United States Environmental Protection Agency
Office of Pesticide Programs

Dietary Exposure Evaluation Model

User's Guide

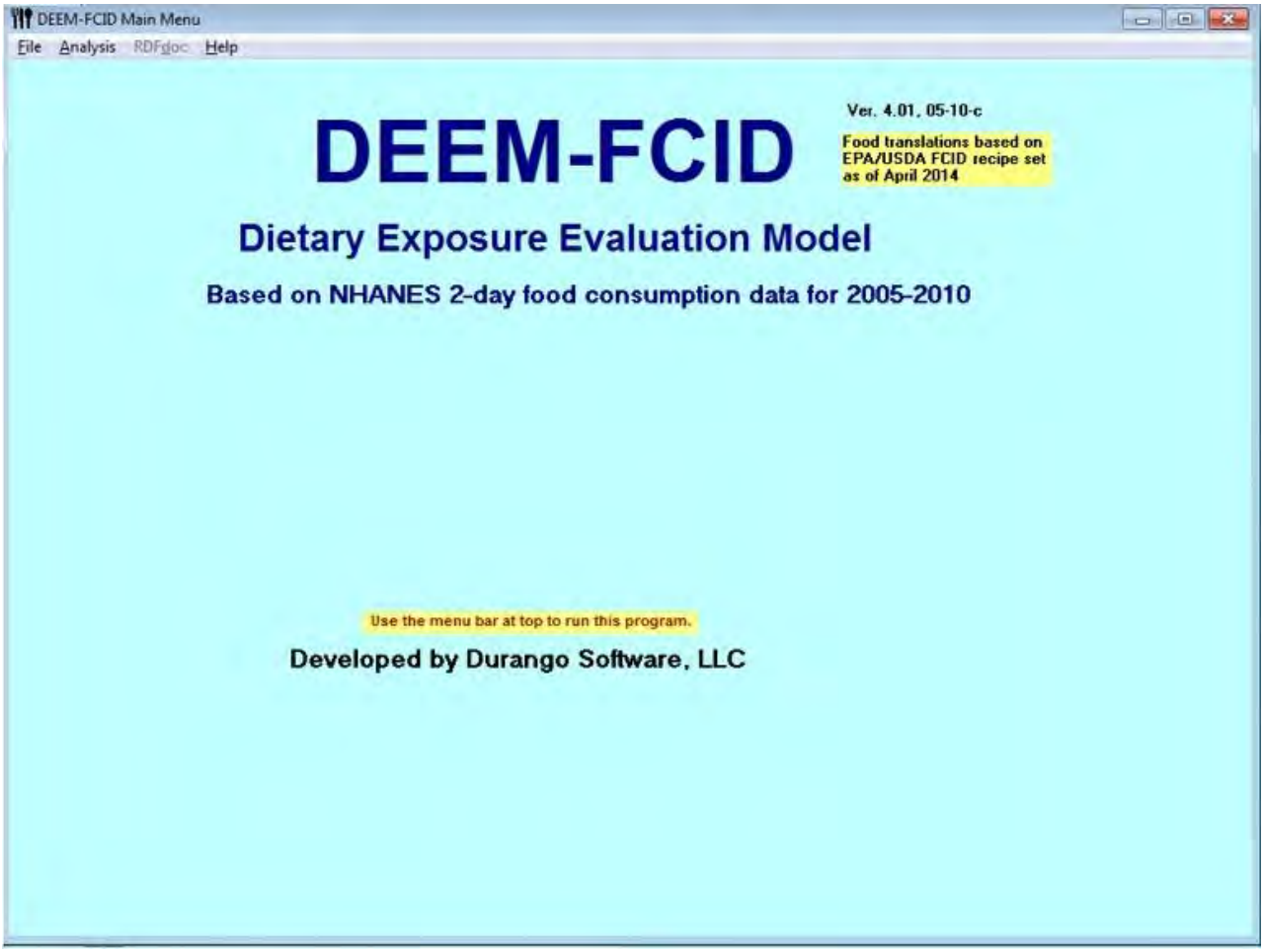
September 30, 2014

Note: Though the current version of DEEM is 4.02, the screenshots used in this DEEM Quick Guide are based on "working" Beta Versions 4.00 and 4.01. Users should not find a significant visual difference in v. 4.02.

Table of Contents

General Overview of DEEM-FCID

DEEM-FCID is a dietary exposure model that is used to **estimate** exposure to pesticides in foods in the diets of the U.S. population. The software was developed by Durango Software, LLC and is based on food consumption data from the National Health and Nutrition Examination Survey (NHANES), What We Eat in America (WWEIA). DEEM-FCID Version 4.02 is based on more recent food consumption data (2005-2010) than Version 3.18 (2003-2008). Version 4.02 also uses commodity codes for two groups (Tropical Fruits with edible peel, and Tropical Fruits without edible peel) that have not been published in the Federal Register as of this release date.



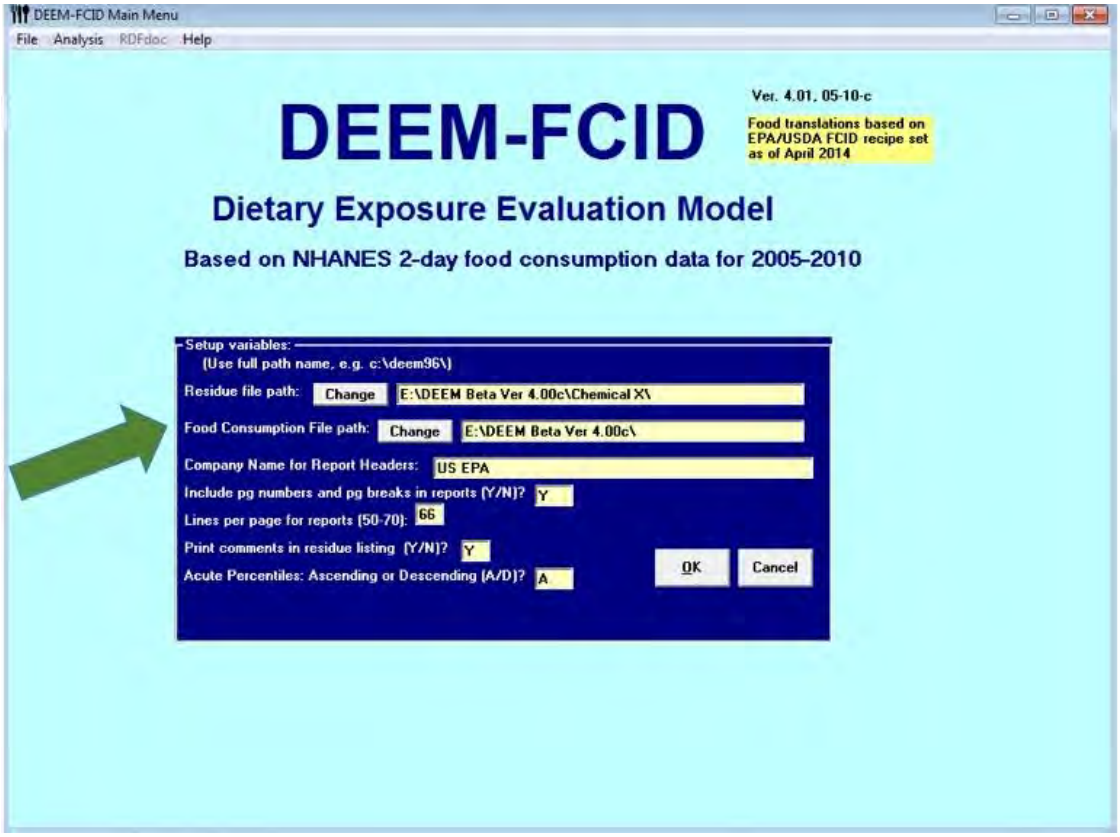
The main DEEM-FCID module is used to launch the residue file editor to create and edit residue files for specific chemical or cumulative applications, and to launch the DEEM-FCID Acute and Chronic/Cancer analysis modules. The DEEM-FCID software itself is also integrated with Calendex, an aggregate exposure assessment software application used when combining dietary and residential (non-dietary) exposures. To conduct either acute, chronic, and/or cancer risk analyses using DEEM-FCID software, the user must provide three types of information: (1) the pesticide's toxicological data that are directly relevant to both the length of time or duration of interest and the evaluation of the significance of estimates of exposure by the oral route. These data should include a toxicology endpoint based on chronic (long-term) exposure such as the

cancer potency factor (Q_1*), the No Observed Effect Level (NOEL) or No Observed Adverse Effect Level (NOAEL), Reference Dose (RfD), Population Adjusted Dose (PAD), or Margin of Exposure (MOE) {*This guide uses the acronym 'NOEL' rather than 'NOAEL' following the label used by the DEEM-FCID software.*}; (2) the residue concentrations in the foods and/or food forms which can be a theoretical level (such as the tolerance or MRL (maximum residue limit)) or a level of residue anticipated to be present in the food of interest; and (3) any adjustment factors directly relevant to potential constituent levels in the diet to more accurately reflect likely exposures (e.g., processing factors or estimates of percent of the crop treated).

The acute and chronic analysis of DEEM-FCID can be used to estimate total exposure for both the U.S. population as a whole and subgroups of the population. Subgroups are divided by age, gender, or ethnicity. The Commodity Contribution Analysis can be used to identify the contribution of residues in individual foods (and food forms) to the overall estimate of dietary exposure.

The purpose of this User's Guide is to familiarize users with the DEEM-FCID interface. The first part depicts how to create a DEEM-FCID Residue file for a hypothetical Chemical "X". The case study shows how to input toxicological parameters for Chemical X, and single value residue inputs for apples, almonds and drinking water. The DEEM-FCID model is then used to calculate estimates of chronic and acute dietary exposures for select populations. The second part shows how to construct and assign empirical residue distributions and to perform acute probabilistic or Monte Carlo Analysis (MCA) using DEEM-FCID.

Getting Started: Creating a Chemical Residue File (R10)

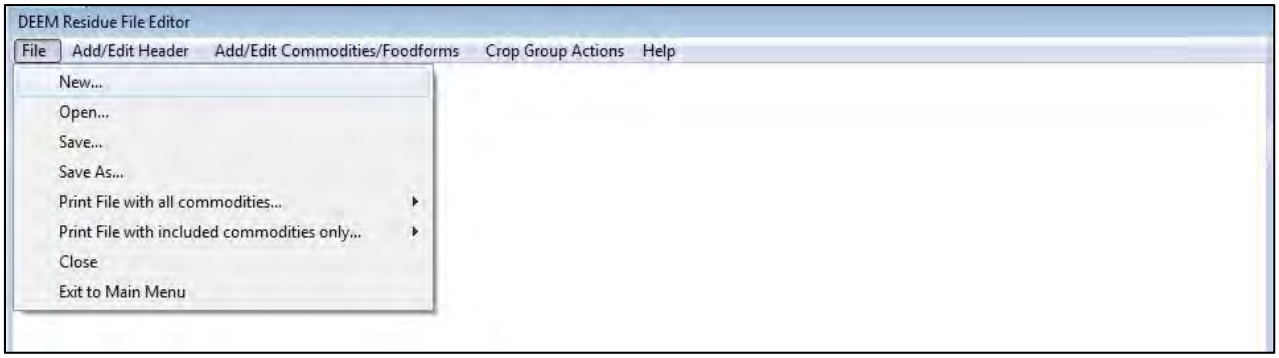


1) Go to "File" and select "Set Up" from the main menu screen. If the DEEM-FCID defaults are correct, click the "OK" button. For the case study, the DEEM-FCID software and residue inputs for Chemical X are stored on a thumb drive (E).

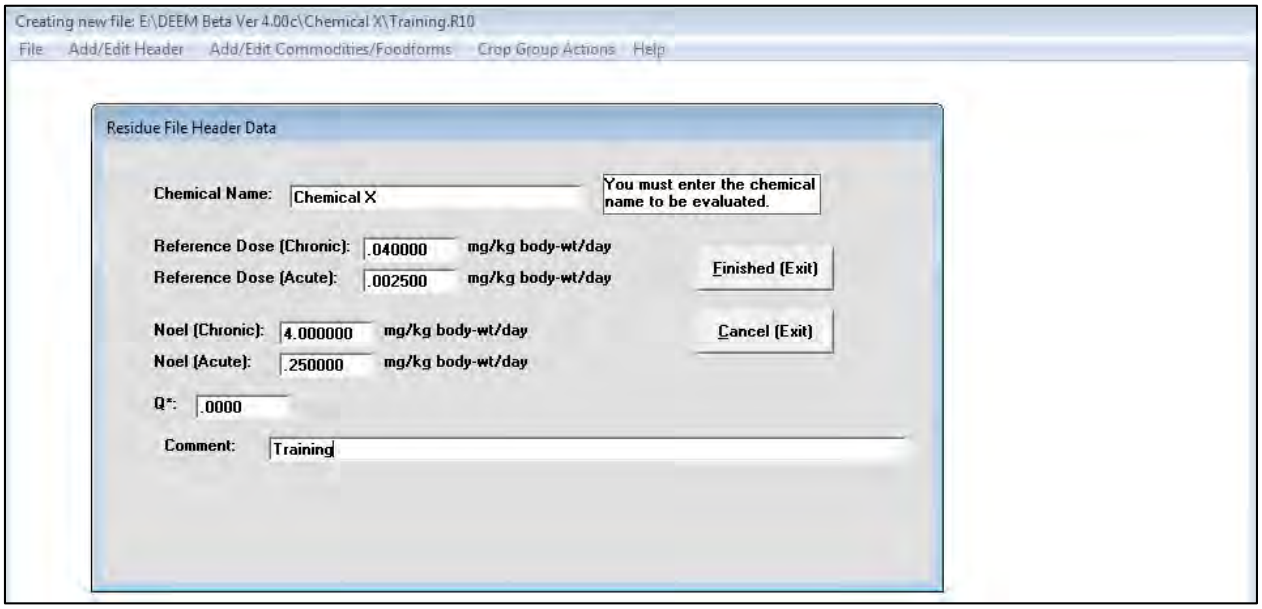
[*If you want to save the software and inputs on your PC, then enter the name of the directory where you would like the residue files that you will be creating to be saved; next, enter the name of the directory where the food consumption files are located. Also, indicate the number of lines per page that will accommodate your printer, page breaks in reports that are generated by DEEM-FCID, identification of printer port, displaying the acute exposure percentiles in ascending or descending order.*]

2) Go to "File" and select "Residue File Editor" from the main menu screen. Next, click on "File" and select "New" to create a new file. You then will be prompted to enter the name of the file. This is your R10 file. For this example, save the file as "Training." Once you have saved the data, click on "Save" to close the screen.

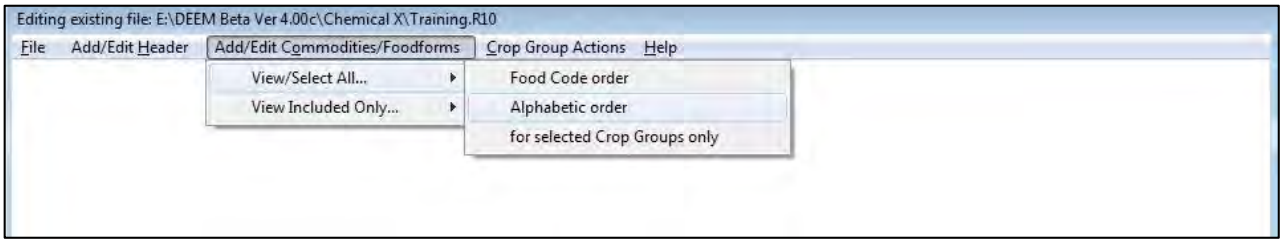
[*Note: When naming a file try not include symbols, spaces, or special characters, such as commas, parenthesis, etc. as this may prevent DEEM-FCID from recognizing your R10 file. When using RDF files, save the R10 and RDF files in the same directory in order to facilitate the use of DEEM inputs on other computers.*]



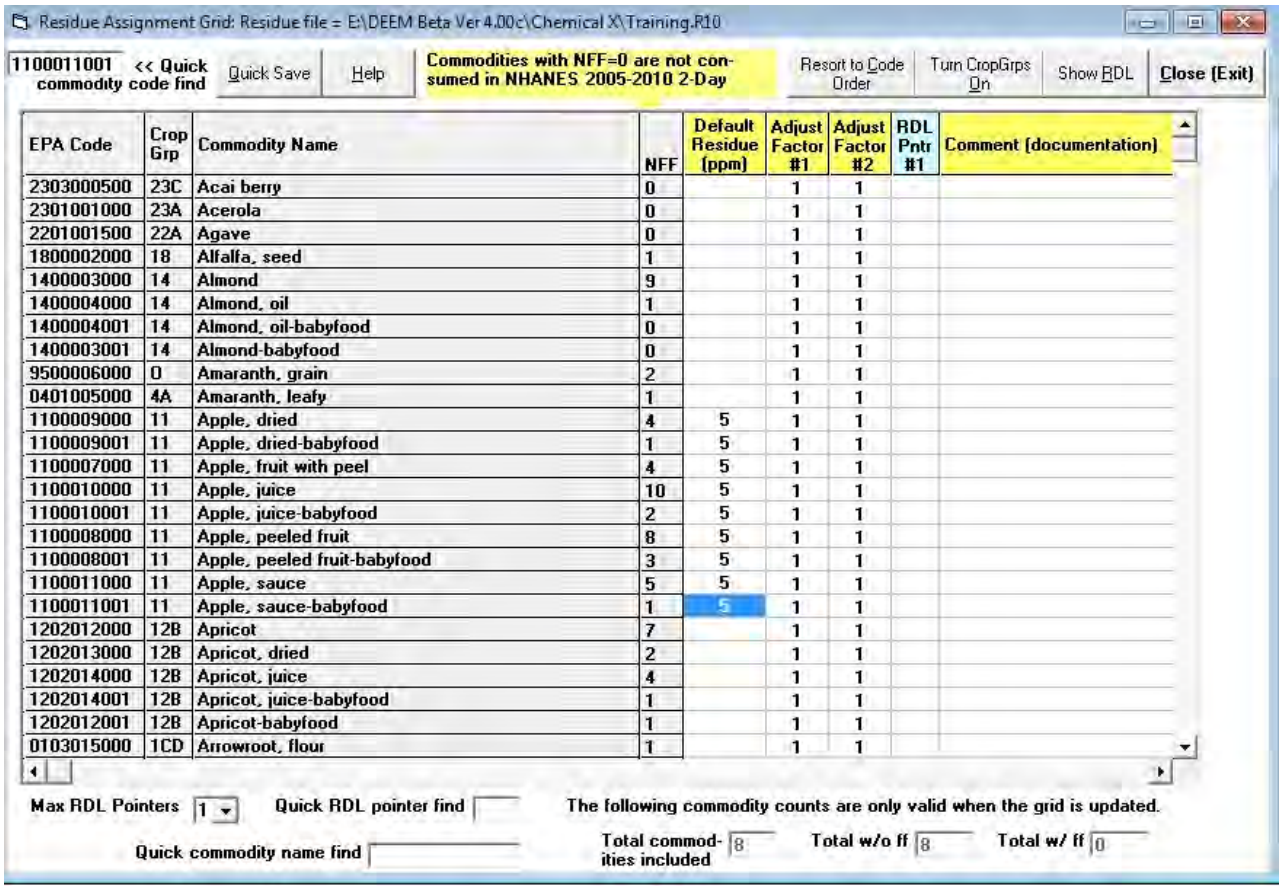
3) Click on "Add/Edit Header" from the main screen then "Open Header." Add the chemical name, NOEL, Reference Dose (RfD) or the Population Adjusted Dose, and Q_1* if applicable. You may also add comments, which will appear on all subsequent DEEM- FCID analyses. Once you have completed entering the data, click on "Finished" to close the screen.
[*You may move from field to field with either the <Tab> key or the mouse. In addition to presenting acute dietary exposures at various per capita percentiles in the summary results report, DEEM will also present those exposures as a percent of the acute Reference Dose (Acute), based on the value in the "Reference Dose (Acute)" blank. If the user inputs a value in the "Noel (Acute)" box, then DEEM will also present those estimated exposures as a Margin of Exposure (=Exposure/Value).*]



4) Click on "Add/Edit Commodities/Foodforms" option from the menu bar. You may sort foods by food code or alphabetic order. Select "View/Select All" and by Alphabetic order.

