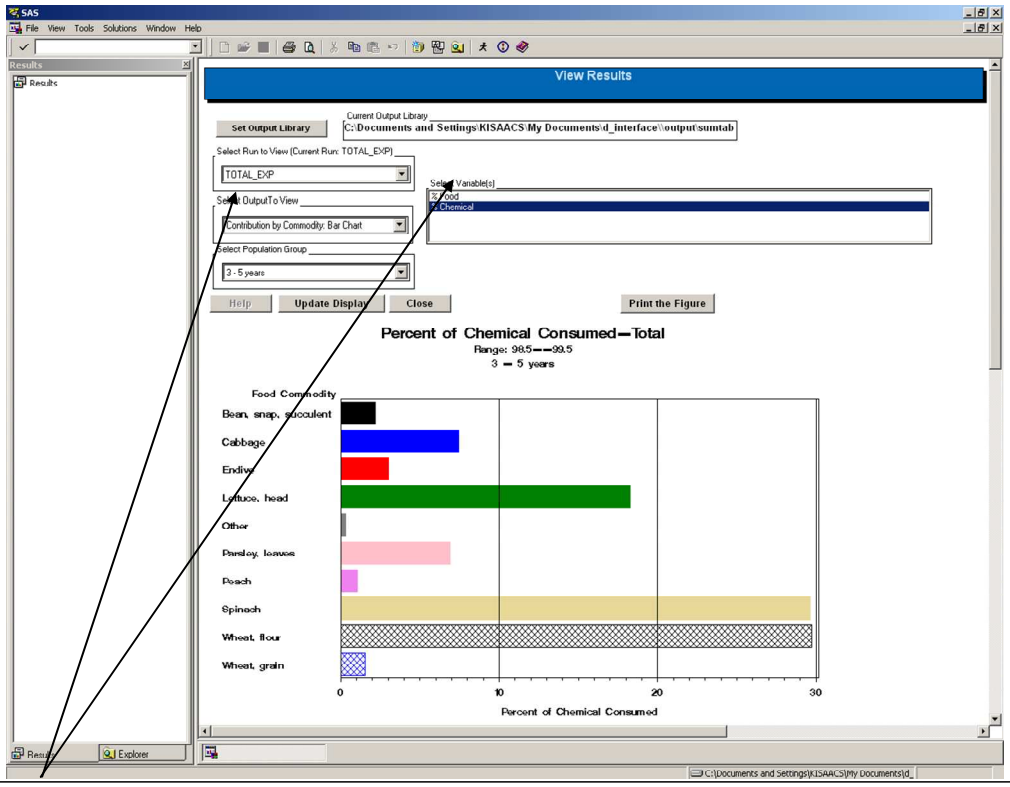
Select “Exposure: Percentile Table” from list. Click <Update Display>.

12) Repeat this process by selecting “Exposure and %APAD: Summary Table” and again updating the display.



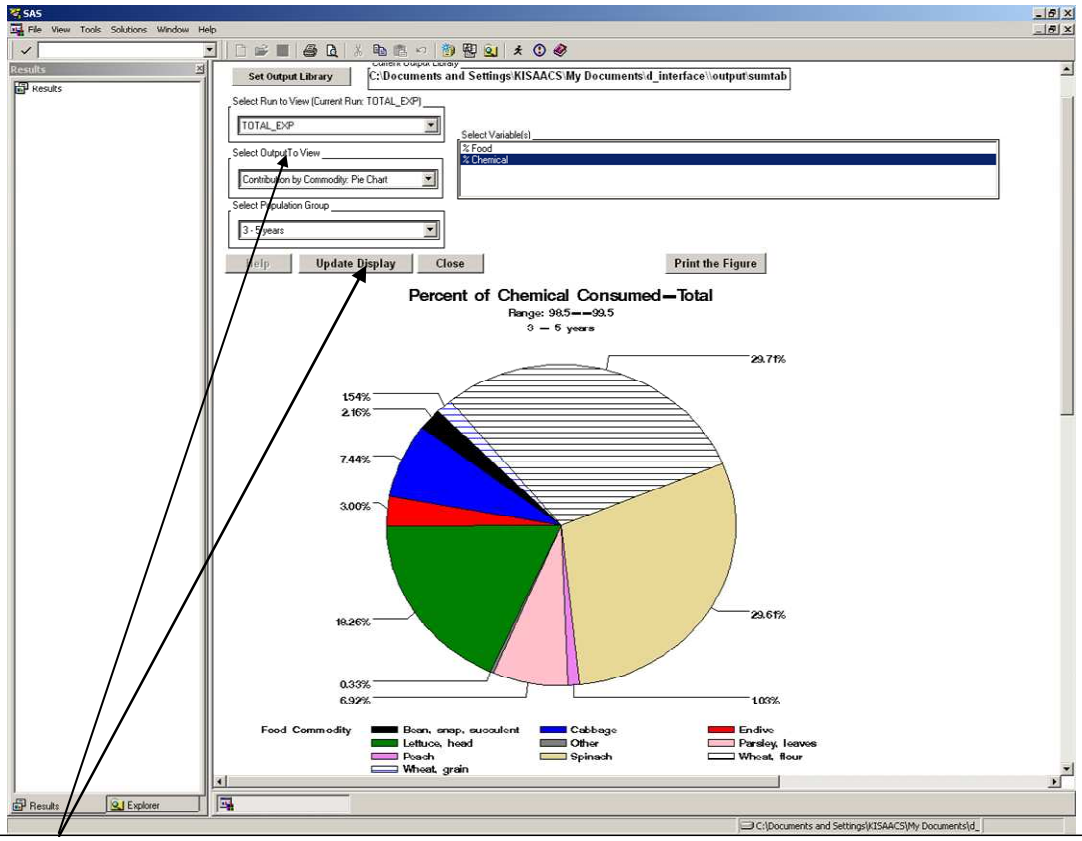
Select “Exposure and %APAD: Summary Table” from list. Click <Update Display>.

