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Background Document for the Sessions:
Dietary Exposure Evaluation Model (DEEM™)
and
DEEM™ Decompositing Procedure and Software

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The DEEM™ Dietary Exposure Model and Software

The purpose of this paper is to provide comprehensive documentation of the algorithms used by the Novigen Sciences' Dietary Exposure and Evaluation Model (DEEM™) to estimate dietary exposure in order to allow facilitate the peer review of this software by the EPA Science Advisory Panel (SAP). Each of these algorithms has been applied to a wide variety of different intake estimate problems – ranging from estimating the intake of pesticides to the intake of nutrients during development of the program. Since its development, various scientists have used the software for conducting scores of dietary intake assessments. Since the algorithms must be evaluated in the context of their intended applications, the paper begins with a brief discussion of those applications. The algorithms themselves are presented in subsequent sections. The corresponding computer codes for the computational algorithms are provided in Appendix 2. This paper also includes a discussion of the data that are used by DEEM™. DEEM™ has undergone extensive QA/QC testing. The results of those tests are summarized for the SAP in this document. The fidelity of the process used to incorporate the data into DEEM™ has been verified through testing that is also described in this report. DEEM™ is currently licensed to government (US EPA, EPA Canada and the California Department of Pesticide Regulations and to more than 20 other clients). Licensees actively participate in improving the capabilities of DEEM™ through User group meetings and by providing Novigen examples of analyses and options. The software is routinely tested and frequently upgraded through the addition of more advanced calculation capabilities and new data bases as they become available. Each new version of the software undergoes thorough testing including in-house testing and subsequent “beta” testing by users prior to release of software that can be used for analyses conducted under the requirements of the Good Laboratory Practices (GLP) regulations.

The algorithms in DEEM™ also form the basic platform used for aggregate assessments in CALENDEX™. DEEM™ contains a representative population (e.g., weighted to be representative of the entire U.S. population) that provides a sample frame with both demographic information and food consumption data.

1. Intended Applications for DEEM™ and Related Software Including CALENDEX™

DEEM™ consists of four software modules: The main DEEM™ module, the Acute analysis module, the Chronic analysis module, and the RDFgen™ residue distribution module. The main DEEM™ module is used to create and edit residue files for specific chemical or cumulative applications, and to launch the DEEM™ Acute, Chronic, and RDFgen™ modules. The RDFgen™ module automates single analyte and cumulative residue distribution adjustments and the creation of summary statistics and Residue Distribution Files based upon USDA Pesticide Data Program (PDP) monitoring data or user-provided residue data. The Acute analysis and Chronic analysis modules provide dietary exposure assessment models based on USDA consumption data. The DEEM™ software itself is also integrated with CALENDEX™, an aggregate exposure assessment software application focusing on combined dietary and residential (non-dietary) exposures (Figure 1).

The DEEM™ dietary exposure assessment modules can be used to estimate the intake of toxicants, nutrients, pesticides, food additives, and natural constituents -- in short for any chemical component of food or water. These substances can include inorganic and organic chemicals as well as microorganisms or toxins produced by microorganisms. They can be naturally or synthetically created.

The mere presence of a substance in the food supply does not imply any adverse health consequence. In fact some substances of interest are essential nutrients. However, virtually all substances are toxic at some dose. Even essential nutrients are toxic, albeit at levels that are higher than the levels that are essential. Therefore, exposure levels should guide the understanding of the significance of the presence of any substance in the diet. Although the interpretation of the results may be different, the methodologies for estimating exposure are similar for toxins, nutrients and microorganisms.

Ingestion will contribute varying amounts to exposure since foods will contain different amounts of each substance on different days. Furthermore, the diets of individuals vary - both between individuals and by the same individual from day to day. DEEM™ is designed to allow the user to tailor the analysis to provide the most appropriate estimates and to allow the user to understand the factors that have the most impact on those estimates.

2. Background

2.1 Dietary Exposure Assessment

The goal of dietary exposure assessments is to characterize the exposure of the population of concern and to identify the variability of that exposure. Typically, the primary objectives are to estimate the level of ingestion of the substance and to identify the sources of both variability and uncertainty in the estimate. In addition, the exposure assessment can also be useful in aggregate exposure assessments to identify the potential importance of diet relative to other pathways of exposure and to indicate where consumption of a particular food commodity or other unique characteristic (i.e., age, regional and ethnic preferences), would indicate the potential for unique exposure patterns.

To assess the ingestion pathway to total exposure, three types of data are required (1) potential levels in food and water; (2) frequency of occurrence of the substance in food or water; and (3) amounts of foods that are consumed by the population being evaluated.

The basic dietary exposure model is of the form:

$$\textit{Consumption} \times \textit{Residue} = \textit{Dietary Exposure}$$

The selection of the most appropriate methodology for an exposure assessment will depend upon (1) the intended application for the exposure assessment, (2) the biological properties of the substance, (3) the physical and chemical properties of the substance, (4) the route of entry into

food and water, and (5) relative contribution of ingestion to overall exposure. Some of the important considerations for each of the five areas are discussed below:

The purpose of the assessment will play a critical role in determining the most desirable methodology. Different methods will be desirable if the assessment is designed to be conservative (as is often the case for regulatory decision making applications) than when it is designed to be as realistic as possible. Some approaches, such as those that assume the food supply contains tolerance level residues are designed as “screening” methods. The assumption that foods contain residues at the maximum legal limit produces a worst-case intake estimate, often called the theoretical maximum daily intake (TMDI), which dramatically overestimates exposure. Although it can be very useful for preliminary assessments, for establishing priorities or for designing sampling programs is it not as reliable as an estimate of actual intakes.

Screening methods, such as the EPA OPP Tier 1 procedure (see Section 2.3.2), sacrifice accuracy of estimate for speed, simplicity, and known over-estimation of exposure. In the case of the evaluation of toxic effects, results that predict that intakes will be less than an acceptable intake level are assumed to mean that exposures will be acceptable. It is further assumed that there is no need to expend resources to collect better data or to apply more sophisticated techniques in search of greater accuracy.

The length of dosing that is required to elicit a specified biological effect should define the key exposure assessment parameters. That is, the biological effects that are the result of a single or at most few doses will be compared to dietary exposure on a single day. Correspondingly, toxic effects that arise as a result of long term exposure will be compared to average dietary exposures (usually over a year).

Other considerations include whether any breakdown products are of toxicological significance and the metabolic pathways in plant and animal systems. Potential biological effects must be carefully considered in planning an exposure assessment. Factors of interest include dose-response relationships, the length of exposure required to produce an adverse effect, potentially sensitive populations, and variability and uncertainty factors.

Often when estimating intake of a substance in food, it is necessary to define or characterize the substance in terms of attributes such as structure, volatility, and solubility. Issues that are related to the substance’s properties once they are in the food or water include: whether the substance breaks down during storage, during processing, or during cooking.

The American diet is highly processed. Therefore, for most assessments it will be critical to include estimates of the residues in the products as they are consumed (Chin, 1991; Elkins, 1991). The DEEM™ software is designed to allow this information to be added as one or more adjustment factors.

If it is possible to group foods into categories it may be possible for data for one food to be extrapolated to foods for which data are not available. For example, if the levels in oranges were expected to be similar to those in grapefruit, it would then be possible to conduct the exposure analysis for “citrus.” These food categories can then be used to select the most appropriate food

consumption data for the assessment. DEEM™ users can group foods by the EPA crop grouping system or by defining their own food categories.

2.2 Special Considerations for Multiple Compound Assessments

The method used to estimate dietary exposure to multiple chemicals needs to adjust the detected residue levels of each of the chemicals considered, by "relative toxicity factors" that reflect the toxicity levels of these chemicals relative to a "standard" chemical. A total adjusted residue then may be derived for each sample by summing the adjusted residue values corresponding to that sample. An exposure assessment is then conducted using these total adjusted residues. The approach is based on the concepts proposed by the National Academy of Sciences (NAS) for the assessment of joint exposure to organophosphate pesticides, and is similar to that followed by the EPA in the case of dioxin-like compounds. DEEM™ does not specify the procedure for establishing the relative potency, but once the user has determined the relative potency, DEEM™ will adjust the residues accordingly.