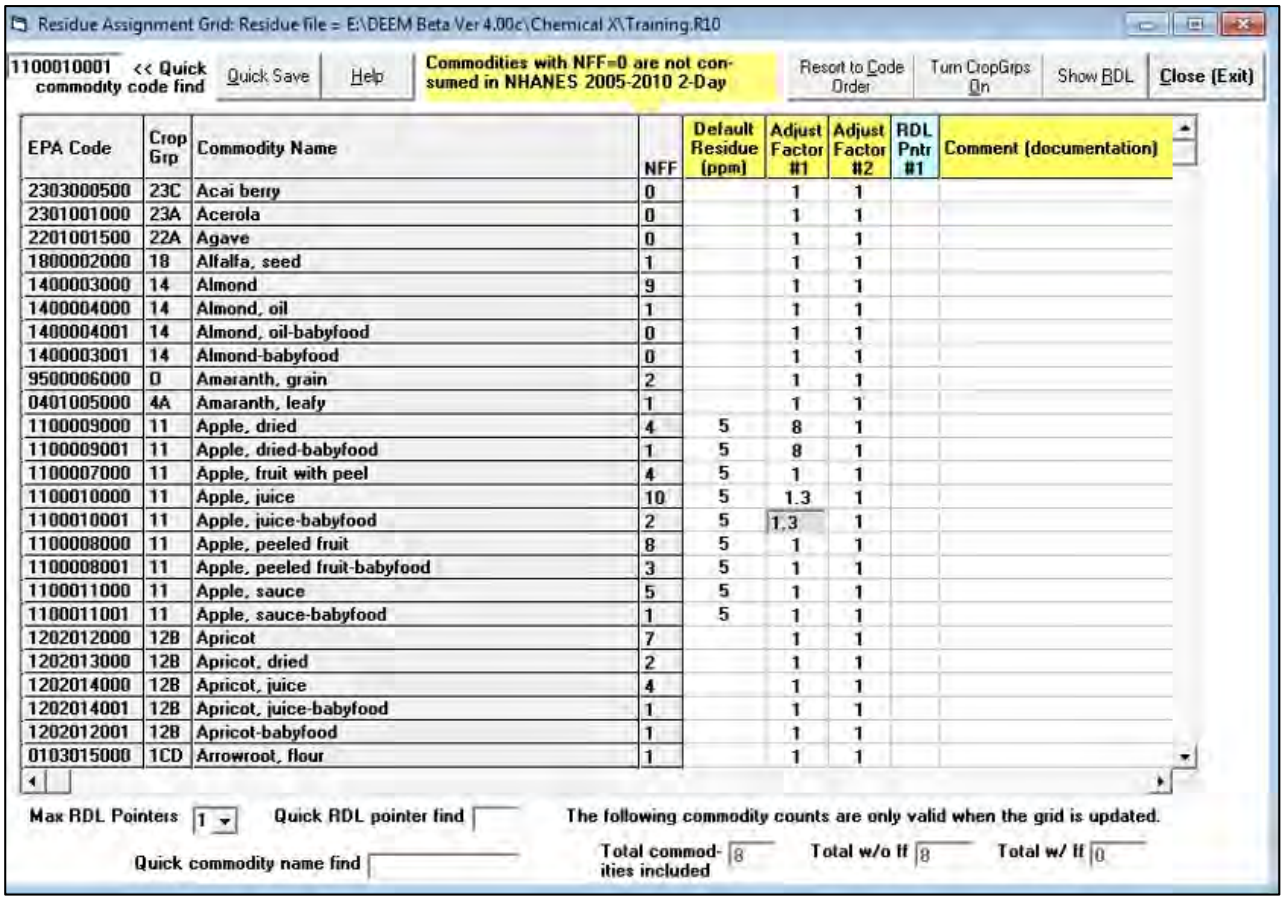


5) In the "Default Residue" column, enter the residue value in ppm for each commodity in your assessment. For this example, use 5 ppm for all apple commodities. [*DEEM-FCID permits entry of values of 0.000001 ppm to 1000 ppm. Note that data entry is restricted to 6 decimals.*]



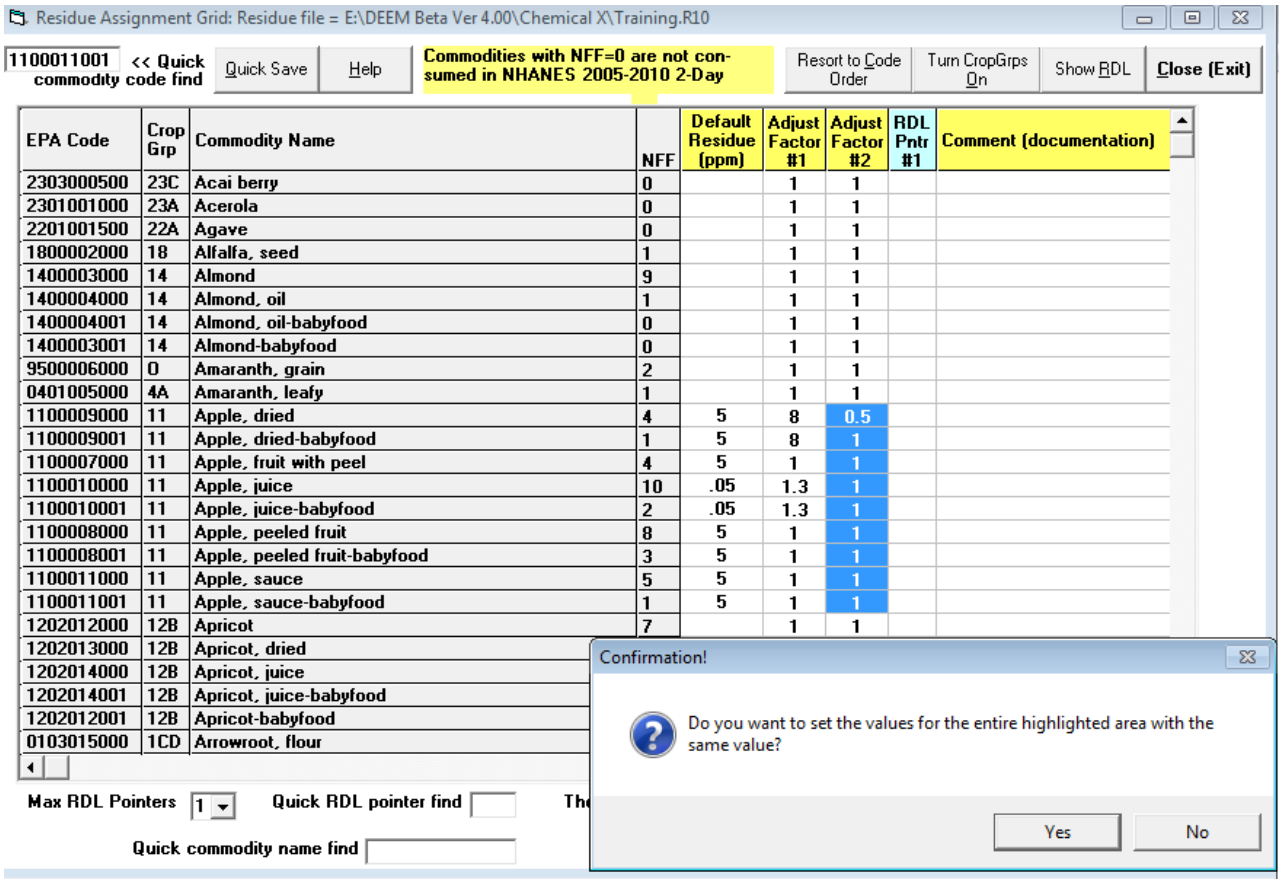
EPA Code	Crop Grp	Commodity Name	NFF	Default Residue (ppm)	Adjust Factor #1	Adjust Factor #2	RDL Pntr #1	Comment (documentation)
2303000500	23C	Acai berry	0		1	1		
2301001000	23A	Acerola	0		1	1		
2201001500	22A	Agave	0		1	1		
1800002000	18	Alfalfa, seed	1		1	1		
1400003000	14	Almond	9		1	1		
1400004000	14	Almond, oil	1		1	1		
1400004001	14	Almond, oil-babyfood	0		1	1		
1400003001	14	Almond-babyfood	0		1	1		
9500006000	0	Amaranth, grain	2		1	1		
0401005000	4A	Amaranth, leafy	1		1	1		
1100009000	11	Apple, dried	4	5	1	1		
1100009001	11	Apple, dried-babyfood	1	5	1	1		
1100007000	11	Apple, fruit with peel	4	5	1	1		
1100010000	11	Apple, juice	10	5	1	1		
1100010001	11	Apple, juice-babyfood	2	5	1	1		
1100008000	11	Apple, peeled fruit	8	5	1	1		
1100008001	11	Apple, peeled fruit-babyfood	3	5	1	1		
1100011000	11	Apple, sauce	5	5	1	1		
1100011001	11	Apple, sauce-babyfood	1	5	1	1		
1202012000	12B	Apricot	7		1	1		
1202013000	12B	Apricot, dried	2		1	1		
1202014000	12B	Apricot, juice	4		1	1		
1202014001	12B	Apricot, juice-babyfood	1		1	1		
1202012001	12B	Apricot-babyfood	1		1	1		
0103015000	1CD	Arrowroot, flour	1		1	1		

6) *Adjustment Factors*: Typically, the first adjustment factor in the DEEM-FCID software is used for reduction or increase of concentrations from processing a commodity, and the second adjustment factor may be used to incorporate pesticide usage estimates for chronic/cancer risk assessments. DEEM always multiplies residues by Adjustment Factor #1. As shown later, users also have the option to have the program multiply anticipated residues by Adjustment Factor #2 when specifying a particular simulation. In this example, the agency's default processing factors are entered for dried apples (8) and apple juice (1.3) under Adjustment Factor #1.



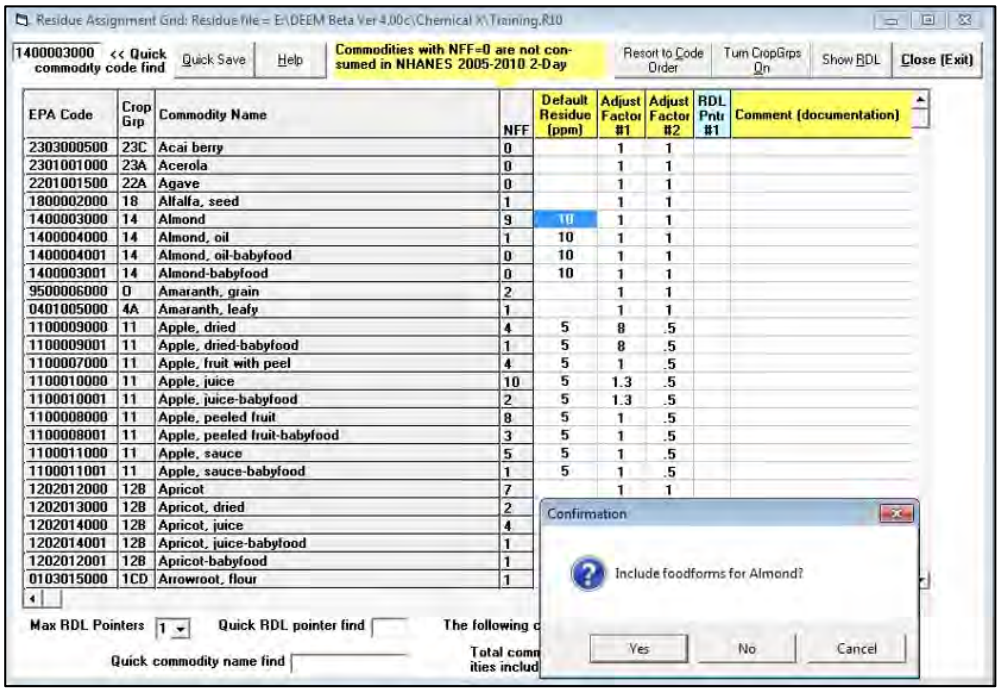
EPA Code	Crop Grp	Commodity Name	NFF	Default Residue (ppm)	Adjust Factor #1	Adjust Factor #2	RDL Pntr #1	Comment (documentation)
2303000500	23C	Acai berry	0		1	1		
2301001000	23A	Acerola	0		1	1		
2201001500	22A	Agave	0		1	1		
1800002000	18	Alfalfa, seed	1		1	1		
1400003000	14	Almond	9		1	1		
1400004000	14	Almond, oil	1		1	1		
1400004001	14	Almond, oil-babyfood	0		1	1		
1400003001	14	Almond-babyfood	0		1	1		
9500006000	0	Amaranth, grain	2		1	1		
0401005000	4A	Amaranth, leafy	1		1	1		
1100009000	11	Apple, dried	4	5	8	1		
1100009001	11	Apple, dried-babyfood	1	5	8	1		
1100007000	11	Apple, fruit with peel	4	5	1	1		
1100010000	11	Apple, juice	10	5	1.3	1		
1100010001	11	Apple, juice-babyfood	2	5	1.3	1		
1100008000	11	Apple, peeled fruit	8	5	1	1		
1100008001	11	Apple, peeled fruit-babyfood	3	5	1	1		
1100011000	11	Apple, sauce	5	5	1	1		
1100011001	11	Apple, sauce-babyfood	1	5	1	1		
1202012000	12B	Apricot	7		1	1		
1202013000	12B	Apricot, dried	2		1	1		
1202014000	12B	Apricot, juice	4		1	1		
1202014001	12B	Apricot, juice-babyfood	1		1	1		
1202012001	12B	Apricot-babyfood	1		1	1		
0103015000	1CD	Arrowroot, flour	1		1	1		

The percent crop treated for apples is 50% and the value 0.50 is entered in the adjustment factor #2 column. The DEEM Residue Editor allows users to copy values for Default Residues or Adjustment Factors to other commodities. To copy the 0.50 value from the first apple commodity to the other commodities, select the cell, left click the mouse, and hold the button down while dragging the highlighted area down to the last cell that you would like to replace. Select "Yes" when the following the screen appears, "Do you want to set the values for the entire highlighted area with the same value?" DEEM will copy that value to the other cells.

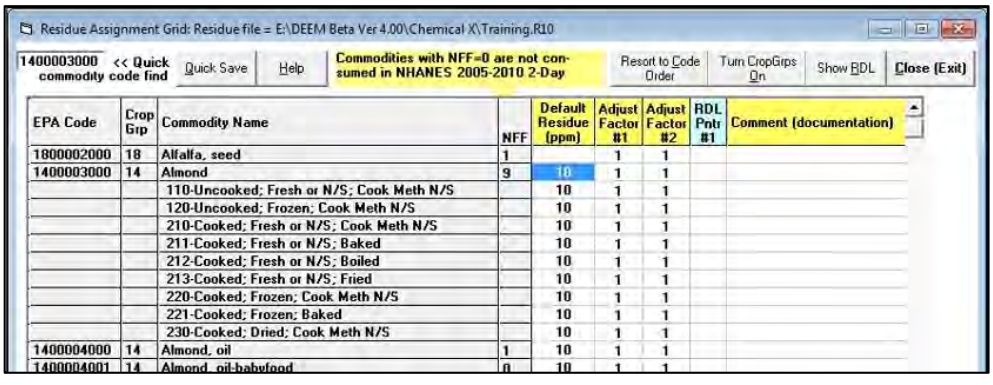


EPA Code	Crop Grp	Commodity Name	NFF	Default Residue (ppm)	Adjust Factor #1	Adjust Factor #2	RDL Pntr #1	Comment (documentation)
2303000500	23C	Acai berry	0		1	1		
2301001000	23A	Acerola	0		1	1		
2201001500	22A	Agave	0		1	1		
1800002000	18	Alfalfa, seed	1		1	1		
1400003000	14	Almond	9		1	1		
1400004000	14	Almond, oil	1		1	1		
1400004001	14	Almond, oil-babyfood	0		1	1		
1400003001	14	Almond-babyfood	0		1	1		
9500006000	0	Amaranth, grain	2		1	1		
0401005000	4A	Amaranth, leafy	1		1	1		
1100009000	11	Apple, dried	4	5	8	0.5		
1100009001	11	Apple, dried-babyfood	1	5	8	1		
1100007000	11	Apple, fruit with peel	4	5	1	1		
1100010000	11	Apple, juice	10	.05	1.3	1		
1100010001	11	Apple, juice-babyfood	2	.05	1.3	1		
1100008000	11	Apple, peeled fruit	8	5	1	1		
1100008001	11	Apple, peeled fruit-babyfood	3	5	1	1		
1100011000	11	Apple, sauce	5	5	1	1		
1100011001	11	Apple, sauce-babyfood	1	5	1	1		
1202012000	12B	Apricot	7		1	1		
1202013000	12B	Apricot, dried						
1202014000	12B	Apricot, juice						
1202014001	12B	Apricot, juice-babyfood						
1202012001	12B	Apricot-babyfood						
0103015000	1CD	Arrowroot, flour						

7) ***Foodforms (FF):*** The FCID recipe database assigned a cooking status (cooked or not cooked), food form (fresh, frozen, canned, dried, etc.) and cooking method (baked, boiled, fried, etc.) to each ingredient in every food item reportedly consumed by WWEIA respondents. We often use the term 'Food Form' (FF) to denote the combination of those 3 characteristics. The number of distinct FFs for each commodity is indicated in the column "NFF". In order to view those FFs, first enter a value in the Default Residue column, then highlight the default residue value (10 ppm) and right click the mouse. In the figure below, 10 ppm is entered for almonds (EPA FCID code=14000003000). Select "Yes" when the following the screen appears, "Include foodforms for Almond?". DEEM will show the expanded list of that commodities' food forms.



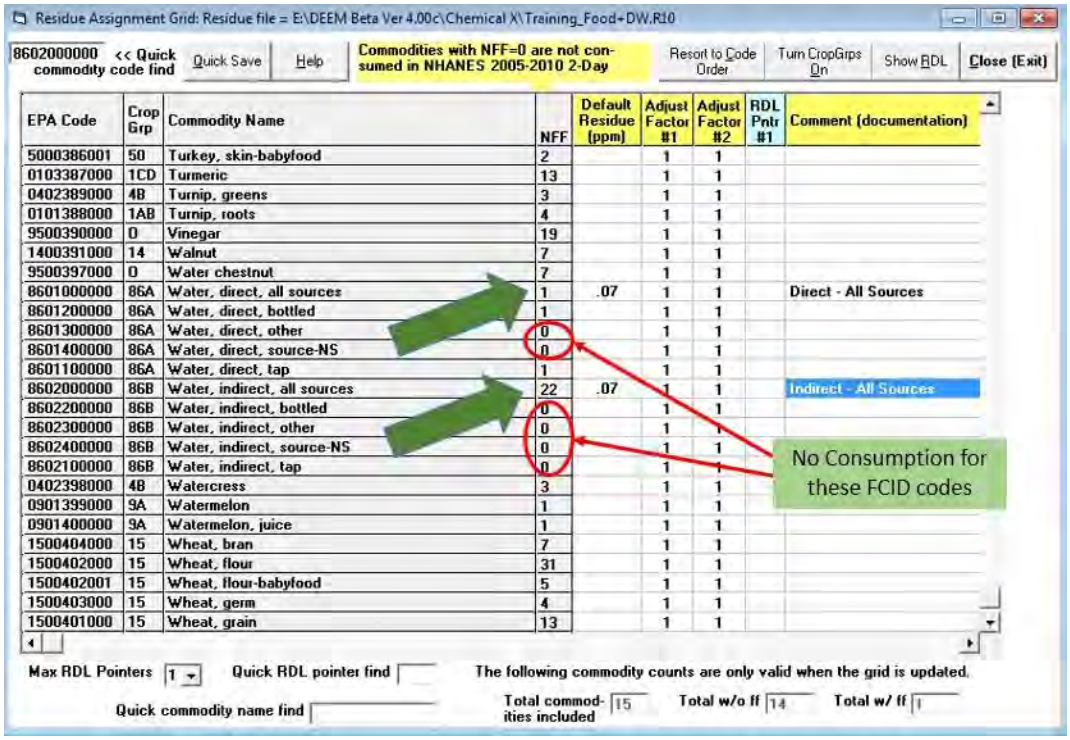
This expanded view enables users to specify different residue data, or appropriate adjustment factors for particular food forms.



Note: If NFF=0, then no one in the WWEIA-FCID 2005-10 database reportedly consumed that commodity in any food form; therefore, assigning residue inputs will not affect dietary exposure. Since there was no reported consumption for "Almond, oil-babyfood" and "Almond-babyfood", those residue inputs will not affect dietary exposures to Chemical X.