13) Selecting “Contribution by Commodity: Bar Chart” as output to view and “%Chemical” as the variable produces a bar chart of the contribution of food types to total chemical exposure.



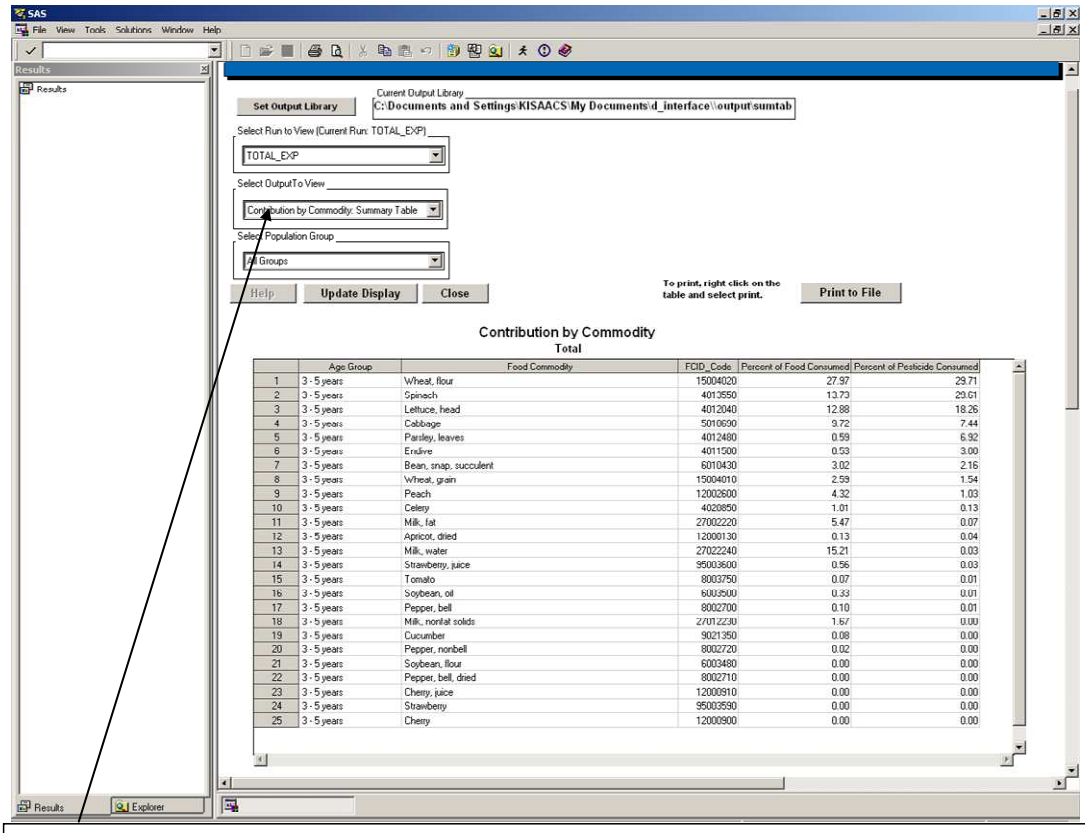
Select “Contribution By Commodity: Bar Chart” from list and %Chemical as the variable. Click <Update Display>.

14) An analogous Pie chart can also be displayed by selecting “Contribution by Commodity: Pie Chart” and “%Chemical”.



Select “Contribution By Commodity: Pie Chart” from list. Select %Chemical. Click <Update Display>.

15) Finally, a contribution table can be created by selecting “Contribution by Commodity: Summary Table” as the output to view.