Based on our experience in conducting cumulative exposures using DEEM™, there are several factors that must be considered in order to estimate reliably the probability of effects from exposure to multiple chemicals. Some of these include:

- Conduct a realistic treatment of the samples with non-detectable residues to reflect actual pesticide usage practices, including the timing of the pesticide applications, and the potential usage of multiple pesticides on the same crop. A probabilistic approach that incorporates information about usage practices is recommended.
- Conduct a realistic treatment of the samples with non-detectable residues to reflect the potential distribution of residue levels below the detection limit. A Monte Carlo approach that incorporates information about the potential association between the detected levels of the various chemicals is recommended.
- Determine consistent procedures for addressing situations where one or more relevant compounds were not estimated or where there is a correlation between the presence of one compound and that of another.
- Develop methodology to permit modeling that will include the differences in time for recovery from potential toxic effects and to account for timing for potential exposure to the population.
- Develop a method for expressing toxicity that is not significantly affected by the experimental doses that were selected for the toxicological testing.
- Identify a common mechanism of action and use that to determine the toxicity, especially in situations where experimental data show that there are multiple mechanisms of action. For example, in the case of organophosphates, some of the chemicals inhibit RBC cholinesterase at higher doses than they inhibit brain cholinesterase, while the reverse is true for others.

- Consider using the dose response patterns in deriving the relative toxicity factors.

2.3 Exposure Assessment Models

There are three general exposure assessment models available in DEEM™: point estimate, simple distribution and probabilistic (Monte Carlo). With appropriate adjustments these models can also be used for estimating cumulative exposures. DEEM™ specifically allows the user to follow the current EPA OPP Tier 1-4 procedures for estimating exposure as described below.

2.3.1 Point Estimate

A point estimate of exposure to a specific chemical by a particular population is a broad estimate generated using one number to represent concentration of the chemical in each food and one number to represent intake of these foods by that population. In estimating chronic exposure, the arithmetic mean of residue concentrations is most commonly used; however, if the distribution of pesticide concentrations is known to be skewed, use of the median (or 50th percentile) concentration is more appropriate (Mosteller and Tukey, 1977). Typically, the most basic models combine data on average intake and average concentration levels of the substance to estimate average exposure.

DEEM™ allows the user to select the most appropriate chemical concentration to be used for each analysis.

2.3.2 Simple Distribution

Single day or "acute" exposures may be computed using a single estimate of the residue concentrations and a distribution of food intake data for a single meal or for the day. A simple distribution of exposure is calculated as follows: a single number chosen to represent concentration of the substance in each of the foods of interest may be applied to a distribution of intake levels for each food. Typically the residue concentration will be a "worst case" residue and the analysis is thus a conservative or screening type analysis.

Current EPA policy is to utilize a tiered approach in assessing acute dietary exposure. Most often the EPA Tier 1 analysis for acute dietary intake utilizes the entire consumption distribution and a single upper-bound residue value (usually the tolerance or highest average field trial (HAFT) residue) for all foods included in the analysis. In the Tier 2 analysis, a single upper-bound residue value is used for those commodities considered to be single serving foods (e.g., a raw apple or an orange); mean field trial residues (or residues from monitoring data) are used for processed or blended commodities (e.g., grains, oils). (Tiers 3 and 4 are discussed below.)

2.3.3 Probabilistic or Monte Carlo Assessment

Probabilistic or Monte Carlo assessments utilize both the anticipated residue distributions and the distribution of intake levels. Consumption levels vary both between and among individuals, similarly residue levels present on foods also vary. The variations in the consumption and chemical concentrations in those foods produce potential variations in the resulting exposure

distributions. Convolution methods can be used to combine the consumption and residue distributions. When the number of observations forming the distributions is large, Monte Carlo techniques can be used (National Research Council (NRC), 1993).

EPA's Tier 3 acute analysis approach incorporates the entire consumption distribution and the entire field trial residue distribution for single serving foods; mean field trial residues or the entire distribution from monitoring programs (under certain conditions) are used for processed/blended commodities. The Tier 3 analysis may also incorporate percentages of the crop that may be treated with the chemical of interest. EPA's Tier 4 analysis utilizes the entire consumption distribution and residue distributions from statistically designed market basket surveys. The EPA's policy regarding use of residue data in dietary intake assessments has been evolving in recent months. The DEEM™ software is able to incorporate residue data according to the EPA's developing data utilization policy.

DEEM™ provides the user with the capability to conduct Tier 1-4 analysis whenever the residue data are available for such analyses. Users can also conduct a combination analysis, using Tier 1 or 2 for some commodities and Tiers 3 and 4 for those where the data permit and/or where those commodities contribute sufficiently to the risk to warrant a more extensive analysis.

3. Data used in DEEM™

Data used by the DEEM™ modules are of two types. The first type of data are those supplied by DEEM™ and cannot be changed by the user, although the user can use a subset of these data. We refer to these data as "hard" data. These are the consumption and demographic profiles of the individuals in USDA's consumption surveys and the translation factors that translate foods as consumed (e.g., pizza) into the corresponding raw agricultural commodities and food forms (e.g., wheat, tomatoes, etc.). The second type of data are those supplied by DEEM™ but that can be modified by the user or data that are provided by the user. We refer to these data as "soft" data. These are the default processing factors and the residue data that can be extracted from USDA's PDP via the DEEM™ RDFgen™ module, and other residue data provided by the user. The user also provides information, such as: the percent of the crop assumed to be treated with the compound of interest and the chemical specific toxicity measures. Toxicity measures used by DEEM™ include the NOEL, the Reference Dose (whether acute (ARfD) or chronic (RfD)), and the population adjusted reference doses (PAD).

3.1 "Hard" data

As described above these are the fixed data that cannot be altered by the user, and refer to the consumption and demographic data of the individuals in USDA's consumption surveys and the translation factors, including the statistical weights developed by USDA. Translation factors transform amounts of foods as consumed, e.g., pizza, into the various raw agricultural commodities (RACs) and food forms, e.g., wheat; processed tomatoes; etc... Appendix #1 lists all RACs and food forms. Translation factors currently being developed by USDA will be incorporated in DEEM™ when USDA makes them available in the spring of 2000.

The dietary assessment modules of DEEM™ currently use data from the 1989-91 and 1994-96 USDA Continuing Surveys of Food Intakes by Individuals (CSFII). In addition, USDA has conducted the Supplemental Children's Survey to the 1994- 96 (CSFII 1998). The CSFII 1998 was conducted in response to the Food Quality Protection Act of 1996, to provide data from a larger sample of children for use by the Environmental Protection Agency in estimating exposure to pesticide residues in the diets of children. The CSFII 1998 was designed to be combined with the CSFII 1994- 96; and will be included in the DEEM™ dietary exposure assessment modules upon their release by USDA.

Each of the CSFII surveys uses a stratified area probability sample of individuals residing in the conterminous US. The primary goal of the sample design for the CSFII surveys is to obtain a nationally representative sample of non-institutionalized persons residing in households in the United States for each of 40 analytic domains defined by sex, age, and income level (an “all-income” group and a “low-income” group). The USDA provided statistical weights that adjusted for the different probabilities of selection and non-response rates and permitted the data from the various years of the surveys to be combined. Fourteen demographic characteristics and month of the interview were used to derive the weights for the individuals in the survey so that the distribution of the weighted sample becomes similar to that of the U.S. population with respect to the demographic characteristics. Weights were derived separately for males age 20 years and older, females age 20 years and older and persons less than 20 years of age. Thus, the CSFII provides a sample frame representing the U.S. population.

The dietary intake information collected by the CSFII 1989-91 refers to three consecutive days, and that collected by the 1994-96 refers to two non-consecutive days. USDA derived statistical weights for the all individuals with records on the first day of the survey, and for those with three days of records, in the case of the 1989-91 CSFII, and two days of records, in the 1994-96 CSFII. DEEM™ uses all individuals in the 1989-91 CSFII with three days of records, and all individuals in the 1994-96 CSFII with two-days of records. Observations from the 1998 Supplemental Children’s Survey will be added to DEEM™ upon the data’s approval and release by USDA.

3.2 “Soft” data

“Soft data” include the default processing factors (which can be changed if data from processing studies are available) and the residue values used in the assessment. The residue data may be based upon residue field trials or taken from monitoring programs, such as USDA’s PDP. The RDFgen™ module of DEEM™ extracts and processes the PDP data for use in the dietary intake assessment. The analyst may also provide residue distribution adjustment parameters, such as estimates of percent crop treated (usually based on market share) and number of units per composite sample (when composite residue data are “decomposed” to estimate residues in single servings). Finally, the analyst also supplies the compound specific toxicity measures.