8) *Drinking Water* DEEM-FCID treats Drinking Water (DW) in a similar manner as dietary exposures from food commodities. Similar to food commodities, DEEM-FCID can accommodate either a deterministic point estimate or an empirical distribution of DW concentrations in acute risk assessments. The Calendex-FCID model also allows users to enter a time series of DW concentrations, including Calendar dates, in order to take into account temporal patterns (autocorrelation) in DW concentrations.

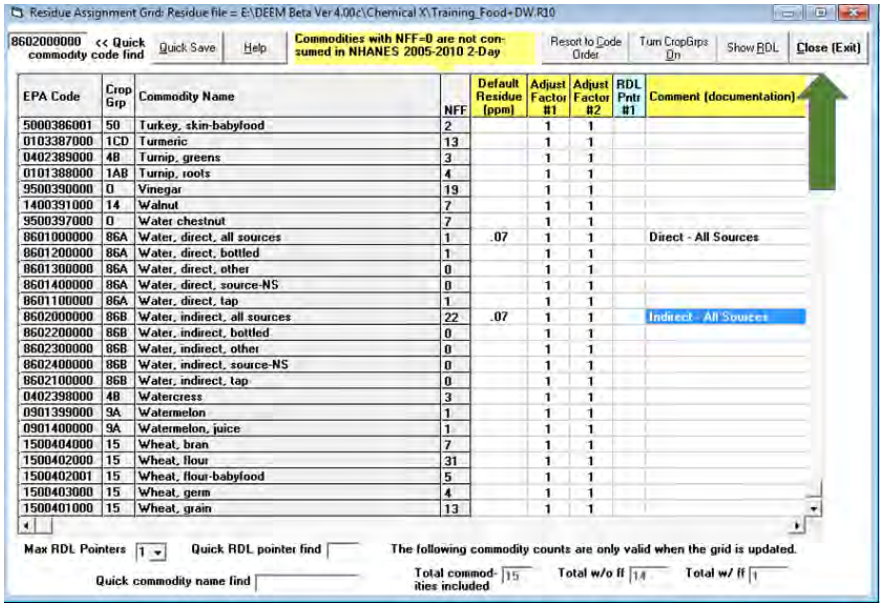
In WWEIA-FCID, Total Drinking Water (DW) consumption consists of Direct Water, "plain water from tap or bottled water", and Indirect Water "water added by respondent for coffee, tea, soups, etc". Attachment 2 provides further description of each component. The user can add DW concentrations to the Chemical X residue file by scrolling down the food list and entering a point value (0.07 ppm) to *Water, direct, all sources* and *Water, indirect, all sources* as depicted below.



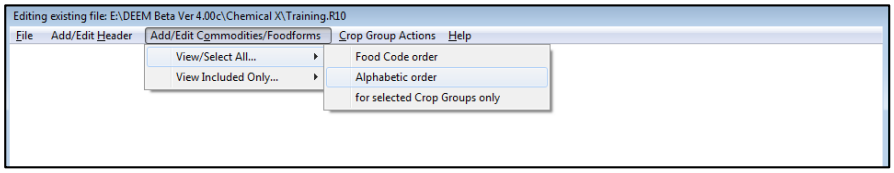
EPA Code	Crop Grp	Commodity Name	NFF	Default Residue (ppm)	Adjust Factor #1	Adjust Factor #2	RDL Pntr #1	Comment (documentation)
5000386001	50	Turkey, skin-babyfood	2		1	1		
0103387000	1CD	Turmeric	13		1	1		
0402389000	4B	Turnip, greens	3		1	1		
0101388000	1AB	Turnip, roots	4		1	1		
9500390000	0	Vinegar	19		1	1		
1400391000	14	Walnut	7		1	1		
9500397000	0	Water chestnut	7		1	1		
8601000000	86A	Water, direct, all sources	1	.07	1	1		Direct - All Sources
8601200000	86A	Water, direct, bottled	1		1	1		
8601300000	86A	Water, direct, other	0		1	1		
8601400000	86A	Water, direct, source-NS	0		1	1		
8601100000	86A	Water, direct, tap	1		1	1		
8602000000	86B	Water, indirect, all sources	22	.07	1	1		Indirect - All Sources
8602200000	86B	Water, indirect, bottled	0		1	1		
8602300000	86B	Water, indirect, other	0		1	1		
8602400000	86B	Water, indirect, source-NS	0		1	1		
8602100000	86B	Water, indirect, tap	0		1	1		
0402398000	4B	Watercress	3		1	1		
0901399000	9A	Watermelon	1		1	1		
0901400000	9A	Watermelon, juice	1		1	1		
1500404000	15	Wheat, bran	7		1	1		
1500402000	15	Wheat, flour	31		1	1		
1500402001	15	Wheat, flour-babyfood	5		1	1		
1500403000	15	Wheat, germ	4		1	1		
1500401000	15	Wheat, grain	13		1	1		

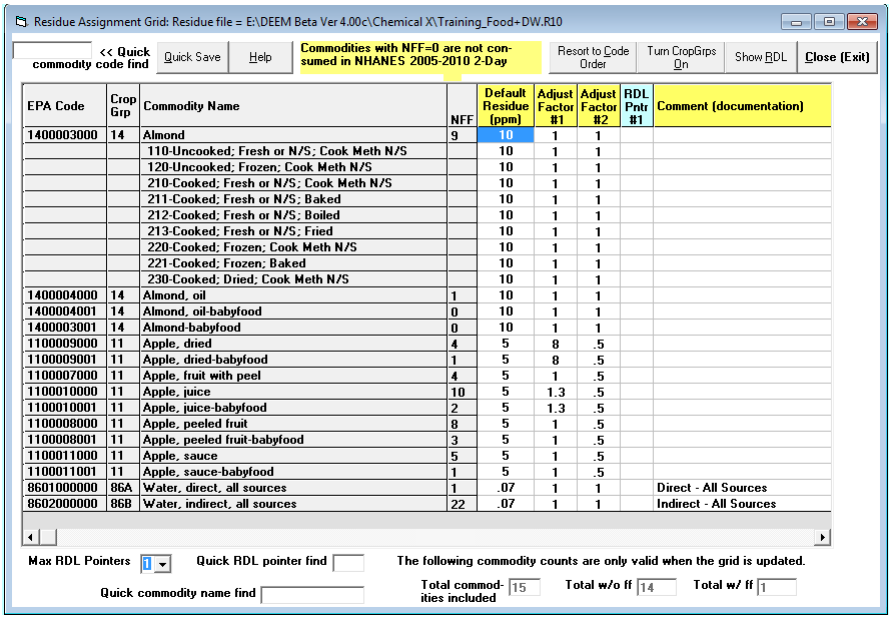
Note: The WWEIA-FCID 2005-2010 database no longer contains DW consumption for the 6 RACs highlighted in red (NFF=0), since WWEIA-FCID 2005-2010 has now collapsed the previous categories into the remaining three; therefore, inputting residues in those rows will not affect dietary (food+DW) exposures. As in previous versions of DEEM-FCID, users can specify different residue inputs for the different forms of water: 1) Direct-Bottled; 2) Direct-Tap; and 3) Indirect-All Sources. That option is not depicted in this user guide since the Agency typically assumes that only a single concentration is selected and applied to all three water forms in a DW assessment.

9) The user can return to the main Residue Editor screen by clicking the “Close (Exit)” button.



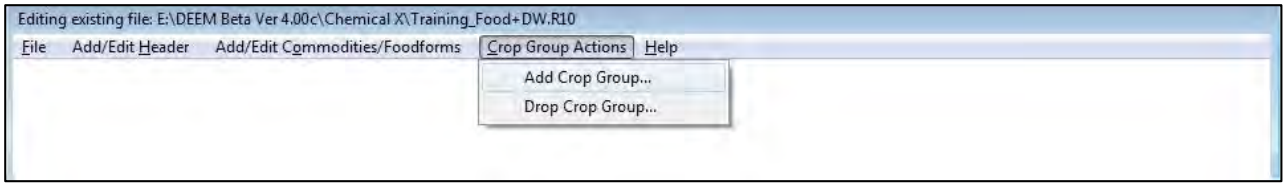
From the main Residue Editor screen, the user can view only those commodities that have assigned residues by selecting “Add/Edit Commodities/Foodforms” and “View Included Only…” option.



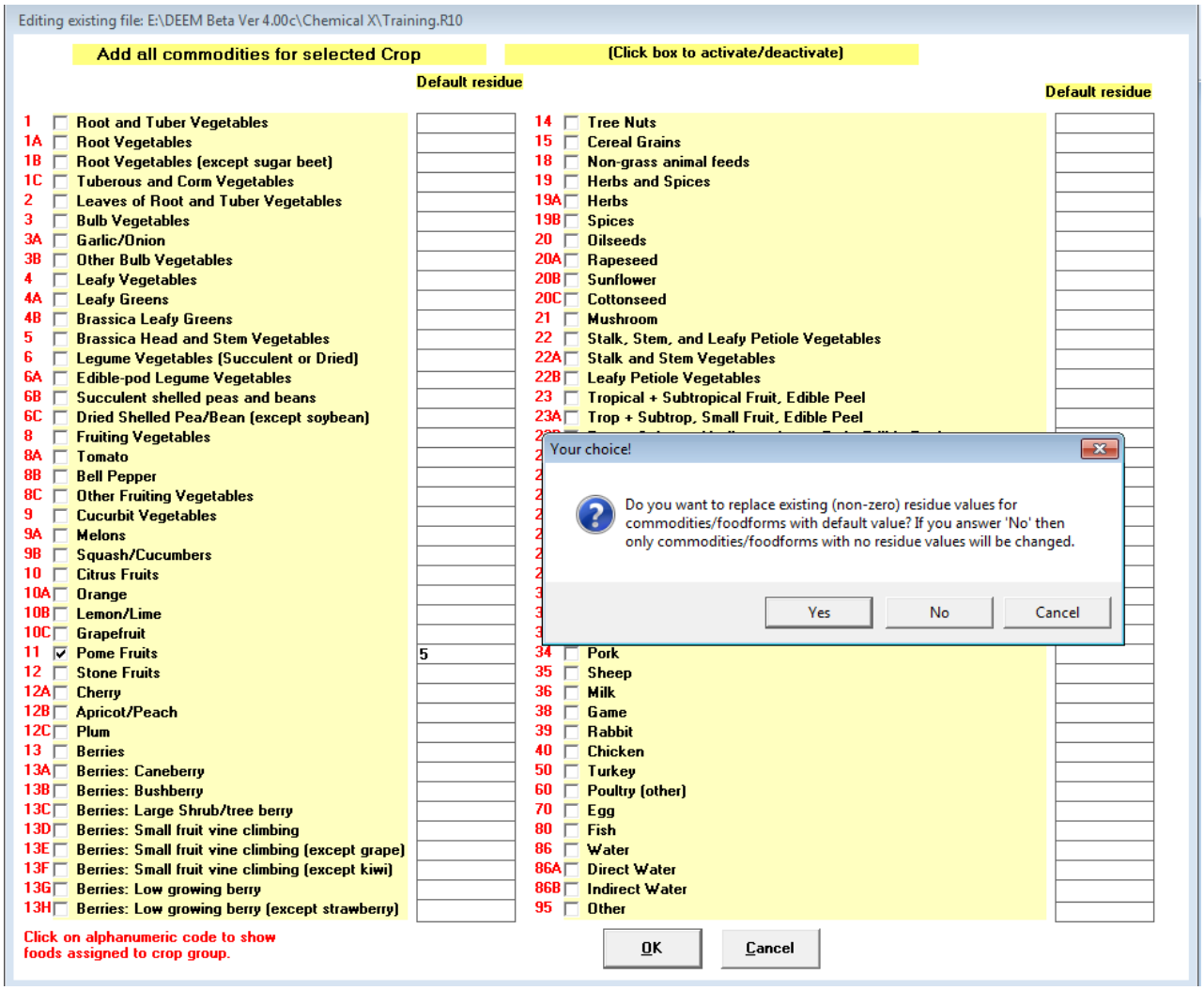


10) ***Additional Features***: ***Crop Groups***

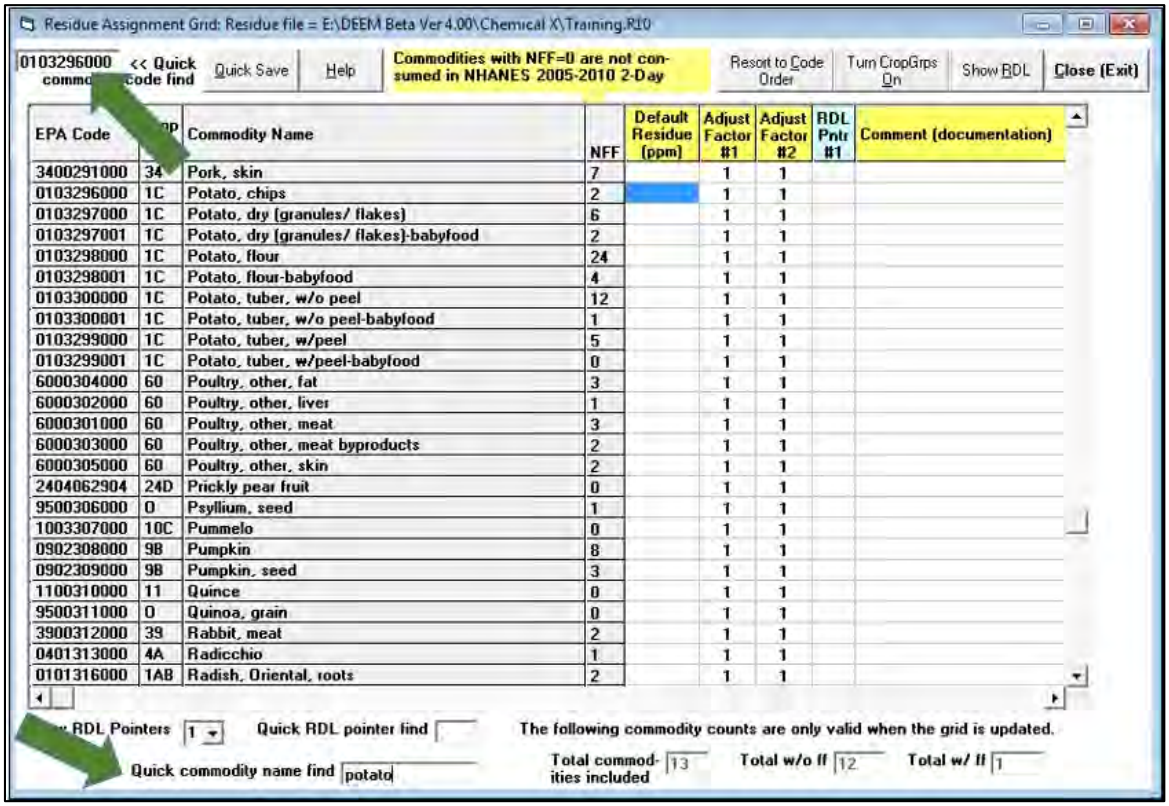
DEEM allows users to assign a single residue value to all commodities in a particular crop group. From main Residue Editor Screen, select "Crop Group Actions", then "Add Crop Group". DEEM will display a table of all Crop Groups and subgroups.



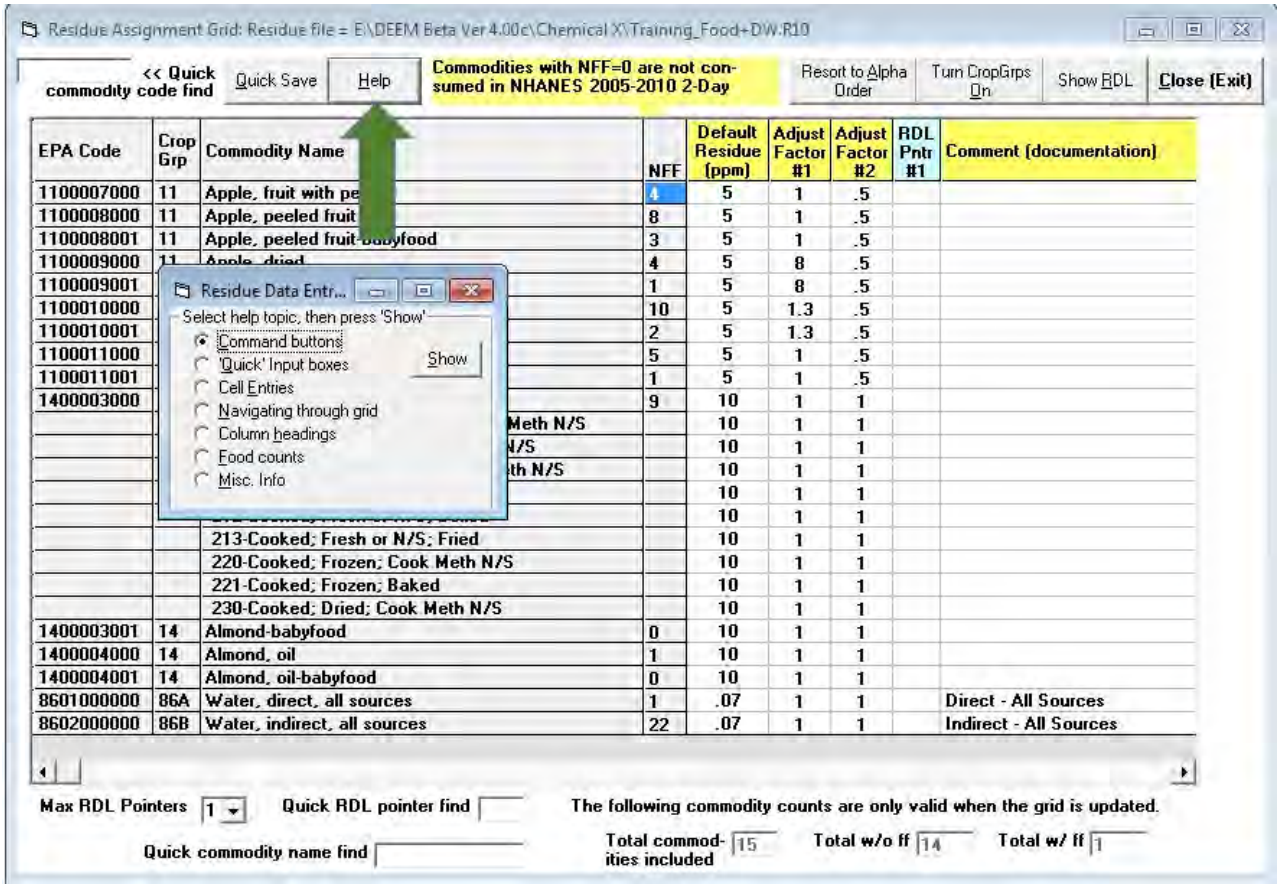
If the user wanted to assign a residue value of 5 ppm to all Pome Fruits, then enter 5 in the "Default Residue" cell, as shown below), and click "OK"; a warning box will appear asking if you want to replace any existing residue values with that default value.



11) The Residue Editor also provides two search fields at the bottom of the window, “Quick Commodity Code Find” and “Quick Commodity Name Find” to move to a specific raw agricultural commodity (RAC) code or food.



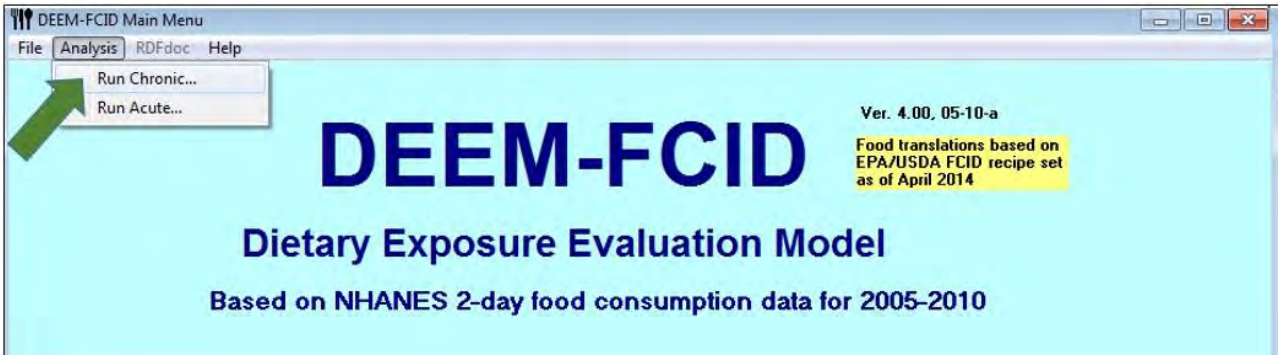
12) The “Help” button provides additional information on the DEEM-FCID Residue Editor.