	Age Group	Food Commodity	FCID_Code	Percent of Food Consumed	Percent of Pesticide Consumed
1	3 - 5 years	Wheat, flour	15004020	27.97	29.71
2	3 - 5 years	Spinach	4013550	13.73	29.61
3	3 - 5 years	Lettuce, head	4012040	12.88	18.26
4	3 - 5 years	Cabbage	5010690	9.72	7.44
5	3 - 5 years	Parsley, leaves	4012480	0.59	6.92
6	3 - 5 years	Endive	4011500	0.53	3.00
7	3 - 5 years	Bean, snap, succulent	6010430	3.02	2.16
8	3 - 5 years	Wheat, grain	15004010	2.59	1.54
9	3 - 5 years	Peach	12002600	4.32	1.03
10	3 - 5 years	Celery	4020850	1.01	0.13
11	3 - 5 years	Milk, fat	27002220	5.47	0.07
12	3 - 5 years	Apricot, dried	12000130	0.13	0.04
13	3 - 5 years	Milk, water	27022240	15.21	0.03
14	3 - 5 years	Strawberry, juice	95003600	0.56	0.03
15	3 - 5 years	Tomato	8003750	0.07	0.01
16	3 - 5 years	Soybean, oil	6003500	0.33	0.01
17	3 - 5 years	Pepper, bell	8002700	0.10	0.01
18	3 - 5 years	Milk, nonfat solids	27012230	1.67	0.00
19	3 - 5 years	Cucumber	9021350	0.08	0.00
20	3 - 5 years	Pepper, nonbell	8002720	0.02	0.00
21	3 - 5 years	Soybean, flour	6003480	0.00	0.00
22	3 - 5 years	Pepper, bell, dried	8002710	0.00	0.00
23	3 - 5 years	Cherry, juice	12000910	0.00	0.00
24	3 - 5 years	Strawberry	95003590	0.00	0.00
25	3 - 5 years	Cherry	12000900	0.00	0.00

Select “Contribution By Commodity: Summary Table” from list. Click <Update Display>.

8 References

Barraj, L.M., Daniels, C.L. 2004. “Drinking Water Consumption Survey”, September 15, 2004, Sponsored by BayerCropScience, Performing Laboratory, Exponent.®, pp.40.

Glen G., Zartarian V.G., Smith, L., and Xue J. (2010). The Stochastic Human Exposure and Dose Simulation (SHEDS)-Residential Model Technical Manual. Prepared for the July 20-22, 2010 EPA FIFRA SAP, Crystal City, VA.

Isaacs K., Xue J., Stallings C., Zartarian V.G. (2010) Stochastic Human Exposure and Dose Simulation (SHEDS) Model for Multimedia, Multipathway Chemicals: Version 1 SHEDS-Dietary Module User Guide. Prepared for the July 20-22, 2010 EPA FIFRA SAP, Crystal City, VA.

Xue J., Zartarian V.G., Nako S. 2010. The Stochastic Human Exposure and Dose Simulation (SHEDS)-Dietary Model Technical Manual. Prepared for the July 20-22, 2010 EPA FIFRA SAP, Crystal City, VA.

Appendix A. Directories, Libraries, and Files

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

A.1 Directories/Libraries

On installation, the directories are laid out as in Table A-1. The indentation of a directory name implies that it is within the directory above it. Each of these directories is also assigned to a SAS library. Default and example SHEDS-Dietary input files can be found in the libraries highlighted in green. The libraries highlighted in blue are the default locations for SHEDS output files. The yellow libraries are those containing model input data that should not be edited by the user. The pink libraries contain model code.

Table A-1. SHEDS-Dietary Directories and Libraries

Directory	SAS Library	Description
<install>/d_interface/Diet_all	diet_all	Contains all the raw dietary data . This includes Food Diaries, Demographics, ADD FCID Recipes and LOOKUP tables: e.g. commodity names, name of eating occasion, food sources.
<install>/d_interface /Output	output	Default directory for cross-sectional output
<install>/d_interface /Output/detail	Odetail	Default directory for detailed output
<install>/d_interface /Output/long	Olong	Default directory for longitudinal output
<install>/d_interface /Output/sumtab	sumtab	Default directory for summary output
<install>/d_interface /User	Usr	Contains the dietary model code
<install>/d_interface /Macro	Macro	Not currently used
<install>/d_interface /Dietary/ Diet_data	Data	Default datasets required by the interface
<install>/d_interface/Dietary/Multi/Bridge	m_bridge	Bridge Files for multi chemical runs
<install>/d_interface/Dietary/Multi/Res	m_ res	Processed residue files for multi chemical runs
<install>/d_interface/Dietary/Multi/RPF	m_ RPF	RPF files for multi chemical runs
<install>/d_interface/Dietary/Multi/PF	m_ PF	PF files for multi chemical runs
<install>/d_interface/Dietary/Multi/Pest	m_ pest	Chemical code files for multi chemical runs
<install>/d_interface/Dietary/Multi/Usage	m_ usage	Usage files for multi chemical runs
<install>/d_interface /Dietary/Prg	prg	Directory containing interface macro code