3.2.1 Default Processing Factors

As a crop item is processed into foods, the chemical or constituents may preferentially segregate into one fraction rather than be distributed equally into the various subparts of the item. For

example, oil-soluble surface residues may remain in the peel. Thus, the resulting concentration in the citrus peel may be higher than the concentration in the whole orange. Similarly, the residue concentration in peeled fruit may be lower than in the whole, unpeeled fruit. To address this situation, DEEM™ multiplies each food consumption estimate by a default “adjustment factor” designed to allow better matching of the residue data with food consumption data. For example, raisin consumption is expressed in terms of consumption of actual raisins. If chemical residue measurements were made in fresh grapes instead, an adjustment factor must be applied to account for the chemical concentration resulting from water loss. This adjustment factor will correctly estimate the potential exposure from the raisins.

Default adjustment factors included in the DEEM™ software are based on yield tables. Sources for these adjustment factors are USDA Handbook 102 (USDA, 1975) and USDA Commodity Maps (USDA, 1982).

Both of these sources provide information on the quantity of processed foods from a unit amount of whole commodity. The USDA Commodity Maps document specifically lists conversion factors (measures of the physical transformation of a commodity from farm gate to processing/consumption) for many foods. The conversion factor is the ratio of the weight of the commodity in one form to its weight in another form. The factors reflect gains or losses in a commodity. For example, the conversion factor reported for apple juice is 0.774 pounds per pound of fresh apples, indicating that one pound of apples converts to 0.774 pounds of apple juice. If residue data are available only for the whole apple, this conversion factor may be used to determine the potential impact on the pesticide residues if treated whole apples are processed to juice. That is, since 1.3 pounds of apples are needed to produce one pound of apple juice, it is assumed that the pesticide level in the RAC apples would concentrate 1.3X in the processed juice ($1 \div 0.774$).

The default adjustment factors in DEEM™ may be considered worst-case because they almost always assume concentration of residues in the processed commodity. The only exception to this is the RAC soybean sprouts for which the default factor is 0.33, suggesting a weight gain (i.e., reduction in pesticide levels) in the processed commodity. If processing studies have been conducted, processing factors derived from the experimental data may replace the default factors included in the DEEM™ software.

Conversion information may change over time as a result of the adoption of new technology in both production and processing as well as variation in the physical properties of commodities from one crop year to another. In addition, as new products become available in the market, new conversion factors may be warranted.

Processing factors can be applied to an entire food or food form using the Residue File Editor in the main DEEM™ module. However, when performing cumulative assessments, processing factors are usually supplied a step earlier in the process, using the Cumulative Mode of the RDFgen™ module to correctly apply distinct coefficients to each analyte included in the assessment prior to combining separate distributions into a cumulative distribution.

3.2.2 Residue Data

Different types of residue data can be used by DEEM™. The type of data used depends on the type of assessment being conducted and on the food or food form it represents. Single point estimates and/or distributions (whether empirical or parametric) may be used. Single point estimates are used in chronic dietary exposure assessments, or in screening levels acute dietary exposure assessments. They can also be used to represent residues in foods that undergo a large degree of blending. Distributions are generally used in more refined dietary exposure assessments and are used to represent foods where residue levels may vary from unit to unit.

Residue data may be provided by the user or may be obtained from monitoring programs such as the USDA PDP monitoring data via the RDFgen™ module of DEEM™. The RDFgen™ module of DEEM™ automates residue distribution adjustments and the creation of summary statistics and Residue Distribution Files (hereafter referred to as RDF files) using the RDFgen™ pre-extracted PDP data sets or user-supplied data. Using the Residue File Editor, the mean value of an adjusted residue distribution calculated by RDFgen™ can be entered for a chronic risk assessment, or an RDF file generated by RDFgen™ can be referenced for an acute risk assessment. RDFgen™ can also perform adjustments to the residue levels in order to generate cumulative RDF files. RDFgen™ will allow the user to do these analyses automatically using the PDP data for samples that have been tested for multiple analytes or manually using user-supplied data. In both situations, the user determines the appropriate adjustment values to use to reflect differences in potency among the chemicals to be analyzed.

The RDFgen™ pre-extracted PDP data sets, at the time of this writing, contain all of the 1994-1997 PDP data. The pre-extracted data sets were compiled from the raw individual sample and residue databases distributed by the USDA PDP. The pre-extracted PDP residue data sets accompanying RDFgen™ begin in 1994, since 1994 was the first year in which the PDP began using a standardized data format where all non-detect samples were explicitly presented in the database and LOD values were explicitly given for each sample. Novigen will integrate PDP data for years after 1997 once USDA release them.

Merits of the PDP pesticide monitoring data for dietary risk assessments include:

- Rigorous statistical design.
- A large number of samples taken of heavily consumed commodities over multi-year periods.
- Sensitive analytical methods.
- Explicit reporting of all analyzed samples (detects and non-detects).
- Good quality assurance.
- Testing of most samples for multiple analytes, enabling cumulative residue operations.

3.2.3 Percent Crop Treated Information

Agricultural commodities are usually grown in several regions and thus may face different pests. Thus, treatments may vary from region to region. In addition, pesticide treatments are not applied to the entire crop of a specific agricultural commodity. Thus, DEEM™ allows the user

to modify residue estimates to reflect the percentage of a crop that is expected to contain residues (“percent crop treated”). This adjustment can be applied through either an adjustment factor used to multiply an average residue value or through incorporation in the residue distribution used in a DEEM™ acute dietary exposure assessment. The latter can be performed automatically on a single analyte distribution or a cumulative distribution using the RDFgen™ module of DEEM™. The user supplies the percent crop treated information.

3.2.4 Toxicity Estimates

Exposure estimates derived by DEEM™ can be compared to compound specific toxicity measures to derive risk estimates. The user provides the toxicity measures to be used in the comparison. The toxicity measure used by DEEM™ depends on the type of assessment being conducted.

Estimates of chronic dietary exposures are usually compared to the chronic reference dose (cRfD), chronic NOEL, or the Q_1^* . DEEM™ allows the user to specify which of these measures to use, and to specify their values. If the RfD is chosen as a measure of toxicity, risk estimates are expressed as a percent of the RfD, while selecting the NOEL will produce Margins of Safety (Exposure). Selecting the Q_1^* permits the user to determine the probability for increased risk of cancer associated with the calculated exposure.

Estimates of acute dietary exposures are usually compared to the acute reference dose (ARfD), population adjusted reference dose (PAD) or the acute NOEL. If the ARfD or the PAD are chosen as measures of toxicity, risk estimates are expressed as a percent of the ARfD, or PAD while selecting the NOEL will produce Margins of Safety (Exposure).

4. Modules

4.1 Dietary exposure assessment modules

4.1.1 Chronic Module

Average chronic exposure is usually estimated on a per-capita consumption basis and is compared to the measure of biological/toxicological results from life-time animal feeding studies or other appropriate test results. The DEEM™ Chronic Module uses the point estimate model described above. The equations are presented in Section 5.1. Exposure and risk estimates are derived for the total US population and 25 subpopulations (26 if using the 1989-91 CSFII data).

4.1.2 Acute Module

Acute dietary exposures are calculated using distributions of daily consumption data. The simple distribution approach is used in the non-Monte Carlo application of the DEEM™ Acute Module, while the probabilistic methodology is used in the Monte Carlo application of this module. The

approach used in the Monte Carlo application of the DEEM™ Acute Module is outlined in Section 5 and in Appendix 2 and follows the method outlined by the NRC (1993). The equations are presented in Section 5.2.

DEEM™ offers two options for estimating acute daily exposures. The first option (“Daily Total”) combines the distribution of total daily consumption levels with the distribution of residue values. The second option (“Eating Occasion”) combines the consumption levels corresponding to each eating occasion with the distribution of residues and sums the resulting estimated exposures to produce an estimate of the daily exposures. For example, if an individual reported consuming a given food twice during the day (say 100 gm and 120 gm), the “Daily Total” option would combine the total daily consumption of that food (220 gm) with a randomly selected residue value. In contrast, the “Eating Occasion” option would combine the first amount consumed (100 gm) with a randomly selected residue value, and the second amount consumed (120 gm) with another (possibly different) randomly selected residue value, and compute a total daily exposure estimate.

4.1.3 Sensitivity Analyses

4.1.3.1 DEEM™ Chronic Module

The DEEM™ Chronic Module allows the user to conduct sensitivity analyses via the Chronic Commodity Contribution Analysis to assess the relative contribution of all the foods and food forms included in a particular assessments to the total exposure or risk. It also allows the user to determine which foods and food forms contribute most to the total dietary exposures of each of the subpopulations considered.