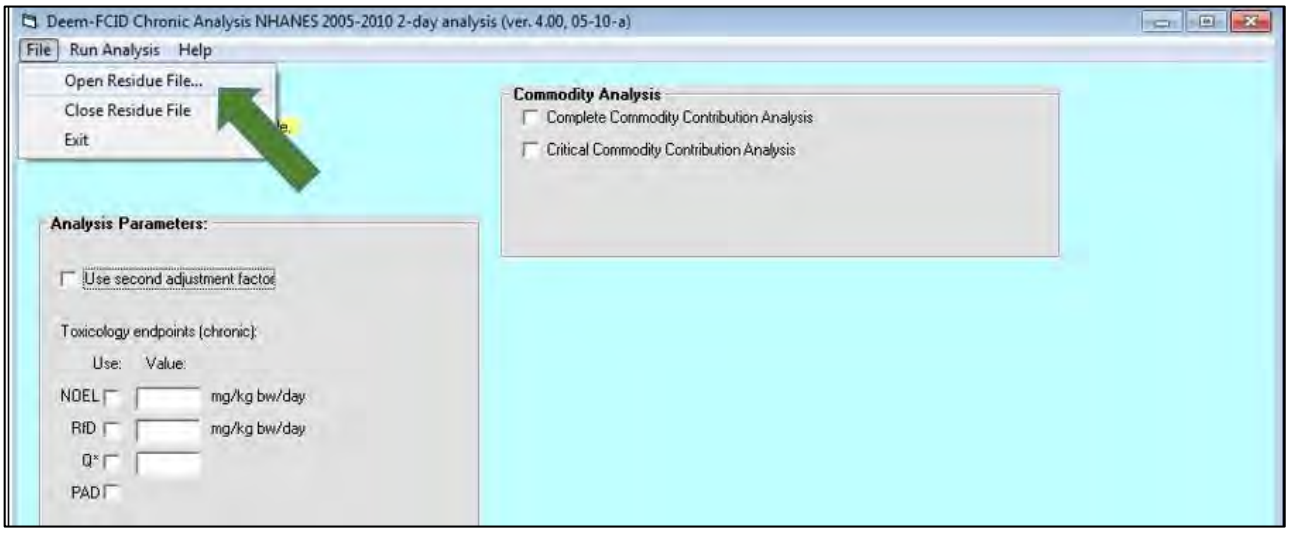
Select the “Close (Exit)” button when you are finished. To save your file for use in the chronic or acute analysis, click “File” and “Save.” For this example, save the file as “Training_Food+DW.” Click “file” and “Exit to Main Menu.”

DEEM-FCID Chronic Dietary Analysis

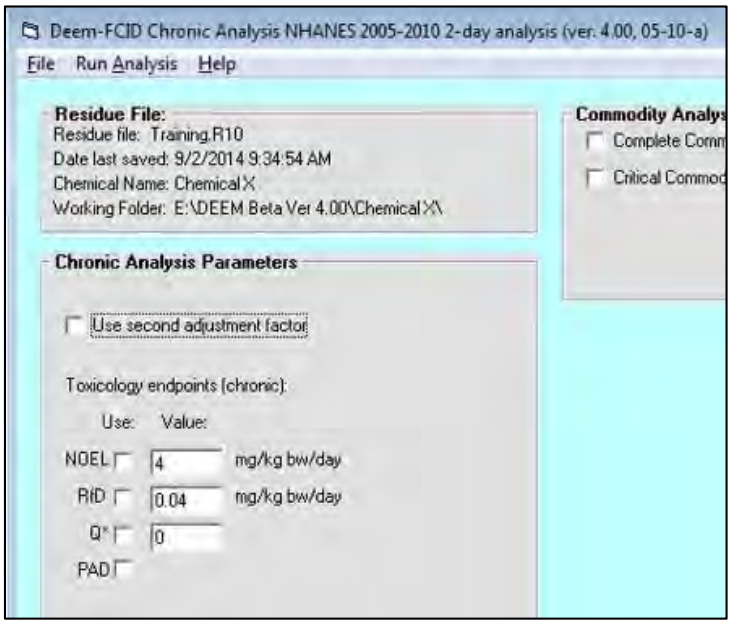
1) To run a DEEM-FCID chronic dietary assessment, go to the DEEM-FCID main menu screen, click on "Analysis" then "Run Chronic."



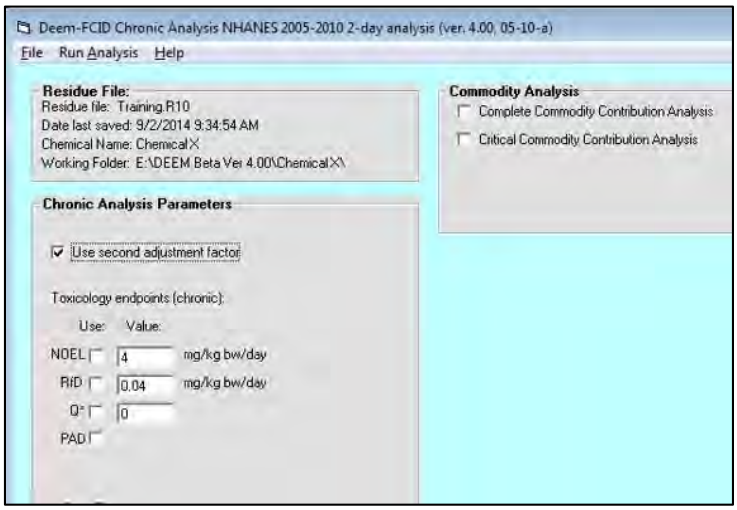
2) Select the file to be analyzed by clicking on "File" from the main menu then "Open Residue File." *Note:* All future run analyses (results files, commodity contribution files) will be saved in the same location as your selected R10 file.



3) Double click the file you want to run. For this example, open "Training.R10." The toxicology endpoints should automatically appear (if you added them in the Edit Header option shown in section 3 of Getting Started). At this point, you will have the option of changing any of the toxicological endpoints identified in the file. You also will be given the option of comparing the exposure results (expressed as mg chemical/kg bw/day) to the chronic RfD, NOEL, both, or to the Q*. Exposure estimates will be expressed as a percent of the RfD; selecting the NOEL will produce Margins of Exposure (MOEs). The chronic exposure value for the general U.S. population will be multiplied by the Q* to yield the lifetime cancer risk estimate. Click on the toxicology endpoints (e.g., NOEL, RfD).

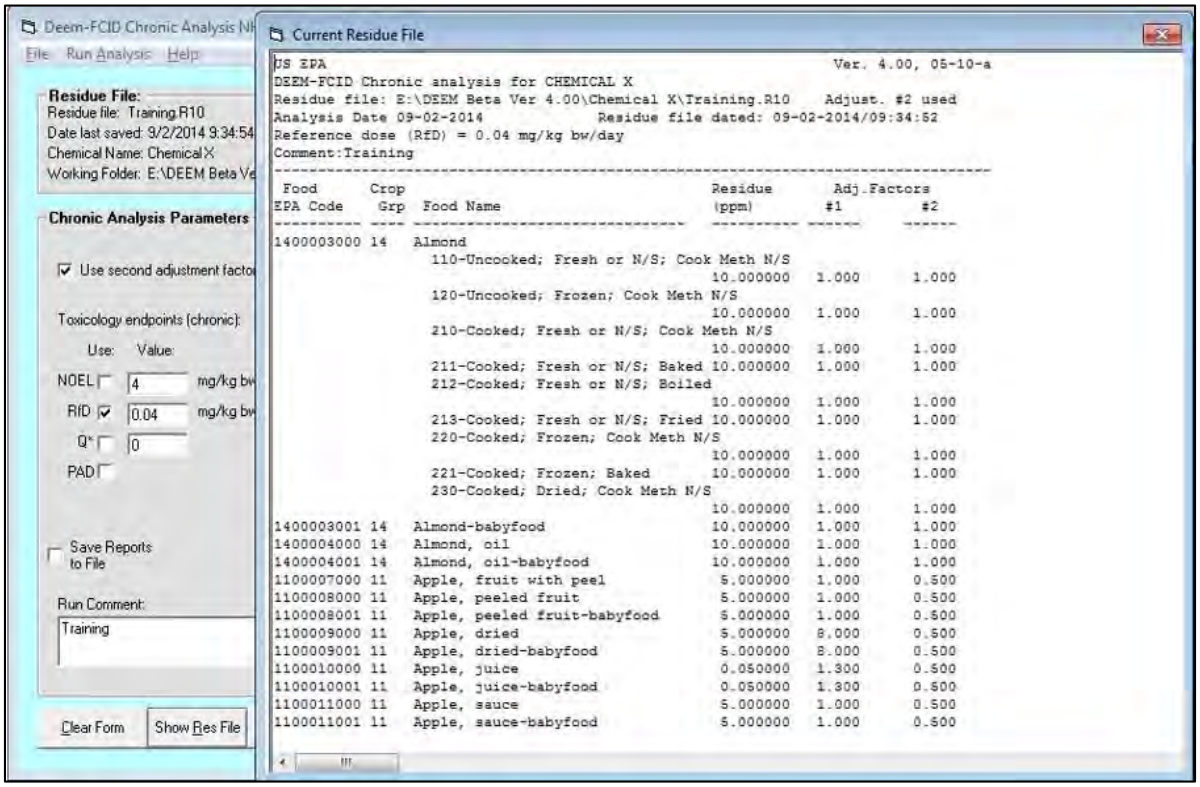


4) Click on the "Use second adjustment factor" (if you added a percent crop treated value in the current analysis). As indicated, DEEM will always multiply the Residue by Adjustment Factor #1 in chronic and acute dietary exposure assessments.

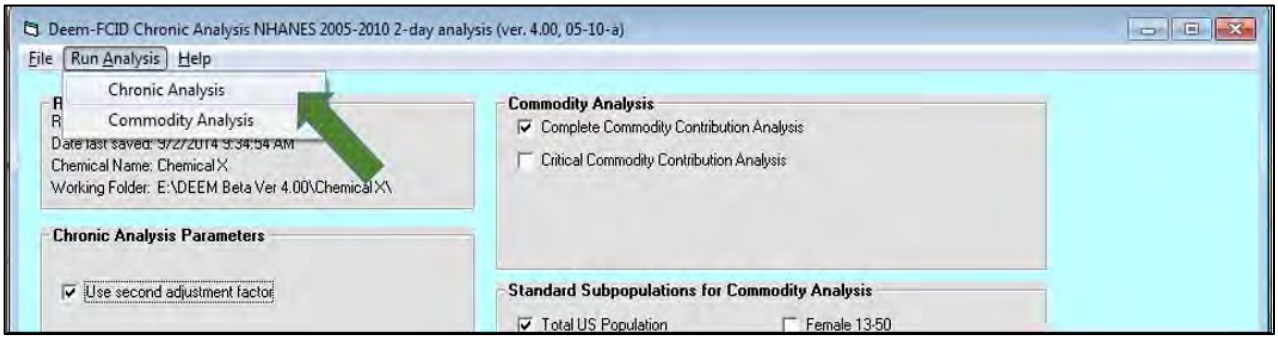


5) If you want to save the chronic analysis report to a file, select "Save Reports to File" option and name the file.

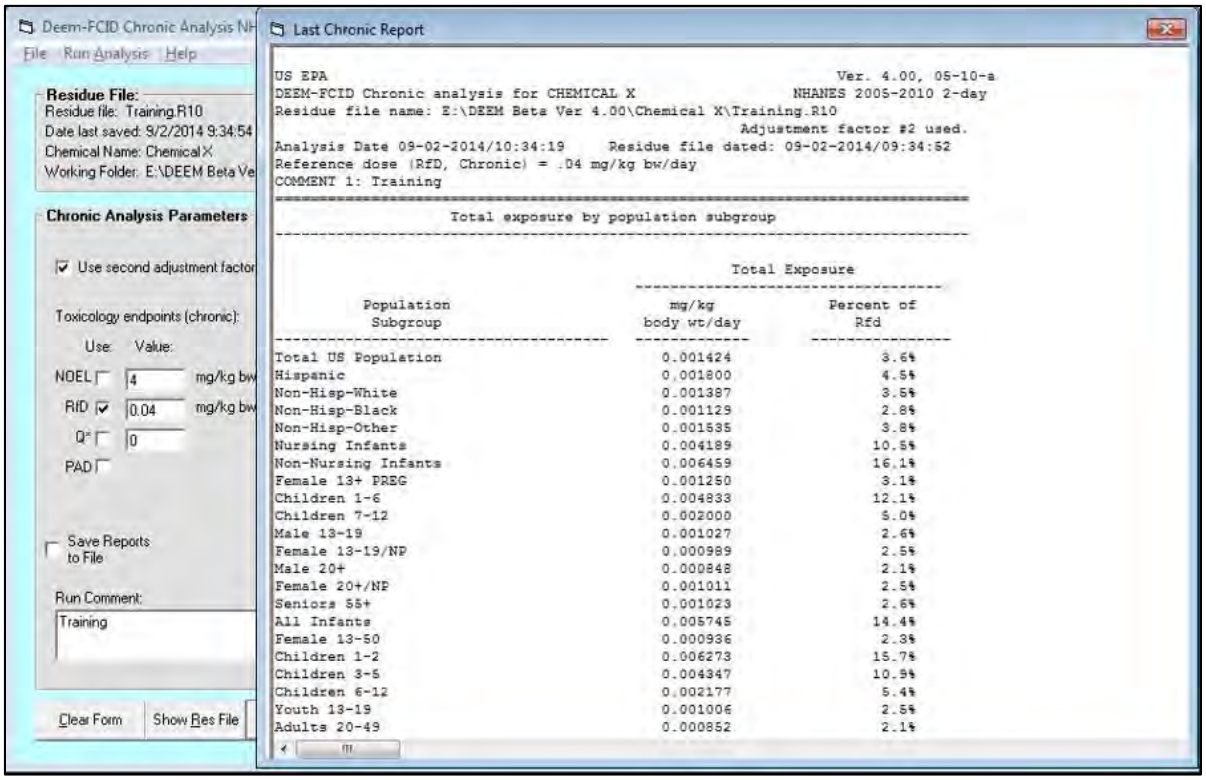
6) Before you perform a chronic (or acute) run, you may view or obtain a hard copy of the residue data used in your analysis by clicking the "Show Res File" button. You will then be prompted to display the report to screen, save to disk, or send directly to printer. DEEM allows you to sort these residue data by alphabetical or crop group order.



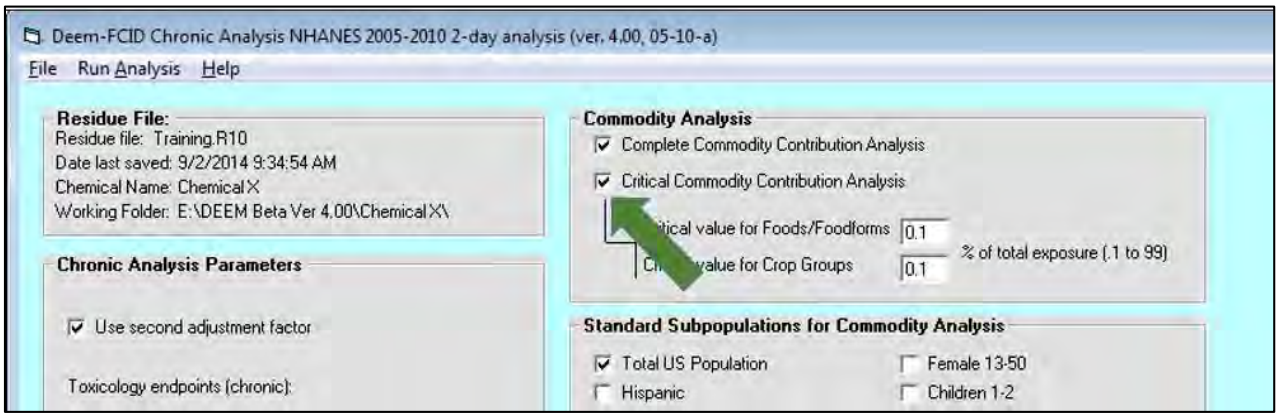
7) To run a DEEM-FCID chronic dietary assessment, click on "Run Analysis," from the main menu, then select "Chronic Analysis." The chronic analysis will run automatically.



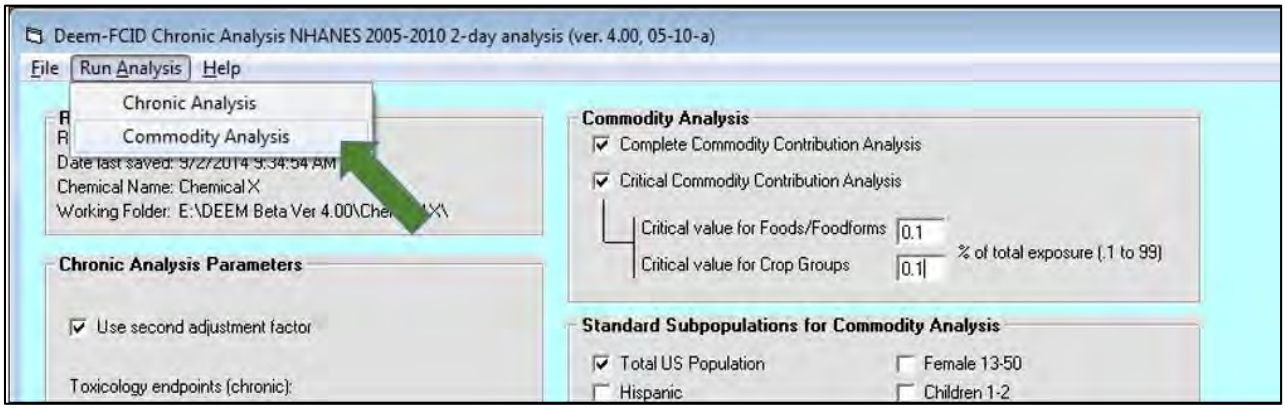
8) The "Show Last Chronic Rpt" button permits the user to display, save, or print the analysis report. If you select to save a report to disk, you will be prompted to enter a file name.



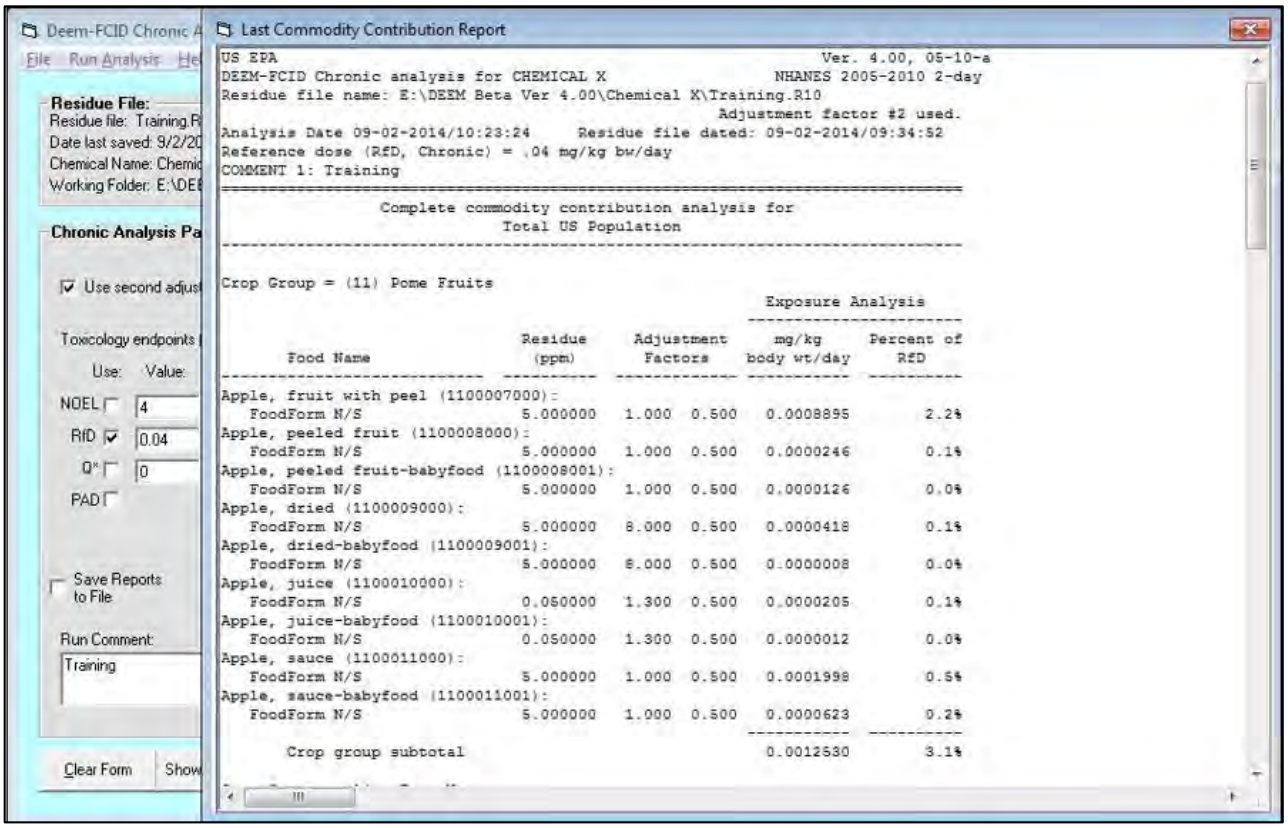
9) Critical Commodity Analysis. To perform a Critical Commodity Analysis, select the "Complete Commodity Contribution Analysis" option and under the Standard Subpopulations for Commodity Analysis select the subpopulations of interest. *[Note: If you click "Total US Population," the results will automatically show the results for all the subpopulations]*



10) To run the Critical Commodity Contribution Analysis, click on "Run Analysis," then click "Commodity Analysis." The commodity analysis will run automatically and you will then be prompted to display the report to screen, save to disk, or send directly to printer.