Directory	SAS Library	Description
<install>/d_interface /Dietary/Runinfo	r_info	Directory containing run information files
<install>/d_interface /Dietary/Runinfo/chemicals	chem	Contains chemical code files for each run; contains PDP database
<install>/d_interface /Dietary/Runinfo/ages	ages	Contains age group files for each run
<install>/d_interface/Dietary/ Single /Bridge	m_bridge	Bridge Files and index files for single chemical runs
<install>/d_interface/Dietary/ Single /Res	s_ res	Processed residue files for single chemical runs
<install>/d_interface/Dietary/ Single /RPF	s_ RPF	RPF files for single chemical runs (not currently used)
<install>/d_interface/Dietary/ Single /PF	s_ PF	PF files for single chemical runs (not currently used)
<install>/d_interface/Dietary/ Single /Pest	s_ pest	Chemical code files for single chemical runs (not currently used)
<install>/d_interface/Dietary/ Single /Usage	s_ usage	Usage files for single chemical runs

A.2 Input Files

This Appendix provides data on the format and contents of the SHEDS-Dietary Input files. This information can be used as guidance for creating such files for different types of runs. Information about the format of food residue distribution files (RDF files) and single chemical Bridge Files are provided in the main body of the manual, as these files can be edited directly within the interface.

A.2.1 The Run Information File

The Run Information File is the main file that controls the SHEDS-Dietary simulation. The contents of the file are given in Table A-2.

Table A-2. Variables in the Run Information File

Variable	Description
ResidueDir	Residue file location (relative to Dietary root)
ByWeight	Risk factors are normalized by weight in kg (Yes/No) (Not currently used)
UsePAD	Use population adjusted dose (Yes/No) (Not currently used)
BySeason	Not currently used
ShwDaily	Add daily totals to output (Yes/No)
ShwDetails	Add details to output (Yes/No) (Not currently used)
ShwEating	Add eating occasions to output (Yes/No)
chronicPAD	Chronic population adjusted dose (Not currently used)
chronicPADF	Chronic population adjusted dose – females (Not currently used, could be used to enter unique data for females)
acutePAD	Acute population adjusted dose (Not currently used)
acutePADF	Acute population adjusted dose – females (Not currently used, could be used to enter unique data for females)

Variable	Description
chronicNOEL	Chronic no adverse effect level (Not currently used)
acuteNOEL	Acute no adverse effect level (Not currently used)
cancerQ	Cancer potency factor (Not currently used)
defaultARFD	Default adjusted reference dose (Not currently used)
ARFD	Adjusted reference doses for age groups 1-9 (group variable also present) (Not currently used)
i_type	Type of run - 1: Single 2: Multiple chemical
i_longtype	Longitudinal type - 1: Generate cross-section and construct longitudinal 2: Construct longitudinal from existing cross-sectional data
a_out_prex	Cross-sectional data prefix
a_loop_num	Number of interaction runs
a_w_res	Water residue file
a_res_final	Final food residue file
a_conv	Residue method: 1: Conversion using bridge 2:Use final residue file
a_grp	Age group dataset for cross-sectional run
a_res	
a_code	Dataset containing pesticides for multichemical run
a_pf	Processing factor file
a_rpf	RPF file
a_bridge	Bridge File
a_res_or	Original food residue file
a_exp_va	Need description from Jim
a_lod	Use pesticide info to fill in LOD for No Detected Value
b_pest	Pesticide to run in a single chemical run
b_pest_cat	Pesticide category
b_long	Type of study - 1: Longitudinal 2: Cross-sectional
b_diet_type	Source of dietary data - CSFII or NHANES
b_year	Year of dietary data (if NHANES) Not currently used.
b_outlib	Output data library for cross-sectional run
b_outlibdir	Location of b_outlib (relative to Dietary installation directory)
b_prex	Prefix for cross-sectional output data
b_diet_water	Pathways modeled - 1: Diet only 3: Diet and water
l_in	Directory containing input cross-sectional data for longitudinal run
l_indir	Location of l_in (relative to Dietary installation directory)
l_out	Output data library for longitudinal run
l_outdir	Location of l_outdir (relative to Dietary installation directory)
l_food_data_num	Number of interaction dietary runs for assembling longitudinal data
l_numPersons	Number of persons to simulate
l_simbegin	Beginning date of longitudinal run
l_simend	Ending data of longitudinal run
l_diarymethod	Diary method: Eight or New
l_diaryD	Population diversity statistic D
l_diaryAmean	Mean population lag-1 autocorrelation
l_agegrp	Dataset containing agegroups for longitudinal run
l_keyvar	Key variable for constructing longitudinal diaries
l_prex	Longitudinal output dataset
l_out_prex	Longitudinal output dataset filename
rr_in	Input library for preprocessing