Two options are available to use to evaluate the contribution of any individual commodity to the exposure estimate:

- **Complete Commodity Analysis**

The Complete Commodity Analysis reports the contribution of every commodity to the total exposure and expresses the contribution both as mg chemical/kg BW/day and as a percent of the Reference Dose (RfD).

- **Critical Commodity Analysis**

The Critical Commodity Analysis reports the exposure from those foods, which contribute a user-specified proportion of the overall exposure, e.g., 1% of total exposure. The critical commodity listing is expressed as both a percent of the RfD and as a percent of total exposure.

4.1.3.2 DEEM™ Acute Module

The DEEM™ Acute Module allows the user to conduct sensitivity analyses, via the Acute Critical Exposure Contribution (CEC) Analysis to determine which foods contribute most to the total exposure of all individuals with exposure levels between user-specified percentiles. The user can thus determine whether a particular food, residue level or individual food “drives” the assessment, and whether more than one food contributes to most of the exposure of the selected individuals.

The computational algorithms used in the CEC are presented in Section 5.2.3 and Appendix 2.

4.2 DEEM™ RDFgen™ Module

RDFgen™ uses QA’ed sets of spreadsheets containing up-to-date monitoring data from the most widely used source, the Pesticide Data Program (PDP) of the U.S. Department of Agriculture (USDA). These sets of spreadsheets are ready for immediate use with RDFgen™, and are referred to by the following titles: “RDFgen™ pre-extracted PDP data set formatted for RDFgen™ Individual Analyte Mode” and “RDFgen™ pre-extracted PDP data set formatted for RDFgen™ Cumulative Mode.”

Additionally, to allow creation of RDFgen™ Cumulative Mode or Individual Analyte Mode PDP residue input spreadsheets filtered for specific sample attributes (such as origin or date collected), Novigen maintains a pre-extracted data set integrating all PDP sample database and residue database information, plus the following helpful standardized fields:

- COMMOD_NAM (Translated version of the two-character COMMOD field, including separation of processed commodities that share COMMOD code with unprocessed commodities, such as green beans/processed green beans and peaches/canned peaches).
- FULL_PESTN (Standardized version of two-character PEST_NAME field).
- BOOKYEAR (PDP data annual report year to which the record belongs).
- YEARY2K (Ensures continued ability to correctly sort and query based on sample date).
- DETECT (Y/N field indicating whether sample is a detect or non-detect sample).
- ORIGINSTD (Standardized version of ORIGIN field, facilitating separation of domestic samples, imported samples, and samples of unknown origin).

This series of spreadsheets is referred to as the RDFgen™ full Pre-extracted PDP data set. Creation of RDFgen™ Cumulative or Individual Analyte Mode PDP residue input spreadsheets or user-defined subsets of the RDFgen™ full Pre-extracted PDP data set is automated by the RDFgen™ Input Generator™ Excel add-in.

RDFgen™ can operate in two primary modes: Individual Analyte Mode and Cumulative Mode. The Individual Analyte mode allows the user to perform the following residue adjustments on any single analyte residue distribution:

- Percent Crop Treated
- Decompositing

The Cumulative mode allows the user to perform the following residue adjustments on any combination of compounds, provided those individual samples have been tested for co-incident residues:

- Percent Crop Treated
- Estimation of concentrations in individual fruits/vegetables based on values in a composite sample (referred to through this document as “decomposing”)
- Relative Potency
- Processing Factors

RDFgen™ may be launched from within DEEM™ or used independently.

The RDFgen™ module of DEEM™ accepts as input any residue data spreadsheet that has been formatted according to a specified format. The user is responsible for the quality and representativeness of the data contained in user developed or modified spreadsheets. In general, Individual Analyte Mode input spreadsheets contain distributions for various commodities tested for a particular chemical, while Cumulative Mode input spreadsheets generally contain distributions for various chemicals tested on a particular commodity. Cumulative Mode should be used when it is desired to combine residue data from multiple analytes into a single distribution. Note that RDFgen™ Cumulative Mode will only use samples from the Cumulative Mode input spreadsheets that have been tested for all of the analytes that are selected for inclusion. Individual analyte mode should be employed when residue distribution adjustments are going to be performed on single analyte’s residue data.

5. Outputs and Algorithms

The computational algorithms and codes used by DEEM™ are presented in Appendix 2. We describe below a representative set of these algorithms.

5.1 The DEEM™ Chronic Module

As discussed earlier, chronic dietary exposures are typically derived as point estimates, using average consumption and residue estimates. The DEEM™ Chronic Module derives estimates of mean per-capita dietary exposure for a pre-defined set of standard populations, and conducts sensitivity analyses by estimating the contribution of the various foods to the total exposure.

5.1.1 Standard populations in the DEEM™ Chronic Module

Chronic dietary exposure estimates are derived for the following standard populations:

U.S. Pop - 48 states - all seasons

Seasonal

U.S. Population - spring season
U.S. Population - summer season
U.S. Population - autumn season
U.S. Population - winter season

Regional

Northeast region
Midwest region
Southern region
Western region
Pacific Region (Used only in CSFII 1989-91 analyses)

Ethnic

Hispanics
Non-hispanic whites
Non-hispanic blacks
Non-hispanic other than black or white

Age and Gender

All infants (<1 year)
Nursing infants (<1 year)
Non-nursing infants (<1 year)
Children (1-6 years)
Children (7-12 years)
Females (13+/pregnant/not nursing)
Females (13+/nursing)
Females (13-19 yrs/not preg. or nursing)
Females (20+ years/not preg. or nursing)
Females (13-50 years)
Males (13-19 years)
Males (20+ years)
Seniors (55+)

The Chronic module uses a data base of pre-calculated per-capita mean food consumption data (g/kg-bw-day) for each raw agricultural commodity (RAC) and food/food form reported in the CSFII surveys. The user can also estimate the same value for user-defined subpopulations by using the per-capita mean estimates provided in the DEEM™ acute module.

5.1.2 DEEM™ Chronic Module Output

5.1.2.1 Default Output

The default output of the DEEM™ Chronic Module consists of the per capita exposure estimates, associated margins of exposure, associated percent of the RfD (Figure 2), or associated risk (Figure 3), depending on which measure of risk is selected, for the US population and each of the standard subpopulations.

5.1.2.2 Sensitivity Analysis Output

The output of the optional sensitivity analyses includes, in the case of the Complete Commodity Contribution, the listing of all the foods included in the assessment together with their contribution to the total exposure and expresses the contribution both as mg chemical/kg bw/day and as a percent of the RfD (Figure 4). If the Critical Commodity Contribution is selected, the

output consists of a listing of all foods in the assessment which contribute a user-specified proportion of the overall exposure, e.g., 1% of total exposure. The critical commodity listing is expressed as both a percent of the RfD and as a percent of total exposure (Figure 5).

5.1.2.3 Residue documentation file

In addition, DEEM™ produces a file listing the residue data used in the assessment, and documenting the options selected in the assessment, e.g., processing factors and whether percent crop treated information was used and at what levels (Figure 6).

5.1.3 Derivation of estimates of chronic dietary exposures

Mean estimates of consumption are combined with residue data from a DEEM™ residue file to determine the mean residue intake (in mg/kg-bw-day) for all individuals in the standard populations.

To conduct the chronic risk analyses using the DEEM™ software, the user must thus input three types of information:

- (1) Concentrations of the constituent or chemical in the foods and/or food-forms. These can include a theoretical level such as the tolerance or MRL (maximum residue limit) or a level anticipated to be found in the food of interest.
- (2) Toxicological information about the compound that will be used to evaluate the significance of the estimates of exposure. These should include a toxicology endpoint based on chronic (long-term) exposure such as the cancer potency factor (Q1*), Acceptable Daily Intake (ADI), chronic population adjusted dose (cPAD) or other chronic Reference Dose (RfD), and chronic No Observable Effect Level (NOEL).
- (3) Adjustment factors to allow the estimation to more accurately reflect likely exposures. These adjustment factors can include proportion of the crop treated, proportion imported, processing factors, etc.