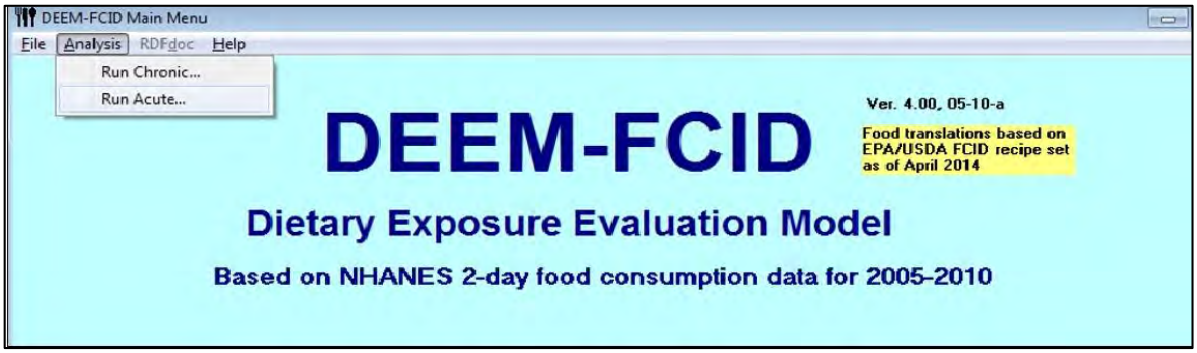
11) The "Show Last Commodity Rpt" button permits the user to display, save or print the analysis report. The user may save the report to file by selecting Save Reports to disk file.



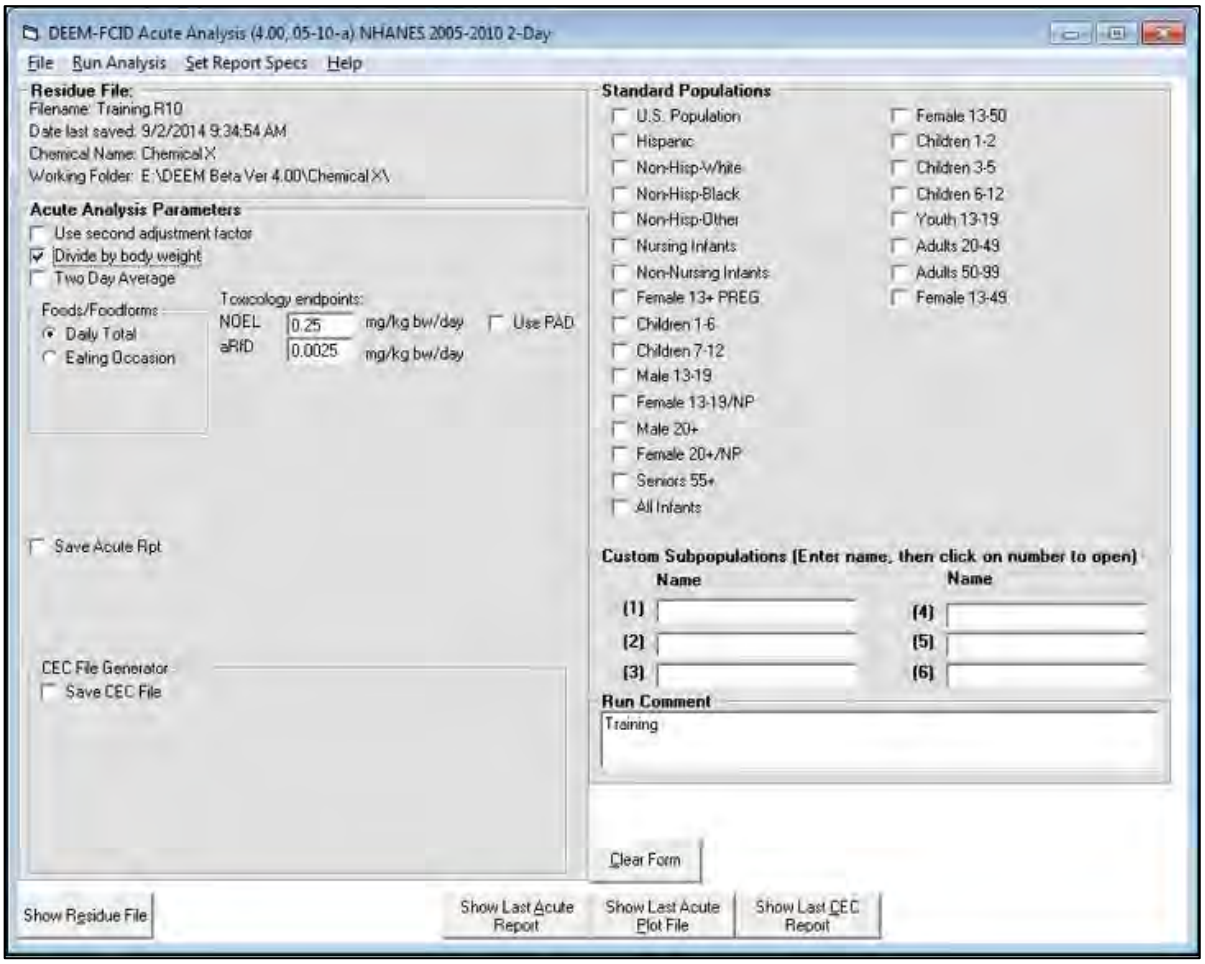
When you have completed your chronic assessment, you may exit the window by clicking on "File" then "Exit."

DEEM-FCID Acute Dietary Analysis (Tier 1 & 2)

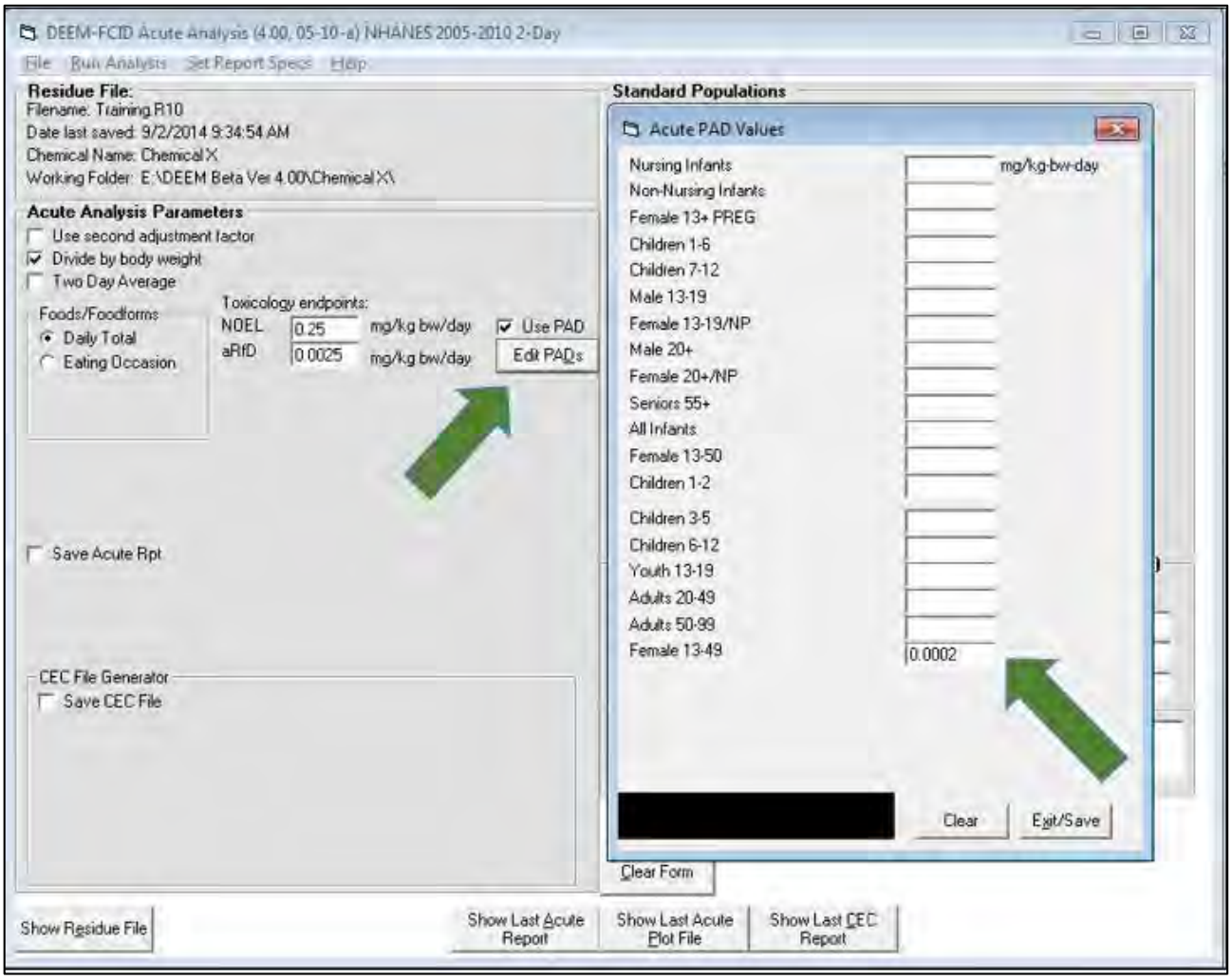
1) To run a DEEM-FCID acute dietary assessment, go to the DEEM-FCID main menu screen, click on "Analysis" then "Run Acute."



2) Select the file to be analyzed by clicking on "File" then "Open Residue File." For this example, open "Training.R10."

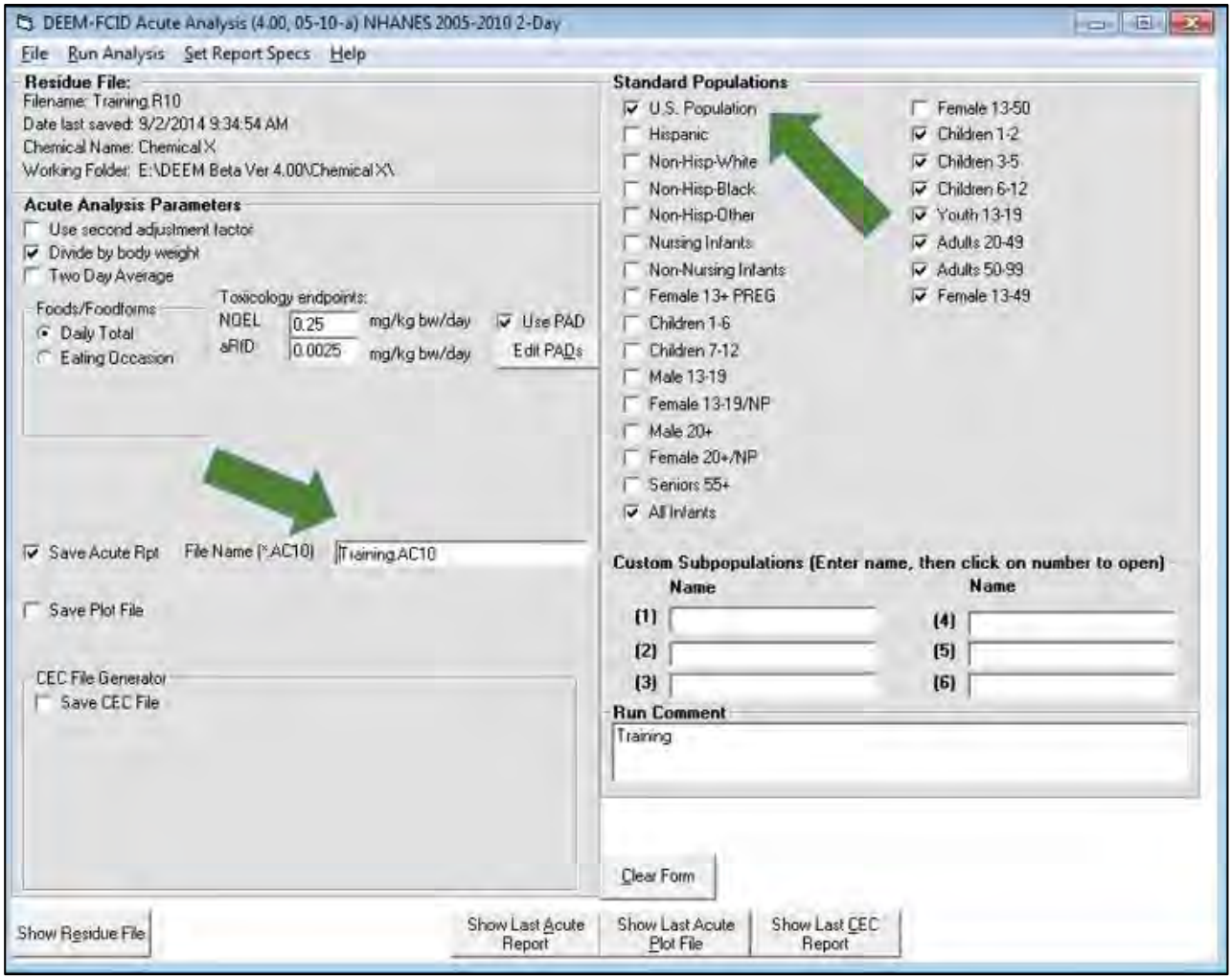


3) The toxicology endpoints should automatically appear (if you added them in the Edit Header option shown in section 3 of Getting Started). At this point, you will have the option of changing any of the toxicological endpoints identified in the file. In particular, for acute analysis, there may be a different toxicology endpoint for females 13-49 yrs. If we want to enter an acute Population Adjusted Dose (aPAD) equal to 0.0002 mg/kg/day for females 13-49 yrs, then click the "Edit PADs" button. A window will appear with a list of population subgroups; enter 0.0002 for Females 13-49 years old, then Click Exit/Save. DEEM will use the default aPAD (0.0025) in the R10 file for all other subpopulations.



Note: Generally, users should not select "Use second adjustment factor" in an acute dietary risk assessment. When performing a deterministic acute dietary exposure assessment, PCT is not used to refine anticipated residues and aggregate dietary exposure at the Per capita 95th percentile is the Percentile of Regulation. In refined dietary exposure assessments, the PCT is used indirectly to determine the expected number of samples that were treated but do not have detectable residues (i.e., number of ½ LODs) and the Per capita 99.9th percentile is the Percentile of Regulation.

4) If you want to Save the results in a separate file, click “Save Acute Rpt” and enter a filename (“Training”) in the blank space.



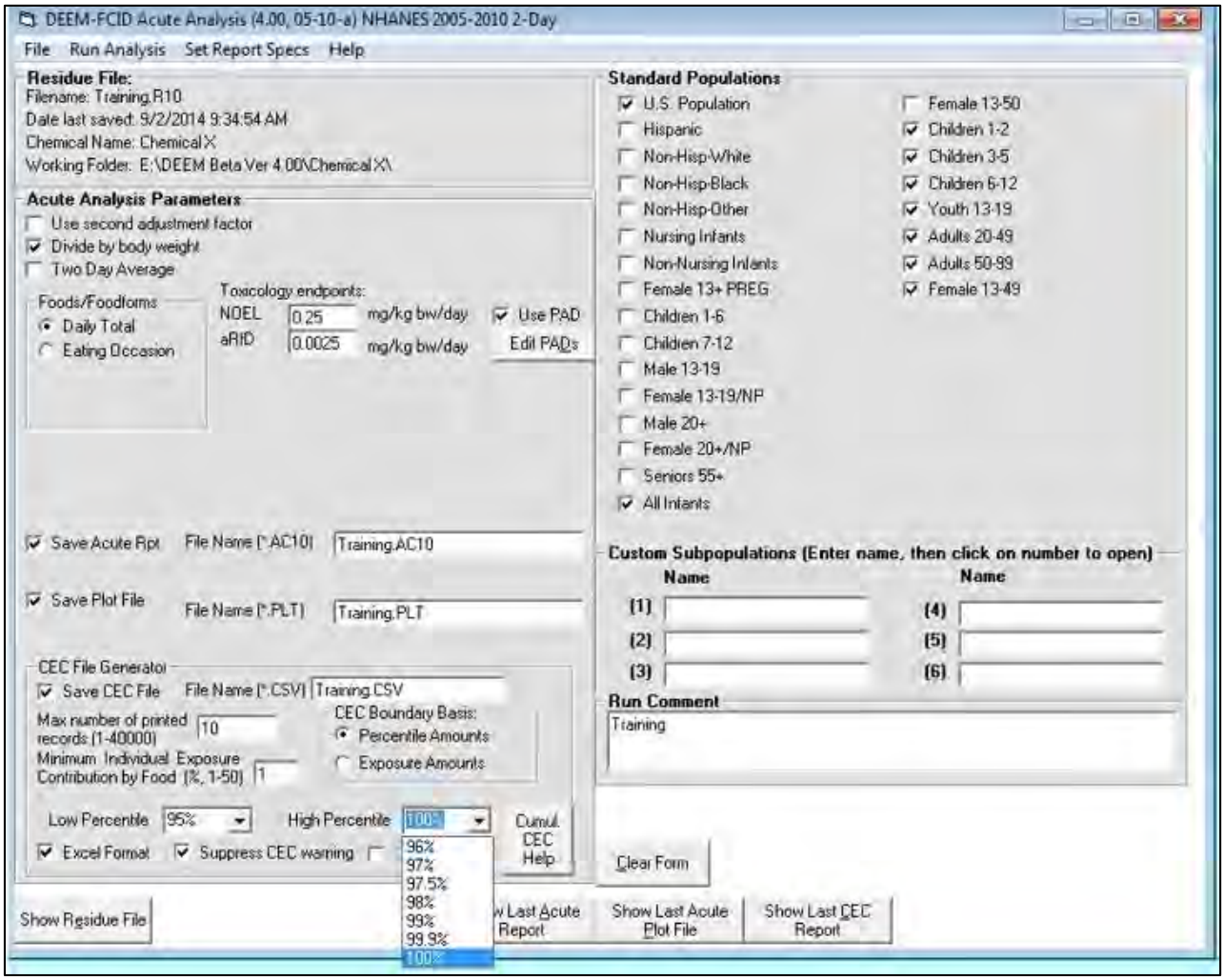
5) The **Plot File** includes information about the actual (unweighted) and weighted number of people-days and user-days in the populations considered. It can be imported in a spreadsheet program for statistical manipulation or to produce graphs. The plot routine runs automatically with the acute analysis, however, if you want the option of viewing the results on the screen, saving it to a disk, or printing it, then you need to Click “Save Plot File” and enter a filename. After the simulation is completed, the Plot file can be accessed clicking the “Last Acute Plot Fl” button.

6) Critical Exposure Commodity (CEC) Analysis. The acute CEC analysis permits the user to identify commodities that are contributing to aggregate dietary exposures within the specified interval. To run a DEEM-FCID acute CEC analysis, select "Save CEC File." You will then be prompted to enter a CEC file name and the desired number of records, minimum exposure contribution, and exposure intervals.