Variable	Description
rr_indir	Input library location for preprocessing
rr_out	Output library for preprocessing
rr_outdir	Output library location for preprocessing
rr_in_prex	Input prefix for preprocessing
rr_out_prex	Output prefix for preprocessing
rr_var	Input ariable for preprocessing
rr_varlabel	Input variable label for preprocessing
rr_loop	Loop number for preprocessing
rr_lowperc	Contribution of lower percentile for preprocessing
rr_upperc	Contribution of upper percentile for preprocessing
rr_diet_water	Pathway for preprocessing- 1: Diet only 3: Diet and water
rr_label	Label for pre-processing

A.2.2 Final (Processed) Residue Files for Single Chemicals

Recall that SHEDS-Dietary can use either individual food residue distribution files (RDF files) or a final processed residue file. The format of the food residue files is discussed in Section 5.5.1. This section describes how a final residue file may be constructed. Like food residue files, final residue files are also used in conjunction with the single-chemical Bridge File discussed in Section 5.6.1. The index set in the Bridge File refers to a record in the final residue file. In this way, the EDFs are linked to the food commodities listed in the Bridge File.

A final residue file is a SAS dataset containing multiple rows, where each row contains data for a single studied food item, and is given an index. All units must be ppm. Each row also contains a comma-separated list of residue values that are assigned to the food commodities listed in the Bridge File via the index. The variables required in the Residue file are given in Table A-3, and an example final residue file is shown in Figure A-1.

Table A-3. Variables in the Final Residue File for Single Chemicals

Variable	SAS Format	Description
Index_num	Numeric	Integer index for the food in question; used to link to the Bridge File: corresponds to Bridge File variable rdl_1 (File Index 1).
resid_n	Numeric	Number of non-zero residue measurements
total_zero	Numeric	Number of zero residue measurements
all_residue	Character (20000 max)	A comma-separated list of all non-zero residue values.

VIEWTABLE: S_res.Final_cisperm_res

	index_num	resid_n	total_zero	all_residue
1	1	1	1289	0.02
2	2	1	2962	0.025
3	3	1	308	0.02
4	4	28	1316	0.079,0.025,0.021,0.004,0.071,0.004,0.015,0.004,0.004,0.0083
5	5	676	1536	0.025,0.052,0.025,0.025,0.025,0.025,0.2,0.025,0.025,0.025,0.0
6	6	1	1483	0.004
7	7	12	968	0.025,0.025,0.027,0.026,0.007,0.037,0.001,0.043,0.049,0.0067
8	8	14	2057	0.026,0.053,0.053,0.025,0.053,0.053,0.053,0.053,0.048,0.053,
9	9	2	1659	0.001,0.02
10	10	9	2757	0.018,0.025,0.018,0.018,0.018,0.018,0.025,0.025,0.044
11	11	6	1470	0.022,0.022,0.022,0.045,0.022,0.022
12	12	2	1425	0.025,0.025
13	13	5	128	0.067,0.065,4.6,1.9,1.4
14	14	6	128	0.02,2,0.19,0.6,1.7,1.1
15	15	357	1821	0.24,0.04,0.061,0.76,0.83,0.92,0.04,0.26,0.28,0.088,0.27,0.32,
16	16	36	1428	0.11,0.025,0.025,0.059,0.025,0.052,0.025,0.025,0.22,0.007,0.0
17	17	1	869	0.02
18	18	73	2734	0.003,0.003,0.01,0.015,0.009,0.016,0.008,0.13,0.006,0.007,0.0
19	19	7	1495	0.12,0.013,0.035,0.04,0.048,0.025,0.04
20	20	261	2513	0.05,0.084,0.025,0.025,0.025,0.064,0.025,0.025,0.025,0.025,0.
21	21	417	99	0.05,0.05,0.05,0.12,0.73,0.74,0.24,0.16,0.05,0.21,0.21,0.54,0.1
22	22	653	398	0.36,0.4,0.4,0.45,0.53,0.95,0.29,0.47,1.3,0.96,0.17,0.51,0.92,0.
23	23	3	382	0.053,0.002,0.009
24	24	98	2940	0.05,0.05,0.053,0.053,0.053,0.053,0.053,0.053,0.013,0.013,0.0
25	25	1	239	0.025
26	26	5	1194	0.028,0.04,0.02,0.02,0.02

Figure A-1. An Example Single-Chemical Residue File.

A.2.3 Final (Processed) Residue Files for Multiple Chemicals

The multichemical residue file provides a database of residue measurements for a number of related chemicals. A multichemical residue file for pyrethroids is provided with SHEDS-Dietary. These residue files can be created in SAS or generated within SHEDS-Dietary via the PDP Generator. The required variables in the file are given in Table A-4. An example is shown in Figure A-2 .

The file has a relatively simple structure. On each observation, the studied food commodity and type are listed along with the year of sample and the measured values for each of N chemicals. All units must be in ppm. Each row of the file lists one residue measurement for each chemical for the studied food commodity and type pair listed. The residue measurements will be linked to standard food commodities listed in the Bridge File via the IDs of the commodity-type pair.