The Chronic analysis module calculates per capita daily mean exposures, for each of the standard populations, by multiplying the pre-calculated mean consumption values by the corresponding residue amount, applying adjusting factors, if applicable and normalizing the exposure amounts to mg/kg-bw-day units. The resulting estimates are added for all the foods in the assessment:

$$\text{ChronicExposureEstimate} = \sum_j \text{Mean}_j \times \text{Residue}_j \times \text{PF}_j \times \text{AF}_j,$$

where Mean_j , Residue_j , PF_j , and AF_j represent the pre-calculated mean consumption value, residue value, processing factor and percent crop treated adjustment factor associated with the j^{th} RAC or food form included in the assessment.

The per capita exposure means for all the standard population groups are reported directly, along with the estimate of risk based on the chronic toxicology endpoints specified by the user. DEEM™ expresses the expected risk relative to either of the RfD (ADI), cPAD or NOEL (chronic), as selected by the user. It also can express the exposure in relation to the results of cancer studies. The slope of the dose-response in cancer studies, the Q_1^* , is used to calculate a dose level relevant to a chosen probability value from a cancer study. Specifying the slope of the dose response permits the user determine the probability for increased risk of cancer. In this case, the DEEM™ output consists of an estimate of the relationship between the population's exposure and the probability of occurrence of increased incidence of cancer.

5.1.4 Steps in the estimation of the chronic dietary exposures

The actual source codes for each step in the calculation is presented in Appendix 2.

- Step 1.** Read in the residue file specific to the analysis
- 1) Read the toxicology endpoints
 - 2) Read the residue amounts and conversion factors for each food/food form in the residue file
- Step 2.** Read the non-food based (NFB) water consumption means for each standard population from supporting file. Note that NFB water consumption is not reported for each drinking occasion, as are other foods, but rather reported as a total daily amount by the individual and included with the demographic records for that individual.
- Step 3.** Open files of per capita food consumption means for the appropriate CSFII survey (1989-91 or 1994-96).
- Step 4.** For each food or food/food form in the residue file (all of which have a default residue amount), retrieve the food consumption record for that food or food/food form from the Chronic data base. Multiply the residue amount by the food consumption amount for each of the populations and sum for this exposure amount separately for each population. The resulting sums are reported as the total daily exposure for each population.
- Step 5.** Calculate the margin of exposure or percent of the cRfD for each population using the toxicology endpoints and report.

5.2 The DEEM™ Acute Dietary Exposure Assessment Module

5.2.1 Populations in the DEEM™ Acute Module

The DEEM™ Acute Module computes exposure estimates for the total US population and/or any of the standard subpopulations listed earlier. In addition within each analysis, the user may specify up to six additional Custom Populations. Criteria used in the selection of the Custom Populations include age, gender, geographic region, season, nursing status, race and ethnicity. The USDA food consumption survey from which the CSFII data were developed was designed

to provide data representative of the various segments of the US population. Nonetheless, the numbers of observations for some populations groups, such as nursing infants, is relatively small. In addition, the DEEM™ Acute Module permits the analyst to define custom populations. Care must be taken not to over-specify a population group for analysis because the number of observations available for the group may, likewise, be relatively small. DEEM™ provides tools (such as the Plot File option, see Section 5.2.2.2) for obtaining the detailed information necessary for the exposure analyst to evaluate the potential impact of the number of observations upon a dietary intake assessment.

5.2.2 DEEM™ Acute Module Outputs

5.2.2.1 Default output

The default output of the DEEM™ Acute Module consists of two summary tables presenting the average and standard deviation and selected percentiles of the estimated per-capita and per-user exposure distributions. The summary tables also provide estimates of the associated risks at each summary exposure mean and percentile (Figure 7).

Each of the individuals in the 1994-96 CSFII survey contributed up to two days (three days for the 1989-91 CSFII survey) of consumption data. As mentioned earlier, DEEM™ uses only those individuals with complete consumption records (i.e., two days for the 1994-96 data and three days for the 1989-91 data). The per-capita estimates use all the person-days, while the per-user estimates use the user-days only, that is, the person-days where consumption of the foods of interest is reported. The term “person day” is used to describe the food consumption data provided by a person during one day of the survey. The term “user day” indicates that at least one of the foods being considered was consumed by the person on that day.

5.2.2.2 Plot file

In addition, DEEM™ produces a “plot” file consisting of the entire per-user exposure distribution. The plot file also includes information about the actual (unweighted) and weighted number of people-days and user-days in the populations considered. The plot file is comma delimited and can be imported in a spreadsheet program for statistical manipulation or to produce graphs (Figure 8).

5.2.2.3 Sensitivity analysis output

In addition to a listing of the analysis parameters (e.g., residue file used, population considered, selected percentiles, minimum contribution), the output of the optional sensitivity analysis, the Critical Exposure Contribution (CEC) analysis, includes the number of records in the selected range and a listing of the foods and foodforms and their contributions to the total exposure (in decreasing order of importance). It also lists the records in the selected range, including selected demographic characteristics, foods contributing to the exposure, consumption level of these foods, residue level, associated exposures, total exposure, and percent of the total daily exposure attributable to the specific foods (Figure 9).

5.2.2.4 Residue documentation file

DEEM™ also produces a file listing the residue data used in the assessment and processing values used (Figure 10).

5.2.3 Steps in the calculation of the acute daily exposure

There are 10 main steps in the acute analysis calculations. The detailed codes and algorithms corresponding to each step are presented in Appendix 2.

- Step 1.** Read in the residue file to be used in this analysis.
- Step 2.** For any RAC without food forms, convert RACs to their constituent food forms, applying the residue information and adjustment factors to each food form as specified for the RAC itself.
- Step 3.** (for the Monte Carlo analyses using RDF files) Preprocess all residue distribution files (RDF) declared in the current residue file and save results to two temporary files. The first file contains summary statistics for each RDF file, including the number of declared zeroes, the number of declared LODs (limit of detection), the LOD residue value, the number of specified residue values, and a location variable showing the starting address of its corresponding list of specified residue values in the second file. The second file contains a vector of the individually specified residue values for all of the RDF files declared in the residue file.
- Step 4.** (for the Monte Carlo analyses only) Compute the approximate mean values for each residue distribution, the cumulative probability of use for the residue distribution functions and the weighted mean for each food/food form and the approximate mean exposure (used to define the interval limits of the exposure distribution).
- Step 5.** Compute the FFFactor! array of preliminary exposure calculations for each food/food form having a defined residue in the current residue file. If the Monte Carlo analysis (MCA) is not used, or there is no RDL pointer for the food/food form, then the FFFactor! is the residue amount, multiplied by the adjustment factors. If MCA is used and one or more RDL pointers are used for any given food/food form, then the exposure represents the adjustment factors only; the residue amount must be determined probabilistically from the appropriate residue distribution function. If a food/food form is not included in the residue file, then FFFactor! = 0 for that RAC or food form.
- Step 6.** Initial pass through the entire food consumption database to compute the approximate mean daily exposure for users (participants who consume at least one of the food/food forms in the residue file) in each population group specified when setting up the analysis. These means will be used to define the interval limits of the exposure distribution.

- Step 7.** (only used when generating CEC file) Make a pass through the entire food consumption data base with 10 iterations (if MCA) or 1 iteration (if no MCA) to determine the approximate user exposure at the 95th percentile for each population selected.
- Step 8.** Calculate the total daily exposure for each individual on each day in the survey and place this exposure amount into the appropriate interval of the exposure distribution for the particular population. Also generate the summation variables needed to compute mean, standard deviation, and standard error of the mean for each population. If the total daily exposure exceeds the preliminary exposure estimate at the 95th percentile, as determined in step 7, save a record of this individual's demographic variables (age, sex, body weight) and daily exposure amount, along with a list of the food/food forms eaten that contribute to this exposure amount, including their consumption amount, residue amount, and adjustment factors. Individual foods/food forms are only included in this list if their percentage contribution to the total daily exposure exceeds the percentage level specified by the user ("minimum exposure contribution by food").
- Step 9.** Call the report subroutine to generate the acute analysis report, which contains user and per capita means, standard deviation, and standard error of the mean, as well as exposure distributions for users and per capita, for all designated populations. For each population of interest, compute the percent of total person-days in the survey that are user days (i.e., at least one of the food/food form combinations in the residue file were eaten)
- Step 10.** (only used when generating CEC file) Generate the CEC file, refining and sorting the list of CEC records saved during the current analysis. Read the temporary CEC records file generated during the last pass through the food consumption data. For each population of interest, find all records in the file and save these to a second file sorted by population type (some records may be included in more than one population). Then read the records for each population individually from the second file; write each record for which total daily exposure falls within the low and high percentile bounds specified by the user in this run, to a third file. Count the number of times each food/food form is found in the records in this subset and sum the exposures for each food/food form. Then divide the sum of exposures for each food/food form by the sum or total daily exposures in this subset to get the percent contribution by each food/food form toward the total exposure in the referenced percentile interval. Sort the individual records in the subset in decreasing order of total daily exposure and print the number of individual records specified by the user to the final CEC report, starting with the individual with the highest exposure. (This is repeated for each population of interest; summaries and record listings for each population of interest are included in the same CEC report.)