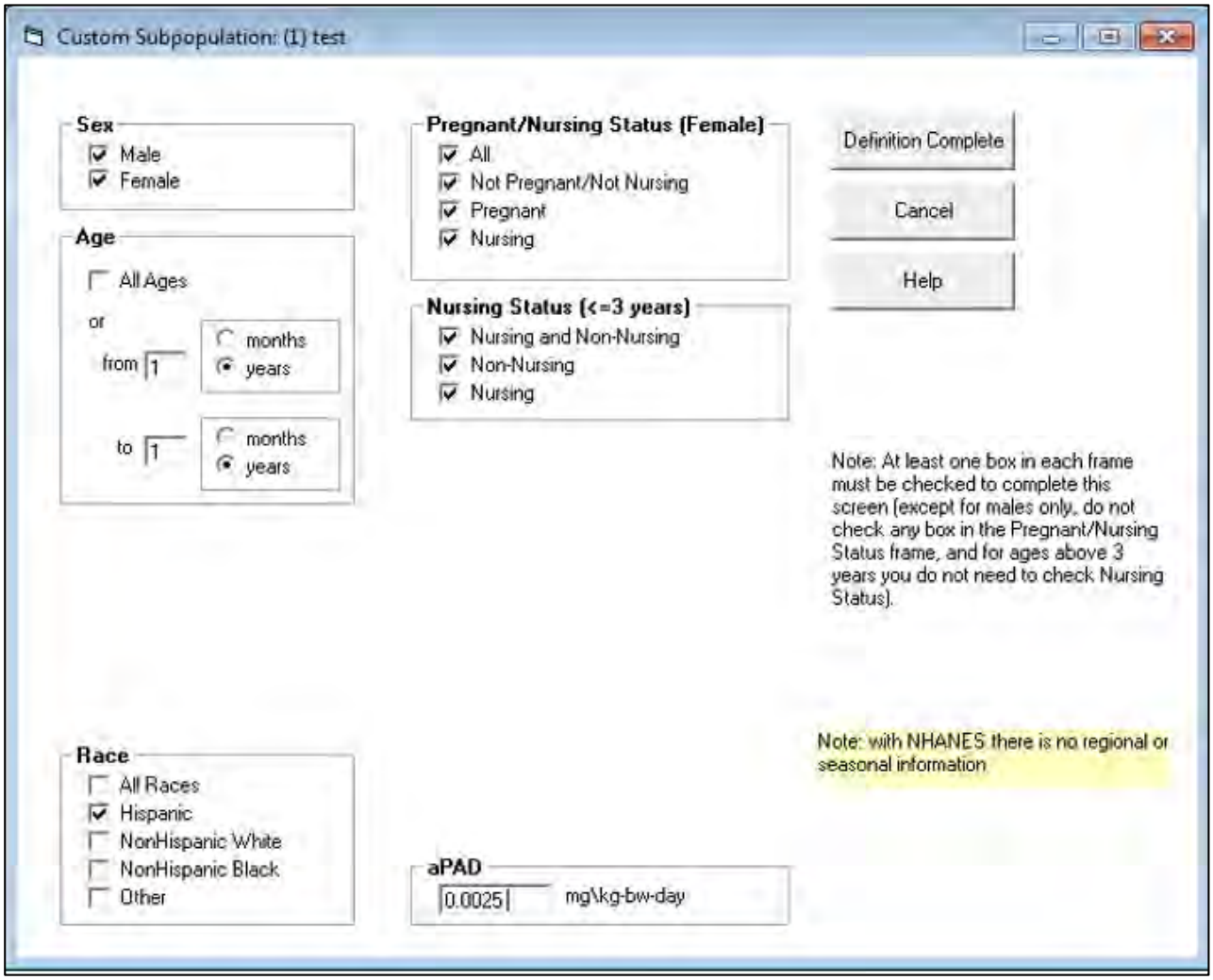
Note: Maximum CEC records (1-40000): This is the maximum number of individual exposure records that can be saved to a CEC file.

Minimum Contribution (1-50%): Only foods/food forms that contribute more than this percentage amount to an individual's total exposure will be included in the CEC printout.

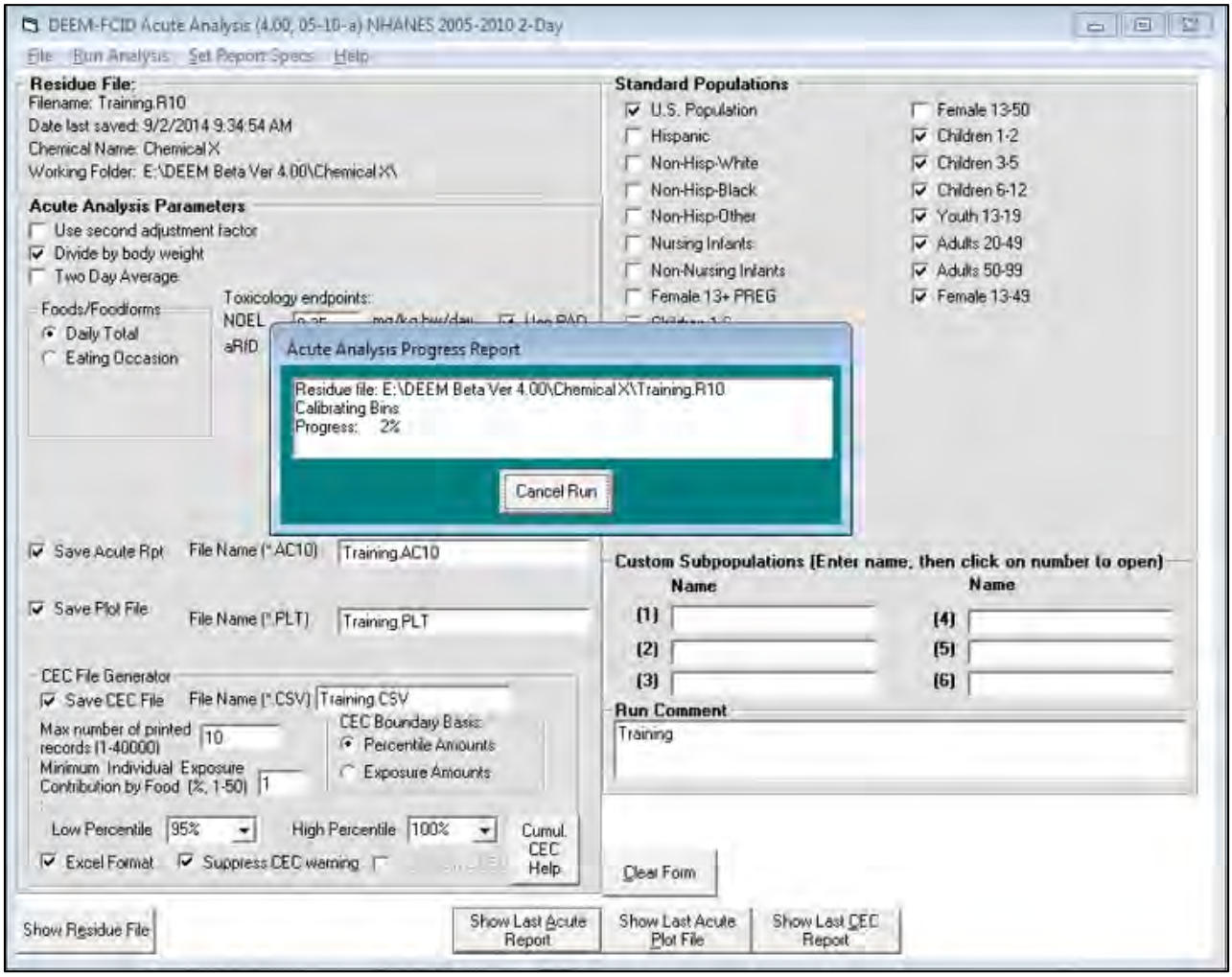
Low/High Percentiles: User-specified interval to determine commodities contributing to exposure between these percentiles. {*The interval 95th to 100th percentile is typically specified for deterministic (Tier 1 or 2) assessments. Select "Excel Format" to facilitate importing into Excel, and "Suppress CEC warning" to allow DEEM to proceed with the analyses.*}



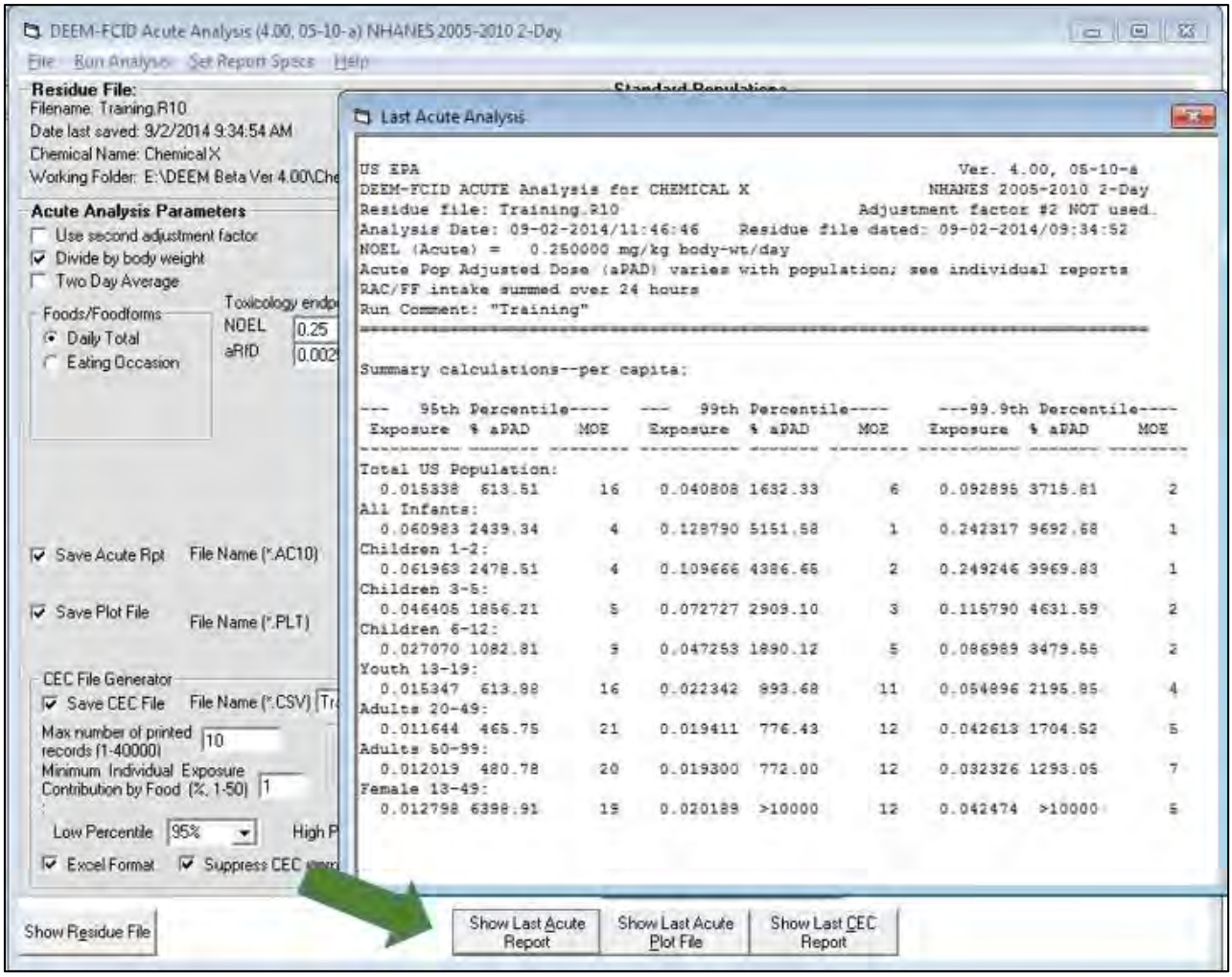
7) Under Standard Populations, select the subpopulations of interest. DEEM-FCID also allows users to create and perform acute dietary exposure assessments for up to 6 **Custom Populations**. To create a custom group, enter a (arbitrary) name for that group in one of the 6 blanks in the "Custom Subpopulations" section and click the number on the left side of that box. This will prompt the Custom Subpopulation menu to appear and you may then select your preferences for the indicated population. In the example below, the custom group 'test' is specified consists of all 1 year olds. Once the population group has been specified, click the Definition Complete button and you will be returned to the DEEM-FCID acute analysis screen.



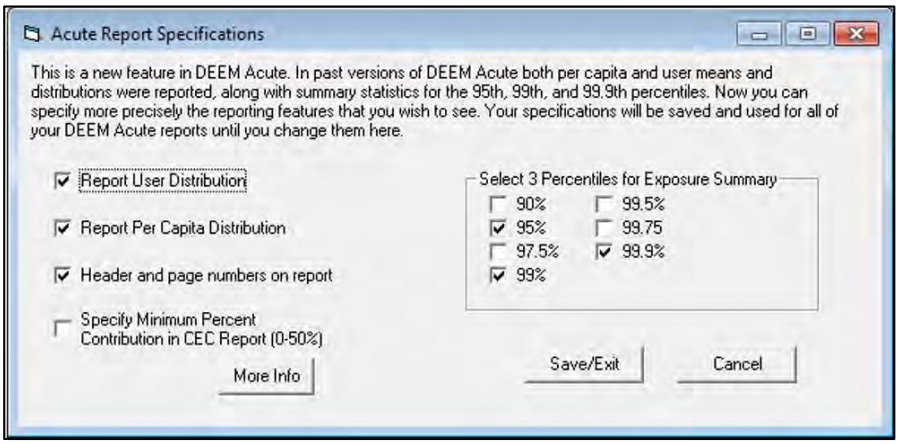
8) Once you have identified the parameters for conducting the analyses and the population groups of interest, click on "Run Analysis" at the top of the Acute Analysis screen. A progress window will appear displaying the status of the analysis.



9) Once the analysis is completed, you will have the option of viewing the results on the screen, saving it to disk, or printing it by clicking the "Last Acute Rpt" button at the bottom of the screen. The other two buttons allow users to view, save and/or print the Plot File and CEC Report.



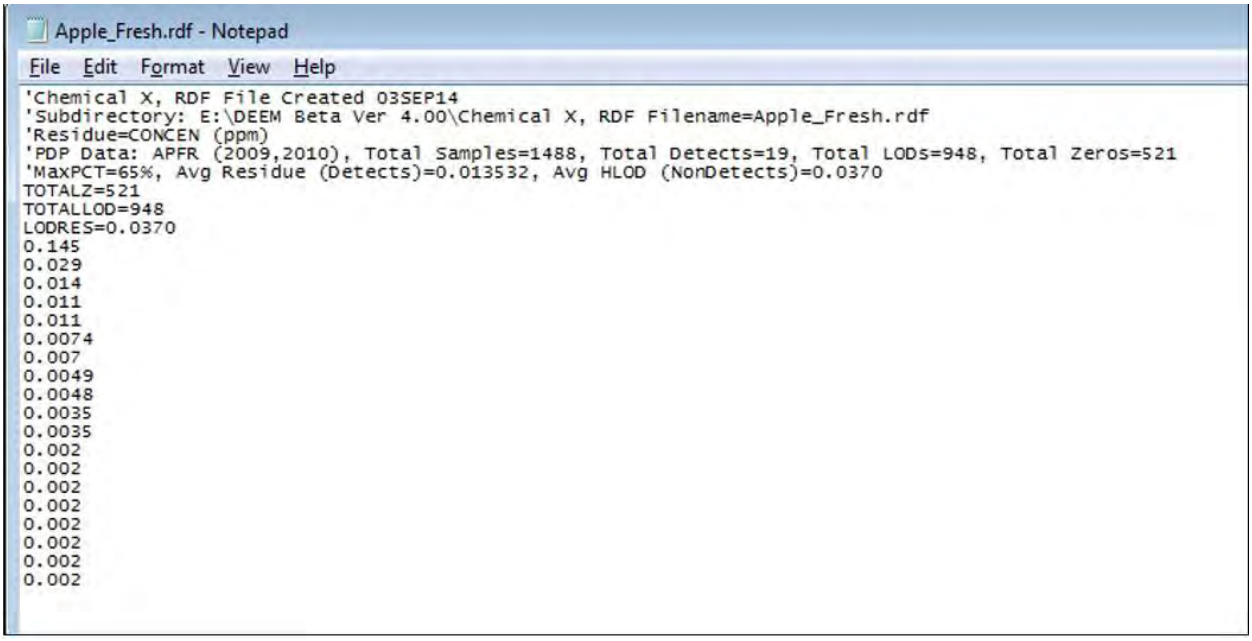
10) DEEM allows users to tailor the results presented in the Acute Report. To edit those specifications, click the Set Report Specs button at the top of the Menu bar and select the parameters (percentiles) that you want to see in the report.



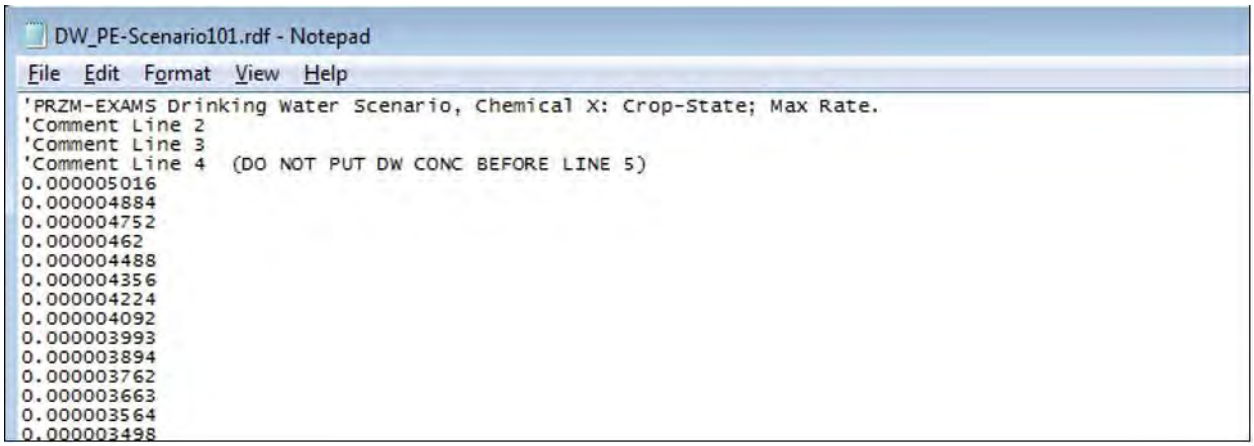
Performing Monte Carlo Simulations in DEEM-FCID

Creating Empirical Residue Distributions

In order to perform an acute probabilistic dietary risk assessment, the user needs to create and assign one or more empirical residue distribution files (rdf) to one or more FCID commodities. Such files may be created in Notepad or Wordpad. The figure below illustrates an rdf file created using residue monitoring data for fresh apples, "Apple_Fresh.rdf". The first five lines begin with a single apostrophe mark and are simply comments. The residue distribution consists of 521 zeros, 948 values at half the LOD (0.0370 ppm), and 19 detects listed below. Attachment 3 provides further details regarding construction of DEEM RDF files.



The next figure illustrates an rdf file "DrinkingWater_PRZMEXAMS.rdf" containing predicted DW concentrations from a PRZM-EXAMS (PE) simulation. As above, the first four lines contain comments, and the DW concentrations follow beginning on the fifth line.