Table A-4. Variables in the Final Residue File for Multiple Chemicals

Variable	SAS Format	Description
Commod	Char	Studied commodity code
Commtype	Char	Studied commodity type
Year	Numeric	Year of sample
Sample_pk	Numeric	
Ppm_XXX	Numeric	Residue concentration in ppm for chemical code XXX (There may be many chemicals in each file, and thus many ppm_XXX variables).

VIEWTABLE: M_res.B_py_res

	COMMOD	COMMTYPE	year	SAMPLE_PK	ppm_222	ppm_223	ppm_781	ppm_070	ppm_597	ppm_930
9884	BZ	FZ	2007	2930	0	0	0	0	0	0
9885	BZ	FZ	2007	2931	0	0	0	0	0	0
9886	BZ	FZ	2007	2932	0	0	0	0	0	0
9887	BZ	FZ	2007	2933	0	0	0	0	0	0
9888	BZ	FZ	2007	2934	0	0	0	0	0	0
9889	BZ	FZ	2007	2935	0	0	0	0	0	0
9890	BZ	FZ	2007	2936	0	0	0	0	0	0
9891	BZ	FZ	2007	2937	0	0	0	0	0	0
9892	BZ	FZ	2007	2938	0	0	0	0	0	0
9893	BZ	FZ	2007	2939	0	0	0	0	0	0
9894	BZ	FZ	2007	2940	0	0	0	0	0	0
9895	BZ	FZ	2007	2941	0	0	0	0	0	0
9896	BZ	FZ	2007	2942	0	0	0	0	0	0
9897	CA	FR	2006	1702	0	0	0	0	0	0
9898	CA	FR	2006	1703	0	0	0	0	0	0
9899	CA	FR	2006	1704	0	0	0	0	0	0
9900	CA	FR	2006	1705	0	0	0	0	0	0
9901	CA	FR	2006	1706	0	0	0	0	0	0
9902	CA	FR	2006	1707	0	0	0	0	0	0
9903	CA	FR	2006	1708	0	0	0	0	0	0
9904	CA	FR	2006	1709	0	0	0	0	0	0
9905	CA	FR	2006	1710	0	0	0	0	0	0
9906	CA	FR	2006	1711	0	0	0	0	0	0
9907	CA	FR	2006	1712	0	0	0	0	0	0
9908	CA	FR	2006	1713	0	0	0	0	0	0
9909	CA	FR	2006	1714	0	0	0	0	0	0
9910	CA	FR	2006	1715	0	0	0	0	0	0
9911	CA	FR	2006	1716	0	0	0	0	0	0
9912	CA	FR	2006	1717	0	0	0	0	0	0
9913	CA	FR	2006	1718	0	0	0	0	0	0
9914	CA	FR	2006	1719	0	0	0	0	0	0

Figure A-2. A Final Residue File for Multiple Chemicals (Pyrethroids).

The assignments of chemical names to chemical codes must be provided in the b_pestcode input file contained in the m_pest library. This file contains a list of chemical codes and their corresponding names; is shown below in Table A-5 and Figure A-3. If the user is going to run their own chemicals they would need to add the codes and names they are going to use to this file.

Table A-5. Variables in the Final Residue File for Multiple Chemicals (Pyrethroids)

Variable	SAS Format	Description
Pest_code	Numeric	Pesticide code
Test_class	Character	Pesticide class
Pest_name	Character	Pesticide name
Rpf	Numeric	Relative potency factor

See Section A.2.6 for a list of the available pesticide classes.

VIEWTABLE: M_pest.B_pestcode

	PEST_CODE	TEST_CLASS	PEST_NAME	rpf
1	930	O	Bifenthrin	1
2	781	O	Cyfluthrin	1
3	597	O	Cypermethrin	1
4	714	O	Esfenvalerate	1
5	546	O	Fenvalerate	1
6	222	O	Permethrin cis	1
7	223	O	Permethrin trans	1
8	070	I	Piperonyl butoxide	1

Figure A-3. A Pesticide Code File for Pyrethroids

A.2.4 Bridge Files for Multiple Chemicals

The form of the Bridge File for multiple chemicals is different than that for single chemicals, it serves an analogous purpose: to assign the residue measurements present in the multi-chemical residue file to food commodity IDs. Like the single chemical Bridge File, the multi-chemical file contains a single of food commodity, form, and type on each row. Each of these commodities is then assigned one or more of the commodity-type pairs for which measurements are present in the residue file. The variables present in the file are given in Table A-6; and example is shown in Figure A-5.