5.2.4 Additional description of DEEM™ algorithms

The DEEM™ Acute Module combines the food and food form consumption values for each individual in the population of interest with the residue value associated with the food or food form. In the Monte Carlo assessment, if a food or food form is associated with a residue

distribution, the food and food form consumption values for each individual in the population of interest is combined with a randomly selected value from the distribution of residues.

5.2.4.1 Calculating the daily total exposures for each person-day in the survey

In the “daily total” assessments, the consumption values correspond to the total daily consumption of the food or food form. In the “eating occasion” assessment the consumption values correspond to the consumption levels at each eating occasion. The total daily exposure estimate for each individual is obtained by summing the calculated for each food or food form reported consumed during that day and dividing by the persons body weight.

Thus, in the “daily total” assessments, the total daily exposure for the k^{th} individual on i^{th} day of the survey is obtained as:

$$TotalDailyExposure_{k,i} = (\sum_j TC_{k,i,j} \times Residue_j) / BW_k,$$

where $TC_{k,i,j}$ represents the total daily consumption by person k on day i of food or food form j , $Residue_j$ represents the residue value associated with the food or food form and BW_k represents the body weight of the k^{th} individual.

In the “eating occasion” assessments, the total daily exposure for the k^{th} individual on i^{th} day of the survey is obtained as:

$$TotalDailyExposure_{k,i} = (\sum_l \sum_j TC_{k,i,l,j} \times Residue_{l,j}) / BW_k,$$

where $TC_{k,i,l,j}$ represents the consumption by person k on the l^{th} eating occasion reported on day i of food or food form j , $Residue_{l,j}$ represents the residue value associated with the food or food form and BW_k represents the body weight of the k^{th} individual.

5.2.4.2 Calculating the daily mean exposures

The per user daily exposure mean is calculated as:

$$PerUserMean = \sum_i \sum_{k=1}^{K_i} TotalDailyExposure_{k,i} \times sw_k / \sum_i \sum_k^{K_i} sw_k,$$

where sw_k represents the statistical weight assigned to the k^{th} individual, and K_i represents the number of consumers on day i of the survey.

The per capita daily exposure mean is calculated as:

$$PerCapitaMean = \sum_i \sum_{k=1}^{K_i} TotalDailyExposure_{k,i} \times sw_k / \sum_i \sum_k^N sw_k,$$

where sw_k represents the statistical weight assigned to the k^{th} individual, and N represents the number of individuals in the population of interest.

5.2.4.3 Calculating the interval (bin) limits of the exposure frequency distribution

In the Monte Carlo mode, the software performs the required number of iterations (typically 1,000 iterations) for each user-day. Thus, in the DEEM™ version that uses the 1994-96 CSFII, a 1000 iteration analysis for Infants could produce 718,000 observations, while analyses with the same number of iterations for children 1-6 years or the entire US population could result in up to 6,074,000 and 30,606,000 observations, respectively. The software resorts to “binning”, i.e., summarizing the data in frequency intervals, to simplify the task of storing and sorting these observations for subsequent use in deriving the exposure distributions.

The bin widths are defined to be a constant percent of the lower bin limit (namely, 1%). This approach provides a method in which the maximum potential error introduced by binning is limited to a fixed value throughout the entire range of bins and does not result in an inordinate number of bins. The potential error for a bin, defined to be the percentage difference between the actual exposure value and the mid-point (or end-point) of the bin in which it is placed is thus at most 0.5% (1%) of the exposure value. For exposures that are larger than the mean exposure, the upper bin size of each bin i , $i = 1$ to n , can simply be defined as (the mean $\times 1.01^i$). The procedure allows for up to $n = 1100$ bins above the mean. Thus, the upper limit of the last available bin is 56,690 times the per-user mean, which provides assurance that high end consumption amounts of foods usually eaten in small quantities will not exceed the maximum bin. For exposures less than the mean, the method creates 100 bins, of width equal to (the mean $\times \frac{i}{100}$).

5.2.4.4 The algorithm used in the Monte Carlo simulations

The algorithm used in the Monte Carlo assessment for the “daily total” analysis follows the approach used by the NRC (1993), and includes the following steps:

1. The consumption of food 1 by individual 1 on day 1 of the survey period is multiplied by a randomly selected residue value from the residue distribution for food 1.
2. Step 1 is repeated for all foods identified in the assessment that were consumed by individual 1 on day 1 of the survey.
3. An estimate of the total exposure for person 1 on day 1 is obtained by summing the exposure estimates for all the foods.
4. Steps 1 to 3 are repeated I times (I is the number of iterations specified by the user), still using the consumption data for person 1 on day 1.
5. The I exposure estimates for person 1 on day 1 are stored as I frequencies in the exposure intervals.

6. Steps 1 to 5 are repeated for person 1 on subsequent days of the survey period.
7. Steps 1 to 6 are repeated for all individuals in the sub-population.
8. The frequency distribution of the exposure estimates for all individuals on all days is used to derive the percentile estimates.

The detailed algorithms and source code segments are presented in Appendix 2.

5.3 Algorithms used in the DEEM™ RDFgen™ module

5.3.1 RDFgen™ outputs

RDFgen™ output spreadsheets contain basic data attributes (such as units) and summary statistics for all distributions in the source data spreadsheet, a summary of user-specified parameters for residue distribution adjustments, and a listing of the residue distribution(s) at each phase of adjustment.

RDFgen™ Individual Analyte Mode output spreadsheets also contain single point estimates to be used for chronic exposure assessment. RDFgen™ generates individual analyte or cumulative Residue Distribution Files (RDF) ready for immediate use in the DEEM™ Acute module.

5.3.2 RDFgen™ functions

Primary function of RDFgen™ include: (1) percent crop treated adjustment and (2) decomposing of the residues associated with composite samples to produce single serving residue distributions. In addition, the Cumulative Mode includes processing factor and toxicity adjustments.

5.3.2.1 Individual Analyte Mode

5.3.2.1.1 Percent Crop Treated Adjustment

Percent crop treated adjustment in the Individual Analyte Mode is performed according to ChemSAC guidelines (ChemSAC memo dated 1/25/99, “ChemSAC decision re: calculation of anticipated residues”). Specifically, for a commodity that is not considered blended, e.g., apples, bananas, etc.:

- The percent of samples with detectable residues (PD) is compared to the percent crop treated (PCT).
- If $PD \geq PCT$, then all samples with non-detectable residues (if any) are assumed to be non-treated and are assigned a zero residue value.
- If $PD < PCT$, then a proportion equal to: $(100 - PCT) / (100 - PD)$ of the samples with non-detectable residues, is assumed to be non-treated and assigned a value equal to zero. The remaining samples with non-detectable residues are assumed treated (“implied treated”)

and are assigned a value equal to half the limit of detection of all samples with non-detectable residues.

On the other hand, all blended commodity samples (e.g., corn oil) are assumed to contain residues, and thus all samples with non-detectable residues are assigned a value equal to half the limit of detection of all samples with non-detectable residues. In other words, for blended commodity samples, the algorithm described above is applied, but with PCT always set to 100%.

5.3.2.1.2 Decompositing

- **Assumptions**

Food and agricultural commodity samples collected by monitoring programs or field trials are generally analyzed as composite samples. Assessment of the potential acute exposure to a specific contaminant require information about the distribution of residues in individual units of food for those foods likely to be consumed as “single-serving,” e.g., raw apples, bananas, baked potatoes, etc. It thus becomes necessary either to analyze these foods as individual units or, alternatively, to use the information from the distribution of residues in the composite samples to “predict” in the residues of the single units making up each composite sample. The purpose of decompositing, then, is to predict single serving residues in the absence of single serving data.

Agricultural commodity samples collected by the USDA PDP are analyzed as composite samples, one composite per location. The treatment history of the samples collected by the PDP is not available. It thus becomes necessary to make assumptions about the proportion of the individual samples in each composite that are treated with the compound of interest. These assumptions are based on information about sample collection and typical packing and shipping practices of the agricultural commodities being studied. In the case of the PDP samples, samples within a composite are likely to have come from the same field, or from fields in the same region. Since samples grown in the same region are likely to have faced the same climate and pest conditions, the single units within PDP composite samples are likely to share the same treatment “history.”