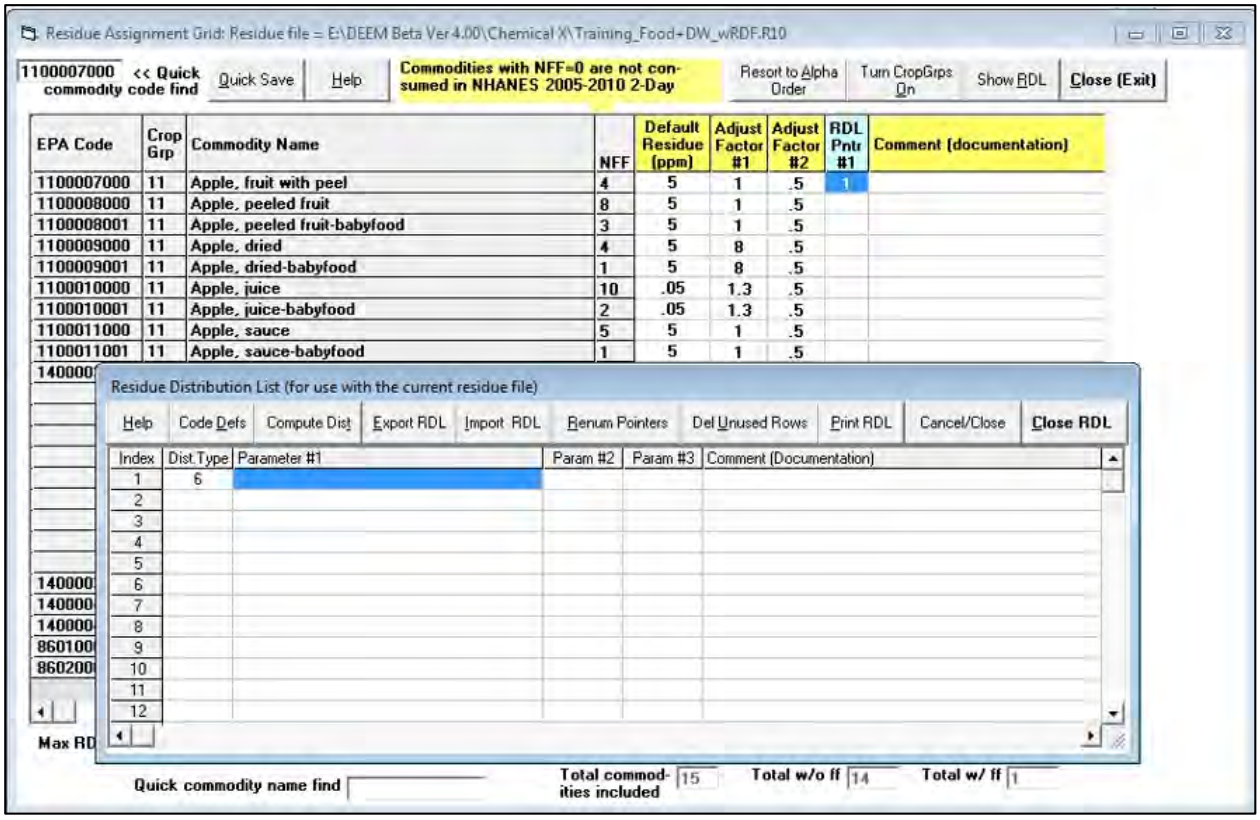


When Creating DW Inputs (RDF Files) from PE data for DW Assessments make sure to:

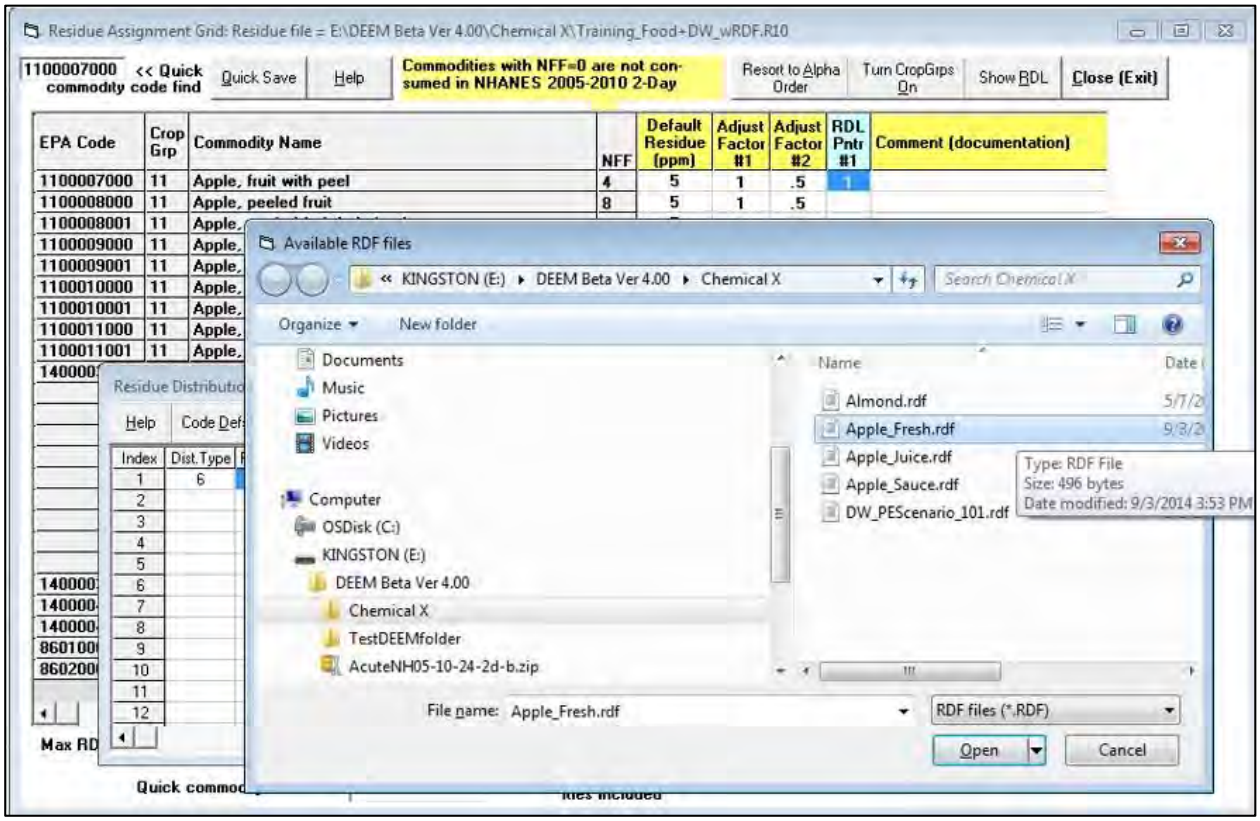
i. Check that DW concentrations are in ppm, and begins on January 1
ii. Delete the entire 1st Year of Simulations (if not already done so) since there are no DW concentrations before the overall 1st app,
iii. Make sure last record is December 31st (complete year); otherwise, delete records for partial years (the last day of some PE outputs contain the first day of following year (e.g., Jan 1st, 1992),
iv. Add Header and Comments in first four rows-DEEM-FCID assumes that the empirical residue data begins after the 4th row (unless otherwise specified), and
v. Save file with *.rdf extension.

Assigning Empirical Residue Distributions

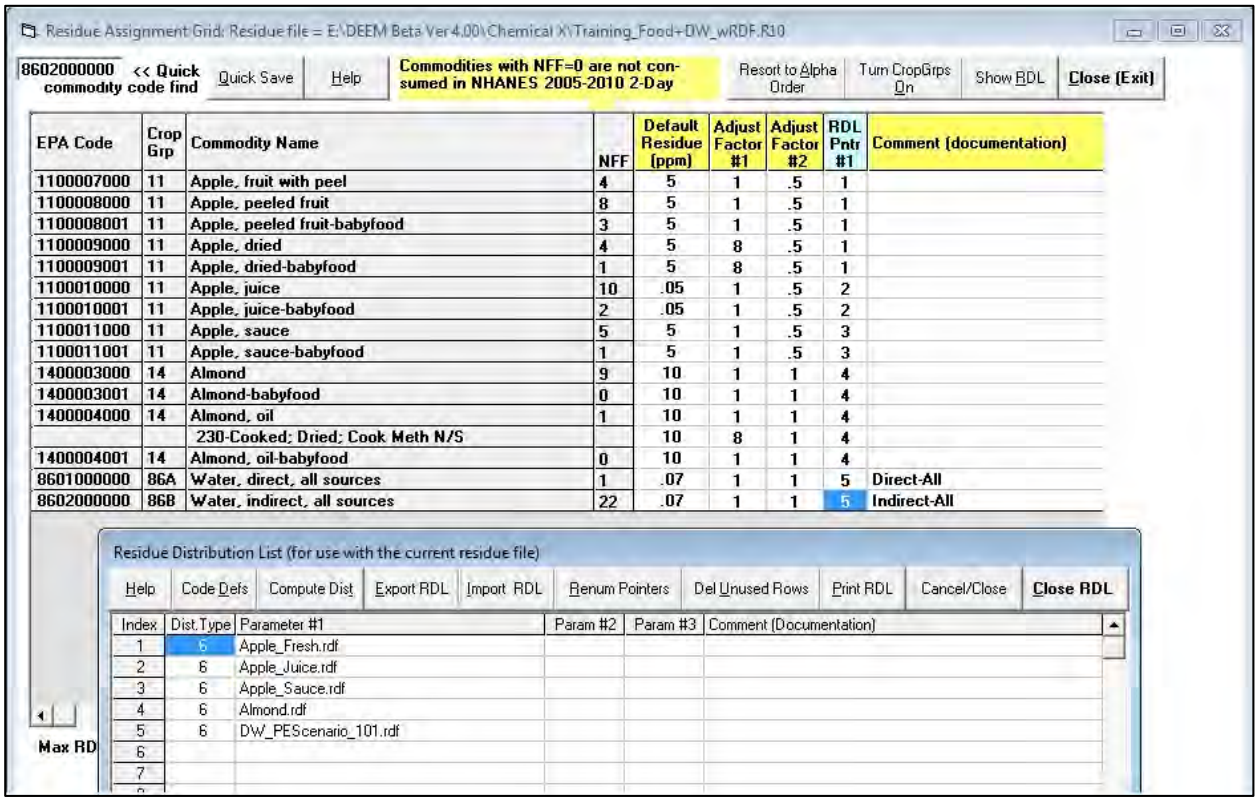
To assign empirical residue distribution (RDF file), enter a number in the "RDL Pntr #1" column, click the "Show RDL" button and wait for DEEM to open a Residue Distribution List (RDL) dialog box. Click on the cell under "Dist. Type", and type in the value "6" to specify an Empirical Distribution, then click the next cell under "Parameter #1"; the DEEM Residue Editor will open an Explorer Window-navigate the "Available RDF files" window.



Navigate the Explorer Window to the appropriate subdirectory and select the desired RDF file. The first column "Index" matches with the index listed in the "RDL Pntr #1": "Apple, fruit with peel.rdf" is assigned to RDF Index=1. Repeat the procedure for other commodities, then save the file as: Training_Food+DW_wRDF.R10.

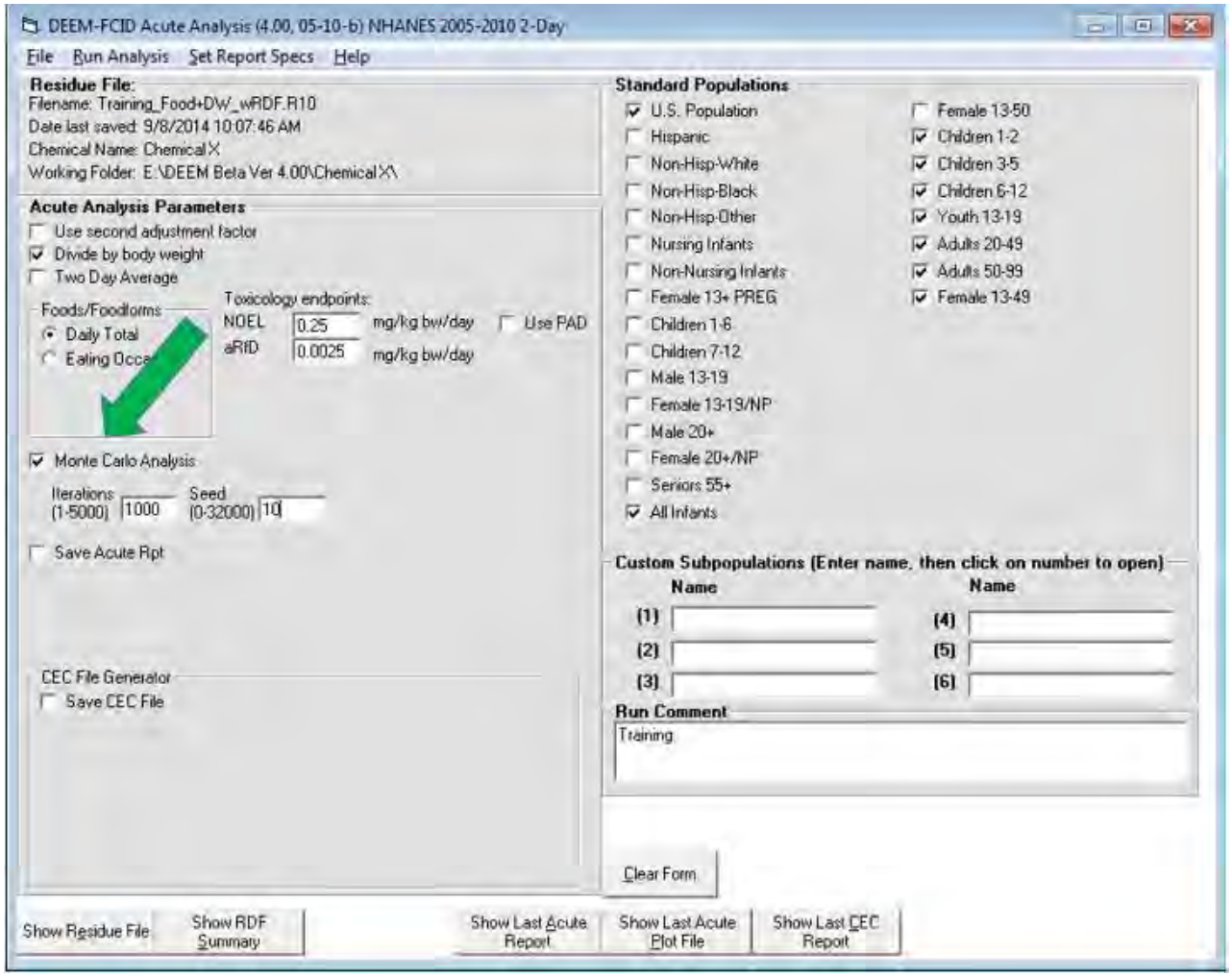


The file "Training_Food+DW_wRDF.R10" contains 5 empirical residue distributions (3 for apples, 1 for almonds, and 1 for DW) assigned to the corresponding commodities.

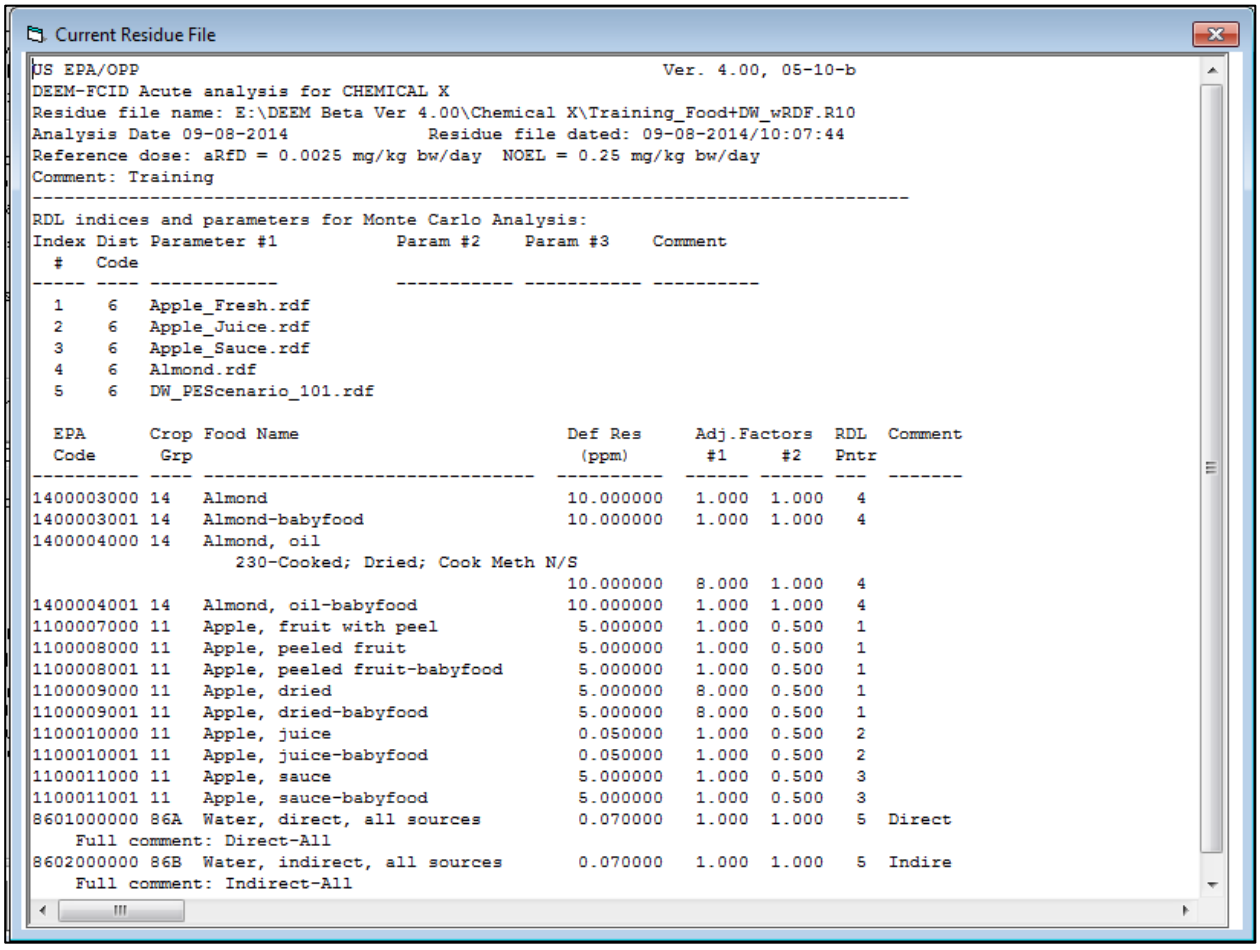


DEEM-FCID Probabilistic Acute Dietary Analysis

If a residue assignment file (R10) contains one or more residue distributions, the DEEM-FCID Acute Dietary Assessment Dialog Window will include a check box option for "Monte Carlo Analysis". If the user checks this option, then DEEM prompts the user to enter values for number of iterations performed per food diary, "Iterations (1-5000)", and a seed value for the pseudo random number generator, "Seed (0-32000)", to allow users to reproduce results on other computers.



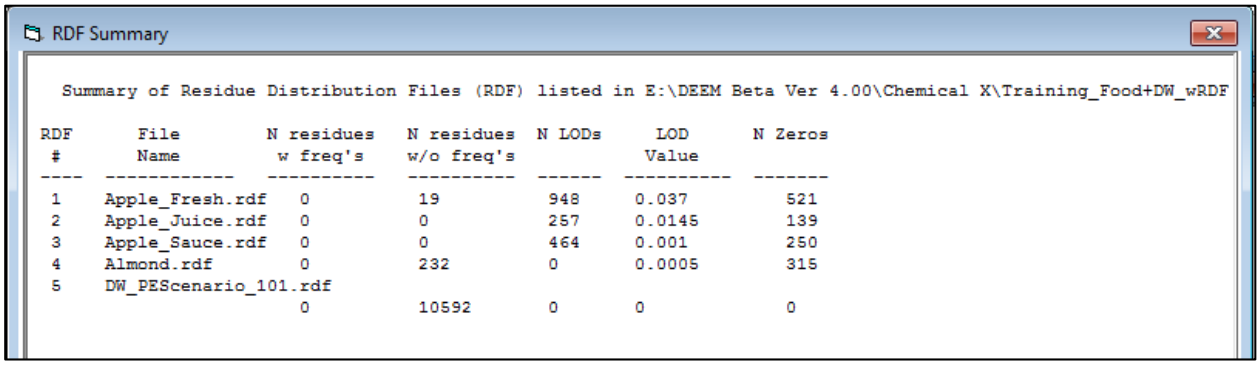
As before, the "Show Residue File" and "Show RDF Summary" buttons allow users to view the residue assignments and summary statistics on the residue empirical distributions (RDF) before performing a Monte Carlo Simulation.