Table A-6. Variables in the Bridge File for Multiple Chemicals

Variable	SAS Format	Description
Com_ff	Character	Commodity food form
Commod_Code	Character	Commodity code
Commtype	Character	Commodity type
ZZ_Code	Character	List of commodity codes from residue file (commod in that file). ZZ_code and ZZ_Type together define commodity-type pairs to assign to this food form
ZZ_Type	Character	Corresponding list of commodity types from residue file (commtype in that file). ZZ_code and ZZ_Type together define commodity-type pairs to assign to this food form

VIEWTABLE: M_bridge.B_py_bridge

	com_ff	Commod_Code	commtype	ZZ_Code	ZZ_Type
1	11000110_221	11	01	AC,AC,AC,AC,AC	CA,GJ,NP,OT,PC
2	11000110_212	11	01	AC,AC,AC,AC,AC	CA,GJ,NP,OT,PC
3	11000110_211	11	01	AC,AC,AC,AC,AC	CA,GJ,NP,OT,PC
4	11000110_210	11	01	AC,AC,AC,AC,AC	CA,GJ,NP,OT,PC
5	11000110_110	11	01	AC,AC,AC,AC,AC	CA,GJ,NP,OT,PC
6	11000111_240	11	01	AC,AC,AC,AC,AC	CA,GJ,NP,OT,PC
7	11000110_240	11	01	AC,AC,AC,AC,AC	CA,GJ,NP,OT,PC
8	11000100_240	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
9	11000101_240	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
10	11000101_230	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
11	11000100_211	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
12	11000100_213	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
13	11000100_230	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
14	11000100_210	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
15	11000100_120	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
16	11000100_110	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
17	11000100_214	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
18	11000100_212	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
19	11000100_130	11	02	AJ,AJ,AJ,AJ,AJ	CA,CO,FZ,OT,RE
20	95002640_230	11	03	PB,PB,PB,PB,PB	CA,GJ,NP,OT,PC
21	95002640_120	11	03	PB,PB,PB,PB,PB	CA,GJ,NP,OT,PC
22	95002640_110	11	03	PB,PB,PB,PB,PB	CA,GJ,NP,OT,PC
23	95002640_211	11	03	PB,PB,PB,PB,PB	CA,GJ,NP,OT,PC
24	95002640_210	11	03	PB,PB,PB,PB,PB	CA,GJ,NP,OT,PC
25	95002640_240	11	03	PB,PB,PB,PB,PB	CA,GJ,NP,OT,PC
26	13020570_230	11	05	BB,BZ	FR,FZ
27	13020570_211	11	05	BB,BZ	FR,FZ
28	13020570_120	11	05	BB,BZ	FR,FZ
29	13020570_110	11	05	BB,BZ	FR,FZ
30	13020570_130	11	05	BB,BZ	FR,FZ

Figure A-4. Example Bridge File for Multiple Chemicals

A.2.5 Processing Factor Files (Multiple Chemicals)

These files are required for multichemical runs. They include processing factors that can be used to adjust residue values based on the anticipated change in residue concentration during the processing of raw food. Processing Factor files can be created in SAS or generated within SHEDS-Dietary via the PDP Generator. The contents of this file are given in Table A-7. An example Processing Factor File is shown in Figure A-5.

Table A-7. Variables in the Processing Factor File for Multiple Chemicals

Variable	SAS Format	Description
Com_ff	Character	Commodity food form ID
PF_XXX	Numeric	Processing factor for each commodity for chemical XXX; one column for each chemical in the simulation.

	com_ff	pf_539	pf_597	pf_781	pf_930
1	01010500_110	1	1	1	1
2	01010500_212	1	1	1	1
3	01010500_221	1	1	1	1
4	01010500_230	1	1	1	1
5	01010500_232	1	1	1	1
6	01010500_240	1	1	1	1
7	01010500_242	1	1	1	1
8	01010500_250	1	1	1	1
9	01010501_211	1	1	1	1
10	01010501_240	1	1	1	1
11	01010780_110	1	1	1	1
12	01010780_130	1	1	1	1
13	01010780_150	1	1	1	1
14	01010780_210	1	1	1	1
15	01010780_211	1	1	1	1
16	01010780_212	1	1	1	1
17	01010780_213	1	1	1	1
18	01010780_215	1	1	1	1
19	01010780_220	1	1	1	1
20	01010780_221	1	1	1	1
21	01010780_222	1	1	1	1
22	01010780_230	1	1	1	1
23	01010780_232	1	1	1	1
24	01010780_240	1	1	1	1
25	01010780_242	1	1	1	1
26	01010781_211	1	1	1	1
27	01010781_240	1	1	1	1
28	01010790_110	1	1	1	1
29	01010790_240	1	1	1	1
30	01011900_110	1	1	1	1
31	01011900_150	1	1	1	1
32	01011900_210	1	1	1	1
33	01011900_240	1	1	1	1
34	01012510_210	1	1	1	1
35	01012510_212	1	1	1	1
36	01012511_240	1	1	1	1

Figure A-5. Example Processing Factor File

A.2.6 Chemical Code Files (Multiple Chemicals)

Chemical code files contain a list of chemicals that can be run in a multichemical simulation. The information that is included in this file is given in Table A-8. An example chemical code file is shown in Figure A-6. Chemical code files can be created in SAS or generated within SHEDS-Dietary via the PDP Generator.