Thus, a proportion of the composite samples (equal to PCT) is assumed to have been grown in treated locations. Specifically, as described in the previous section, all composite samples with detectable residues and a sub-sample of the composite samples with non-detectable residues are assumed to have been grown in treated locations (if applicable). All individual units in each of these composite samples are assumed to have been treated. If necessary, and if the required data are available, the proportion of the composites assumed to have been grown in a specific treated location may be allowed to differ from the national estimate of PCT to reflect regional differences in treatment history and sampling practices.

For each “treated” composite, the distribution of single serving residues making that composite is assumed to follow a lognormal distribution (Ott, 1988).

- **Parameter estimates**

The residue value detected in the composite sample value is used to estimate the mean of the lognormal distribution used to represent the residue distribution of the single serving samples making that particular composite. The approach used to estimate the standard deviation of the lognormal distribution depends on whether additional information is available about the relative variability, or coefficient of variation, = $(\frac{\text{standard deviation}}{\text{mean}})$ of the single serving residues.

Residue data from field trials are often available and may be used to estimate that relative variability. If that information is available, the standard deviation of the distribution of single serving residues in a particular composite is estimated by multiplying the value detected in the composite sample by the coefficient of variation. Thus, for each treated composite, n single serving residues are drawn from a lognormal distribution with the following parameters:

$$\begin{aligned} \text{Mean} &= \text{Composite value} \\ \text{SD(ind)} &= \text{Composite value} \times \text{Coefficient of variation}^1 \end{aligned}$$

If no information is available, an estimate of the standard deviation is derived assuming the composite samples are “repeated” samples from the same population of residues. Thus, for each treated composite, n single serving residues are drawn from a lognormal distribution with the following parameters:

$$\begin{aligned} \text{Mean} &= \text{Composite value} \\ \text{SD(ind)} &= \text{SD(comp)} \times \sqrt{n} \end{aligned}$$

Thus, in this case, the estimate of the standard deviation is derived assuming the standard deviation of the distribution of residues detected in the composite samples is an estimate of the standard error of the estimated mean of the individual units. Comparisons of the estimates of the standard deviations derived under this assumption with estimates of the standard deviation derived from observed single serving residues suggests that this approach may overestimate the variability in the residue distribution of the individual units.

- **Sampling single serving residues**

Random samples representing single serving residues for each composite are drawn from each of the lognormal distributions. Sampling is performed using Latin Hypercube Sampling. Specifically:

- Each lognormal distribution is divided into n equal probability intervals, where n represents the number of single servings per composite.
- A random value is selected within each of these intervals.
- The average of these n random values is computed and compared to the corresponding composite value.

¹ This approach has been implemented only recently, and requires further testing by the EPA.

- If the calculated average is within 5% of the composite value, the n individual unit observations are saved, and the algorithm moves to the next composite and associated lognormal distribution.
- If the calculated average is not within 5% of the composite value, the n observations are discarded, n new observations are drawn, their average is calculated and so on until the 5% convergence criteria is met. Note that there is no limit on the number of sets of single unit residue values generated while attempting to achieve convergence within 5% of the composite residue value. Such a limit is not needed because convergence reliably occurs without requiring excessive numbers of attempts. This is a result of the fact that the mean of the lognormal distribution is the composite value itself and because Latin Hypercube Sampling is used to sample the single serving values.
- All generated single serving samples are combined in a single distribution.

5.3.2.2 Cumulative Mode

5.3.2.2.1 Cumulative Percent Crop Treated Adjustment

Percent crop treated is performed for each selected analyte based on the user-specified percent crop treated for each analyte using the same algorithm as in the Individual Analyte Mode, with the following modifications:

- Where the Individual Analyte Mode Percent Crop Treated algorithm replaces n non-detect residue values with a uniform value equal to $\frac{1}{2}$ of the average of the LOD values of the distribution's non-detect samples (as specified by the aforementioned ChemSAC memo); the Cumulative Mode percent crop treated algorithm replaces the n non-detect residues with $\frac{1}{2}$ of the individual sample LOD value from n non-detect samples from the distribution.
- The “Probability of Treatment” algorithm is used to determine a subset of the non-detect samples from each analyte to randomly select from when assigning implied treated ($\frac{1}{2}$ LOD) residue values. By first assuming independence of pesticide use, the “Probability of Treatment” algorithm is able to calculate the expected number of samples that will have been treated with a particular combination of pesticides using the user-specified percent crop treated value for each analyte. For instance:

Illustration of the “implied treated” assignments

This simplified example includes only two compounds; many compounds may be included using RDFgen™, provided that samples exist that have been tested for all of the chemicals included.

- ✓ Assume that $n=200$ samples of a particular crop are available, and that analysis of each of these samples for compounds A and B, resulted in a total of 40 detectable residues for compound A and 35 for Compound B, with the following permutations of each sample:
 - 5 samples with detectable A and B residues
 - 35 samples with detectable A residues, and no detectable B residues

Illustration of the “implied treated” assignments (Cont’d)

30 samples with detectable B residues and no detectable A residues
 130 samples with no-detected A and B residues

- ✓ Assume that the market shares of compounds A and B are 25% and 30%, respectively.
- ✓ Based on the percent crop treated, we expect 50 samples to have been treated for compound A (200 X .25) and 60 for compound B (200 X .3). We compare these expected values with the number of detectable residues, and find that 5 of the samples (40-35) with no detected A residues must be assigned ½ LOD A residue values, and 5 of the samples (35-30) with no detected B residues must be assigned ½ LOD B residue values. Note that if it had turned out that the percentage of samples with detectable residue values for either compound exceeded that compound’s percent crop treated, the percent crop treated value for that compound would have been adjusted upward correspondingly.
- ✓ Under the independence assumption, we would expect:
 - 15 samples with detectable A and B residues (200 X .25 X .3)
 - 35 samples with detectable A residues, and no detectable B residues (200 X .25 X (1-.3))
 - 45 samples with detectable B residues and no detectable A residues (200 X .3 X (1-.25))
 - 105 samples with non-detectable A and B residues (200 X (1-.25) X (1-.3))
- ✓ Count the actual number of samples matching each of these permutations in the source residue data for the two compounds.
- ✓ Adjust each compound for PCT selecting implied treated samples randomly only from the subsets of the non-detect samples from each compound that do not cause the actual count of samples matching each possible permutation to exceed the expected counts.

Excerpt 1 from RDFgen™ spreadsheet output:

DISTRIBUTION HEADING	NUM. OF OBS.	NUM. OF DETECTS
Compound A	200	40
Compound B	200	35

Excerpt 2 from RDFgen™ spreadsheet output:

Compound A	Compound B	Probability:	Expected # of samples matching pattern:	Initial # of samples matching pattern:	# of samples matching pattern after adjusting for PCT:
NT	NT	0.525	105	130	105
NT	T	0.225	45	30	45
T	NT	0.175	35	35	35
T	T	0.075	15	5	15

5.3.2.2.2 Cumulative Decompositing

Decompositing in the Cumulative Mode is performed in exactly the same manner as decompositing in the Individual Analyte mode. However, to avoid creating an artificial correlation between single serving residues from various compounds, the relationship between single serving data points from the different analytes is maintained, randomizing the sequence of residue values within each set of single servings belonging to a particular composite in order to prevent generation of unrealistic cumulative single serving values. For instance, assume the analysis included 2 compounds and 30 composite samples of 6 single servings each. The 6 single serving residues generated for compound A and composite (i) are randomly paired with the 6 single serving residues generated for compound B and composite (i). Note that the “generated” residues for composites assumed not treated for a particular compound are all zeroes.

5.3.2.2.3 Cumulative Processing Factor Adjustments and Cumulative Potency Coefficient Adjustments

All residue values in the distributions for each included analyte are multiplied by the user-specified processing factor and/or potency coefficient before each sample’s composite residue value is finally determined by summing the adjusted residue values for each included analyte. By adjusting for processing at this stage, any differences in processing among different compounds is maintained.

Enhanced versions of RDFgen™ will also include modified RDF specification allowing the component residues to be specified side by side with the cumulative residues to facilitate chemical-based CEC reporting in DEEM™.

6. Quality Audits and Validation

6.1 DEEM™ Dietary modules

DEEM™ outputs and algorithms have undergone extensive validation and quality audits to verify the data transfer, data manipulation, and calculations.