Current Residue File

```
US EPA/OPP                                                  Ver. 4.00, 05-10-b
DEEM-FCID Acute analysis for CHEMICAL X
Residue file name: E:\DEEM Beta Ver 4.00\Chemical X\Training_Food+DW_wRDF.R10
Analysis Date 09-08-2014            Residue file dated: 09-08-2014/10:07:44
Reference dose: aRfD = 0.0025 mg/kg bw/day  NOEL = 0.25 mg/kg bw/day
Comment: Training
--------------------------------------------------------------------------------
RDL indices and parameters for Monte Carlo Analysis:
Index Dist Parameter #1           Param #2    Param #3    Comment
  #   Code
----- ---- ------------           ----------- ----------- ----------
  1    6   Apple_Fresh.rdf
  2    6   Apple_Juice.rdf
  3    6   Apple_Sauce.rdf
  4    6   Almond.rdf
  5    6   DW_PEScenario_101.rdf

  EPA      Crop Food Name                          Def Res     Adj.Factors  RDL  Comment
  Code      Grp                                     (ppm)       #1     #2   Pntr
---------- ---- --------------------------------  ----------  ------ ------ ---  -------
1400003000 14   Almond                            10.000000   1.000  1.000   4
1400003001 14   Almond-babyfood                   10.000000   1.000  1.000   4
1400004000 14   Almond, oil
                   230-Cooked; Dried; Cook Meth N/S
                                                  10.000000   8.000  1.000   4
1400004001 14   Almond, oil-babyfood              10.000000   1.000  1.000   4
1100007000 11   Apple, fruit with peel             5.000000   1.000  0.500   1
1100008000 11   Apple, peeled fruit                5.000000   1.000  0.500   1
1100008001 11   Apple, peeled fruit-babyfood       5.000000   1.000  0.500   1
1100009000 11   Apple, dried                       5.000000   8.000  0.500   1
1100009001 11   Apple, dried-babyfood              5.000000   8.000  0.500   1
1100010000 11   Apple, juice                       0.050000   1.000  0.500   2
1100010001 11   Apple, juice-babyfood              0.050000   1.000  0.500   2
1100011000 11   Apple, sauce                       5.000000   1.000  0.500   3
1100011001 11   Apple, sauce-babyfood              5.000000   1.000  0.500   3
8601000000 86A  Water, direct, all sources         0.070000   1.000  1.000   5  Direct
    Full comment: Direct-All
8602000000 86B  Water, indirect, all sources       0.070000   1.000  1.000   5  Indire
    Full comment: Indirect-All
```

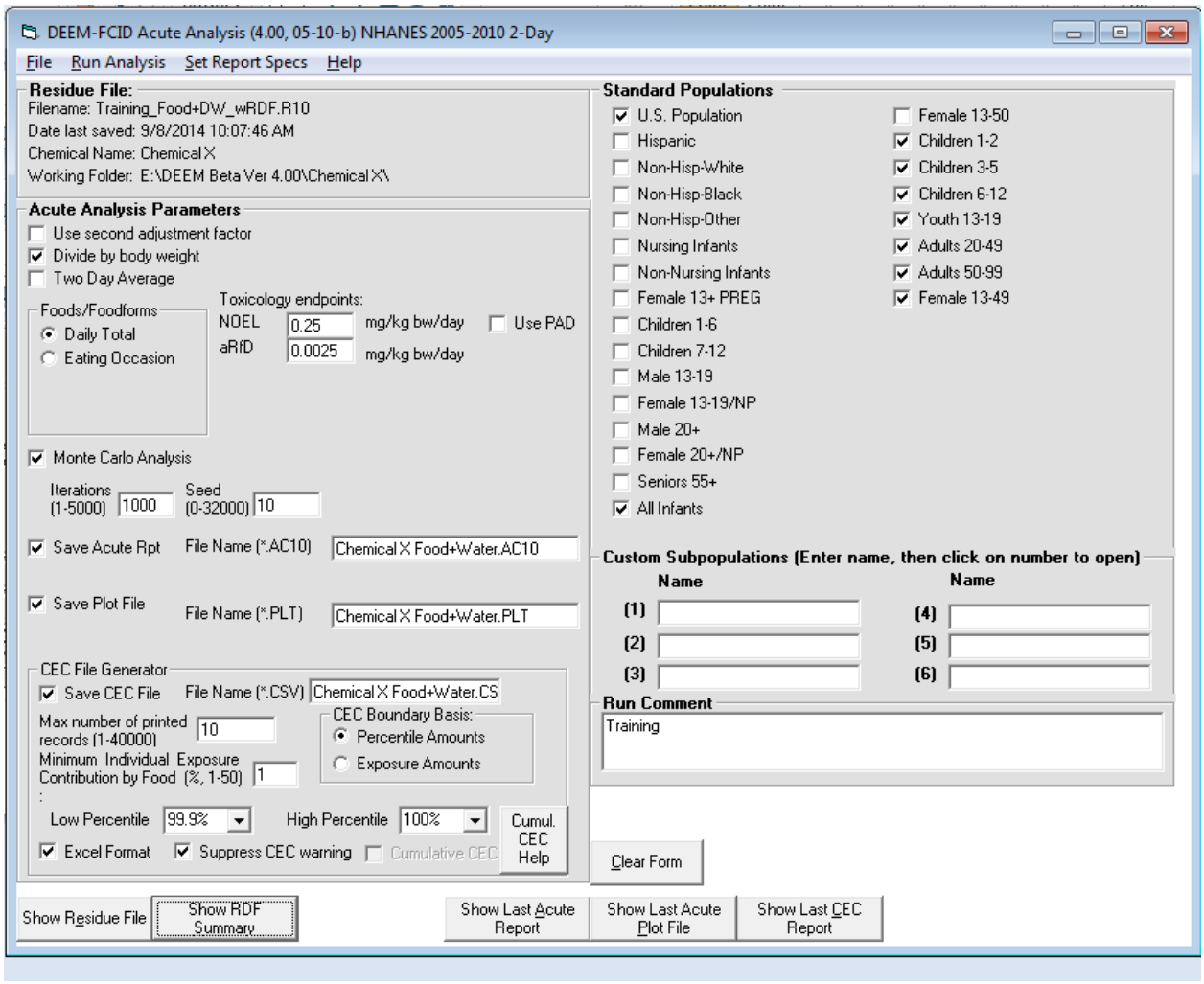


RDF Summary

```
   Summary of Residue Distribution Files (RDF) listed in E:\DEEM Beta Ver 4.00\Chemical X\Training_Food+DW_wRDF

 RDF      File         N residues   N residues  N LODs     LOD      N Zeros
  #       Name          w freq's    w/o freq's            Value
 ----  ------------   ----------   ----------  ------  ----------  -------
  1    Apple_Fresh.rdf    0           19          948     0.037        521
  2    Apple_Juice.rdf    0           0           257     0.0145       139
  3    Apple_Sauce.rdf    0           0           464     0.001        250
  4    Almond.rdf         0           232         0       0.0005       315
  5    DW_PEScenario_101.rdf
                          0           10592       0       0            0
```

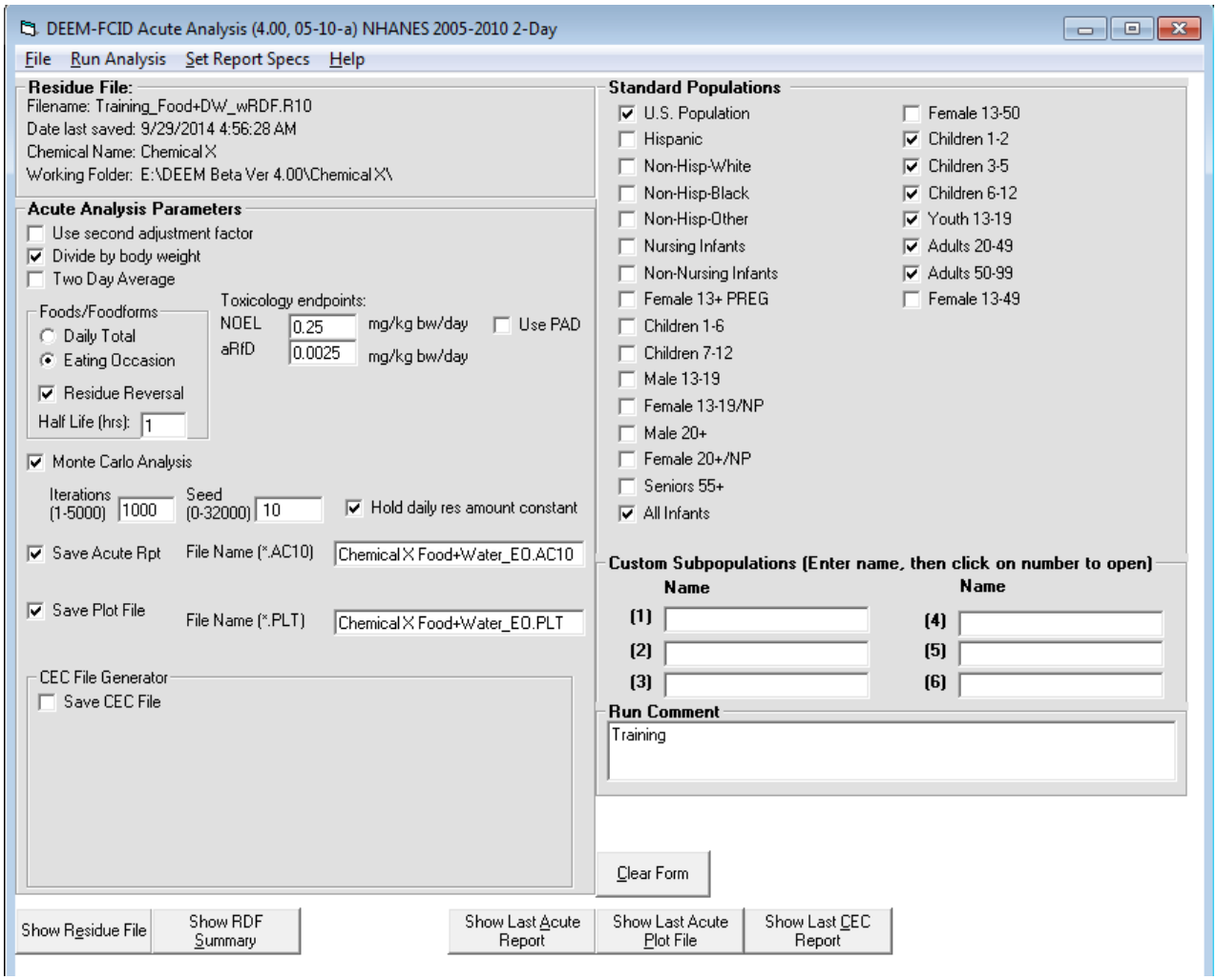
In the example below, 1000 iterations are specified with the Seed value set at 10 (any value can be entered). Agency risk assessments typically specify at least 1000 iterations per diary. As indicated in Attachment 1, the DEEM-FCID database contains a total of 49,346 food diaries, therefore, 1000 iterations will lead DEEM-FCID to simulate 49,346,000 person-days and calculate per capita exposures based on those outcomes.



The "Low", "High" ranges for the CEC analyses are set at 99.9 and 100 percentiles, to match the outcomes exceeding the aPAD in a highly refined acute assessment. As before, click Run Analysis, and select Acute Assessment to perform an acute probabilistic (Monte Carlo) risk assessment. For each person-day, DEEM-FCID randomly selects residue values from the corresponding empirical distributions to calculate dietary exposures for each of the various commodities (RAC-FF). For DW, DEEM-FCID will randomly select a single value from the DW PE file to calculate Total (Direct+Indirect) DW exposures for the corresponding person-day.

DEEM-FCID Acute Eating Occasions Analysis

To perform an Eating Occasions Analysis, select "Eating Occasion" option in the "Foods/Foodforms" box, click "Residue Reversal" option, then **enter a value** for "Half Life (hrs)". In the example below, 1 hour is specified. The option "Hold daily res amount constant", directs DEEM to select only one residue value for each commodity (RAC-FF) even though that person may have consumed that commodity multiple times throughout the day. {*This latter option is consistent with the use of residue monitoring data based on composite samples. For non-blended commodities, such as apples, each composite sample reflects the average residue for that 'bag' of apples. If a person ate four apples on four different eating occasions throughout the day, then DEEM will select one residue and apply that value to calculate dietary exposures from each of those four apples. If single serving residue data were used, then it would be appropriate not to select that option and allow the DEEM model to select a new residue for each eating occasion.*}"



Attachment 1. General Overview of WWEIA-FCID Database

DEEM-FCID Ver 4.00 incorporates food consumption data from the National Health and Nutrition Examination Survey)/"What We Eat in America" (NHANES/WWEIA) dietary survey for the years 2005-2010. The WWEIA survey collected food consumption data from 24,673 respondents. Each WWEIA respondent provided two days of food consumption data, which leads to a total of 49,346 food diaries. DEEM-FCID uses the WWEIA sampling weights to calculate per capita estimates. These weights sum to 296,898,902 million over the 24,673 persons, or a projected total 593,797,804 person-days for these 49,346 food diaries.

WWEIA-FCID 2005-10 Data (2 Day Respondents)

Group	Total Number of Respondents	Total Number of Food Diaries	Total Projected Person-Days
US Population	24,673	49,346	593,797,804
All Infants <1 year old	1,190	2,380	9,249,545
Children 1-2 years old	1,479	2,958	17,110,755
Children 3-5 years old	1,418	2,836	23,173,612
Children 6-12 years old	3,316	6,632	56,169,346
Youth 13-19 years old	3,486	6,972	58,583,237
Adults 20-49 years old	6,974	13,948	247,009,831
Adults 50+ years old	6,810	13,620	182,501,480
Females 13-49 years old	5,543	11,086	158,399,337

In order to improve the utility of the WWEIA food consumption survey for performing pesticide dietary exposure assessments, the U.S. EPA's Office of Pesticide Programs (OPP) developed the Food Commodity Intake Database (FCID), comprised in part of a collection of recipes for each food item in the WWEIA survey in order to translate those food items into Raw Agricultural Commodities.

Further information regarding the NHANES survey and the WWEIA-FCID database can be found at the following web sites: http://www.cdc.gov/nchs/nhanes/nhanes_questionnaires.htm; and http://fcid.foodrisk.org/.

Attachment 2. General Overview of Drinking Water (DW) Consumption

In the WWEIA-FCID database, Drinking Water consists of Direct Water and Indirect Water. The NHANES WWEIA survey collected information on Direct DW Consumption from each survey respondent similar to the information collection on food intake. Direct DW is defined as either plain drinking water, from tap or plain bottled water. The WWEIA Total Nutrient Tables (2005-2010) provide tabulations on Total DW intake for plain tap water for plain bottled water. Prior to the 2011-2012 cycle, those tabulations only included only food code 94100100 "Water, bottled, unsweetened" as Direct Bottled Water; in the 2011-2012 cycle, NHANES-WWEIA added food code 94300100 "Water, baby, bottled, unsweetened" to Bottled Water. The WWEIA-FCID 2005-2010 includes both food codes in Direct DW. The WWEIA-FCID food diaries (DRIFF_0510) contain detailed information on each DW occasion, by type: Direct-Tap (94000100) and Direct-Bottled (94100100, 94300100).

Drinking Water Consumption in WWEIA-FCID

Included as Drinking Water Consumption		
Type	**Components**	**Examples**
Direct Water	**Tap Water**	Water from the tap or faucet; drinking fountain (not water cooler); water served in restaurants or other food service establishment that was not bottled; Tap water that has passed through a water filter (e.g., Brita); Tap water with lemon or lime added.
	Bottled Water	Plain noncarbonated water such as spring water or other water sold in a store (e.g., Evian); Plain noncarbonated bottled water with lemon or lime added; Water from a water cooler (e.g., Poland Springs in an office)
Indirect Water	**Water added to make Beverages and other Foods**	The water component to make Infant Formula or various beverages (e.g., Coffee, Tea), as well as water added to prepare foods (soups-add water; rice, pasta, etc.) are included as part of Indirect Water.
Not Included as Drinking Water Consumption		
Carbonated Water	**Beverages**	Carbonated water includes: Seltzer water, both flavored and plain; Club soda; Perrier and other similar sparkling waters, flavored or plain; Tonic water (regular and diet); Sweetened water beverages such as Clearly Canadian, Mystic, Sparkling water beverage with regular or artificial sweetener. These beverages are not included as Drinking Water Consumption in the FCID recipes
Sodas	**Beverages**	Any water contained in all sodas (including clear sodas, such as Sprite, Slice or 7-UP) are not included as part of Drinking Water consumption.
Food Products	**Ready-to-eat**	The FCID recipes do not include water added by commercial food producers (e.g., soup 'do not add water'), nor the (biological) moisture content in foods.

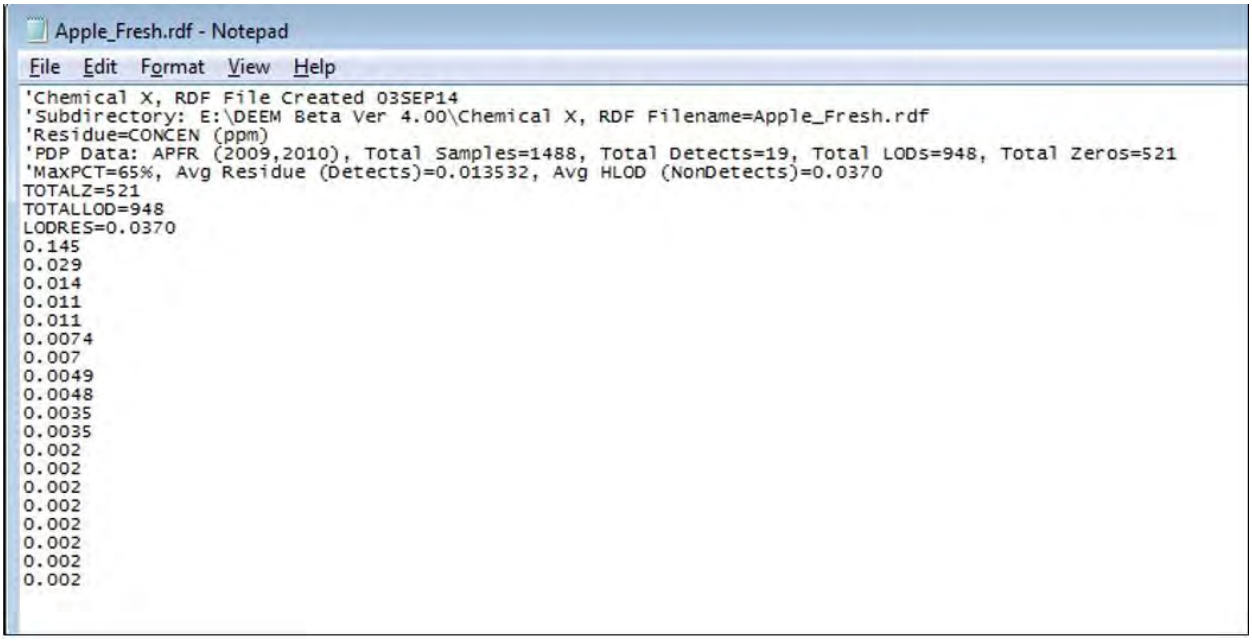
Indirect DW consists of water added by food preparers (individuals or restaurants) to food items and beverages, as presented in the FCID recipes. Carbonated water or water added by a commercial food processors are not included. Therefore, 8 fl oz of infant formula prepared from powder would contribute approximately 207 g (=244 g x 0.85) to DW intake, while ready-to-feed infant formulas and soft drinks (Cola) provides no contribution.

Attachment 3. Creating Empirical Residue Distributions (rdf files)

- Comments are preceded with an apostrophe mark. Comments usually take up the entire row, led with an apostrophe mark in the first Column.
- Residue values can begin at or below Row 5; DEEM will provide a warning if residues are listed in Rows 1-4.

DEEM has optional parameters that can be used to specify an empirical residue distribution. The following 3 options help to clarify the use of PCT in refining the distribution:

- TOTALZ indicates the total number of values that were not believed to be treated-i.e., containing a true Zero (0), based on the Max PCT parameter.
- LODRES indicates DW concentration at 'Half LOD'
- TOTALLOD indicates the total number of values containing a 'Half LOD' value based on the Max PCT parameter.



- If an empirical distribution contains multiple occurrences of one or more residue concentrations, then those values can be specified by listing the number of occurrences, followed by the residue concentration, as shown below:
  - 2,0.011
  - 2,0.0035
  - 8,0.002
- If this option is used, then the number of distinct values must be specified: TOTALFREQ=3.
- Finally, TOTALR indicates the total number of values without FREQuency option. For the Apple_Fresh.rdf distribution above, the TOTALR would be equal to either 19 if TOTALFREQ is not used, or 7 if the TOTALFREQ option is used.