Table A-8. Variables in the Chemical Code File for Multiple Chemicals

Variable	SAS Format	Description
PEST_CODE	Numeric	Chemical code
TEST_CLASS	Character	Chemical class
PEST_NAME	Character	Chemical name
rpf	numeric	Relative potency factor

	PEST_CODE	TEST_CLASS	PEST_NAME	rpf
1	930	O	Bifenthrin	1
2	781	O	Cyfluthrin	1
3	597	O	Cypermethrin	1
4	714	O	Esfenvalerate	1
5	546	O	Fenvalerate	1
6	222	O	Permethrin cis	1
7	223	O	Permethrin trans	1
8	070	I	Piperonyl butoxide	1

Figure A-6. Example Chemical Code File

The defined pesticide classes are as follows:

A Halogenated
B Benzimidazole
C Organophosphorus
E Carbamate
F Organonitrogen
G 2,4-D / Acid Herbicides
H Formetanate HCL
I Other Compounds
J Imidazolinone
K Sulfonyl Urea Herbicides
L Conazoles / Triazoles
N Imidazoles
O Pyrethroids
P Thiocarbamates
R Triazines
S Triazine, Non-Halogenated
T Nitrile
U Uracil
V Pyrimidone
W Morpholine

A.3 Output Files

By default, all output files from the SHEDS-Dietary run are stored in <install>/Output. Cross-sectional output is stored in the main Output library, longitudinal datasets are stored in the Olong library, and summary datasets are stored in Sumtab. However, note that the interface allows the user to choose libraries other than these for writing output.

The general structures of different types of SHEDS-Dietary outputs are provided here.

A.3.1 Cross-Sectional Output Datasets

By default, output from a cross-sectional SHEDS-Dietary run is written to the Output library. These files will begin with the cross-sectional prefix assigned by the user for the run, and food exposure files will end with a suffix "_X" where X is the loop number. Water exposure output files will have an analogous suffix "_X_w". The contents of the cross-sectional files are given in Table A-9.

Table A-9. Variables in the Cross-Sectional Output Datasets

Variable	Format	Description
HHID	Numeric	
SPNUM	Numeric	
Daycode	Numeric	
AGE	Numeric	Age in years (food consumption diary)
SEX	Numeric	Sex
WGT_KG	Numeric	Weight in kilograms
WT4_2DAY	Numeric	Statistical weight
tot_cal	Numeric	Total calories consumed
age_group	Character	Age-group simulated
ARFD	Numeric	Acute reference dose
OCC_TIME	Numeric	Time of eating occasion
comcode (FCID code)	Numeric	EPA commodity code
Ff	Numeric	food form
com_gram	Numeric	grams of chemical consumed
exp_ug (single chemicals)	Numeric	Exposure in micrograms
exp_ug (multiple chemicals)	Numeric	Total exposure in micrograms
ug_XXX (multiple chemicals)	Numeric	Exposure in micrograms for chemical code XXX

A.3.2 Longitudinal Output Datasets

By default, output from a cross-sectional SHEDS-Dietary run is written to the Olong library. These files will begin with the longitudinal dataset name assigned by the user for the run; water exposure files will end with a suffix "_w".

The contents of the longitudinal files are given in Table A-10.

Table A-10. Variables in the Longitudinal Output Datasets

Variable	Format	Description
person_id	Numeric	Person ID
date	Numeric	Date
id	Numeric	Diary ID
loop	Numeric	Loop number for this day
diary_age	Numeric	Age on food diary
age_group	Numeric	Age group
total_cal	Numeric	Total calories consumed
weight	Character	Statistical weight
aRFD	Numeric	Acute reference dose
exp_ug (single chemicals)	Numeric	Exposure in micrograms
exp_ug (multiple chemicals)	Numeric	Total exposure in ug for chemical code XXX
ug_XXX (multiple chemicals)	Numeric	Exposure in ug for chemical code XXX

A.3.3 Summary Output Datasets

The summary output datasets are generated by the Pre-Process Output data screen, and by default written to the Sumtab library. The results are generated for one variable at a time using the Pre-process frame, for either exposure to single chemical, or total exposure (for multi-chemical runs). These files will begin with the prefix assigned by the user when the data is preprocessed. These are the data that can be visualized with the View Cross-Sectional Results screen. The files and their contents are as follows:

PREFIX_contrib: Contribution by commodity to exposure and food consumed**.**

PREFIX_pctl_day: Percentiles for daily exposure: food (dietary), water and total.

PREFIX_ pctl_occ: Percentiles for eating occasion exposure: food (dietary), water and total**.**

PREFIX_ summary_day: Summary percentiles for daily exposure by age group**:** food (dietary), water and total.

PREFIX_ summary _occ: Summary percentiles for eating occasion exposure by age group**:** food (dietary), water and total.

PREFIX_ tab_day: Daily exposure and percent %APAD percentiles by age group: food (dietary), water and total.

PREFIX_ tab _occ: Eating occasion exposure and percent %APAD percentiles by age group: food (dietary), water and total.