6.1.1 Validation of the transfer of the data from the USDA CD-ROM to DEEM™

Comparisons of DEEM™ outputs and summary tables prepared by USDA were used to confirm the data transfer from the USDA CD-ROM to DEEM™. Specifically, unweighted counts of individuals in various subpopulations provided by USDA summary tables were compared to counts in DEEM™ outputs, and confirmed that the transfer was done correctly.

6.1.2 Quality audit of the computational algorithms

6.1.2.1 Quality audits performed

Audits of the computational algorithms used in DEEM™ are conducted by comparing DEEM™ with estimates derived using spreadsheet calculations. These include the algorithms for deriving the interval limits, the allocation of the observations to the intervals, the calculation of the various statistics, including the means, standard deviations, and percentile estimates.

6.1.2.2 Quality audits results

Consumption data for children ages 1 to 6 years were used to test the algorithms. We show below representative examples of these tests. Specifically, we compare the estimates of the weighted percent users, per-user mean, standard deviation and standard error, derived using DEEM™ and those derived using spreadsheet functions.

- **Data used:**

Consumption of raw apples (RAC 54), FF11 for children ages 1 to 6 years from 1994-96 CSFII
 Number of children in the population: 3037, each contributing two days of intake for a total of 6074 person days.

- **Results:**

Parameter	DEEM™	Spreadsheet calculation
Weighted number of person days	49587812	49587812
Weighted number of user days	11996587	11996587
Weighted percent user days	24.19%	24.1926%
Weighted mean (gm/day)	243.0934	243.093437
Weighted standard deviation (gm/day)	201.1288	201.128776
Weighted standard error (gm/day)¹	5.072802	5.07280232

¹ The standard error is calculated using the approach used by Ershow and Cantor (LSRO, 1989).

Thus, estimates derived by DEEM™ and spreadsheet calculations are identical

6.1.3 Assessing the impact of the binning procedure on interval estimates

6.1.3.1 Quality audits performed

Consumption data for children ages 1 to 6 years were used to test the algorithms. Percentile estimates derived using the DEEM™ “binned” distributions were compared to percentile estimates derived using the “unbinned” data and SPSS® “WEIGHT” and “PERCENTILE” functions.

6.1.3.2 Quality audits results

We show below results of a representative test.

- **Data used:**

Consumption of raw apples (RAC 54, FF11) for children ages 1 to 6 years from the 1994-96 CSFII
 Number of children in the population: 3037, each contributing two days of intake for a total of 6074 person days

- **Results:**

Percentile	Estimates (gm/kg/day)	
	DEEM™	No binning SPSS®
10	3.869486	3.8526
20	6.118532	6.0784
30	7.808793	7.7987
40	9.827055	9.7842
50	11.657370	11.6385
60	14.595180	14.6457
70	18.193310	18.2353
80	23.386380	23.3962
90	34.089500	34.2069
95	45.324030	45.5046
97.5	56.054500	56.1214
99	70.996250	71.5096
99.5	84.019320	84.0678
99.75	104.679300	105.0847
99.9	117.245400	117.4737

The percentile estimates are virtually identical.

6.1.4 Validation of the algorithm used in the Monte Carlo assessment

6.1.4.1 Types of validation analyses

Consumption data for children ages 1 to 6 years were used to test the algorithms. Exposure distributions derived from DEEM™ Monte Carlo acute assessment were compared to distributions derived using commercial Monte Carlo software (Crystal Ball®).

6.1.4.2 Results of the validation analyses

Examples using varying degrees of residue data complexity were used. We present below the results of two such examples.

- **Example 1:**

- **Data used:**

Consumption of orange juice (RAC 36) for children ages 1 to 6 years from the 1994-96 CSFII
Residue data: RDF file (empirical distribution) consisting of 106 data points

- **Results:**

Parameter	Estimates (mg/kg/day)	
	Crystal Ball®	DEEM™
Number of iterations	10,000	100
Percentile		
10	0.000004	0.000004
20	0.000009	0.000009
30	0.000016	0.000016
40	0.000029	0.000030
50	0.000057	0.000057
60	0.000092	0.000091
70	0.000129	0.000128
80	0.000183	0.000183
90	0.000302	0.000296
95	0.000519	0.000519
97.5	0.000953	0.000912
99	0.001688	0.001629
99.5	0.002424	0.002274
99.75	0.003303	0.002973
99.9	0.004111	0.004172

Note that the 100 DEEM™ “iterations” correspond to 607,400 iterations in “traditional” Monte Carlo software since, in DEEM™ 100 iterations are performed using each of the 6,074 person-days of intake, while in traditional Monte Carlo software, 100 iterations would correspond to 100 observations drawn from the intake distributions. Percentile estimates derived using DEEM™ and CRYSTAL BALL® are virtually identical.

- **Example 2:**

- **Data used:**

Consumption: RAC 36 and RAC 52 FF 11 for children ages 1 to 6 years from the 1994-94 CSFII. This test provides an evaluation of a relatively complex set of food consumption data and a combination of several types of residue data. Such a scenario would be quite common in an actual dietary intake assessment in which several foods are consumed, and different types of residue data are available for the different types of food.

Residue data:

- RAC 36, FF 11: Constant value (0.002)
- RAC 36, FF 12: Constant value (0.002)
- RAC 36, FF 31: Mixture: 65% zeroes, and 35% from RDF file with 106 observations
- RAC 36, FF 41: Constant value (0.002)
- RAC52, FF11: Mixture: 50% zeroes, and 50% lognormal (0.007, 0.006)

▪ **Results:**

Parameter	Estimates (mg/kg/day)	
	Crystal Ball®	DEEM™
Number of iterations	100,000	500
Percentile		
10	0.000000	0.000000
20	0.000000	0.000000
30	0.000000	0.000000
40	0.000000	0.000000
50	0.000002	0.000002
60	0.000004	0.000004
70	0.000014	0.000014
80	0.000039	0.000039
90	0.000103	0.000104
95	0.000183	0.000182
97.5	0.000286	0.000285
99	0.000599	0.000598
99.5	0.001030	0.001029
99.75	0.001629	0.001579
99.9	0.002439	0.002416

Percentile estimates derived using DEEM™ and CRYSTAL BALL® are virtually identical.

6.1.5 Audit of the randomization algorithms

6.1.5.1 Analyses performed

Analyses were conducted by Novigen and EPA and confirmed that the estimated exposure distribution is not affected by:

- the order in which the residue values are listed in the RDF file.
- the method used to adjust the distribution of residues for percent crop treated.
- the computer used to run the assessment.
- whether the assessment was run separately or in a “batch” file.
- random seed (after allowing for enough iterations).

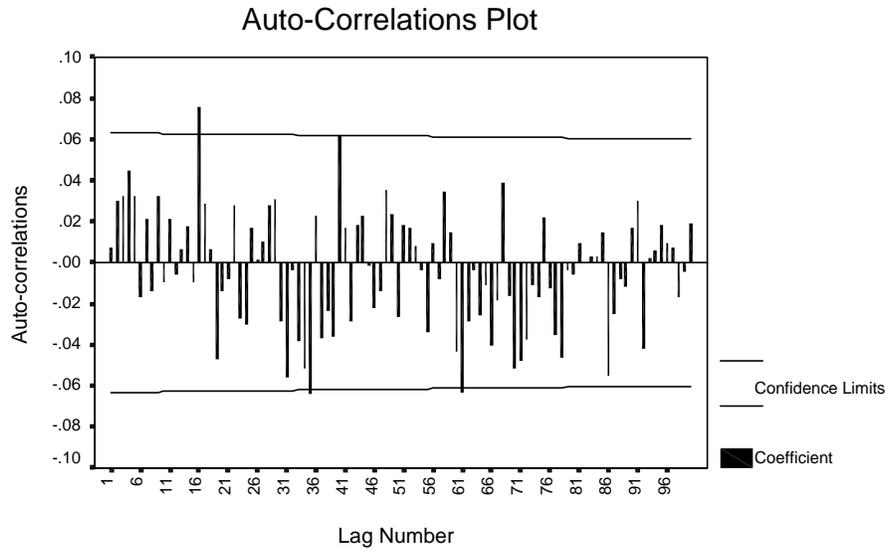
In addition, statistical analyses of sets of random numbers generated by DEEM™ were conducted to confirm that they were indeed uniformly distributed and did not show any correlations or patterns.

6.1.5.2 Results of selected analyses

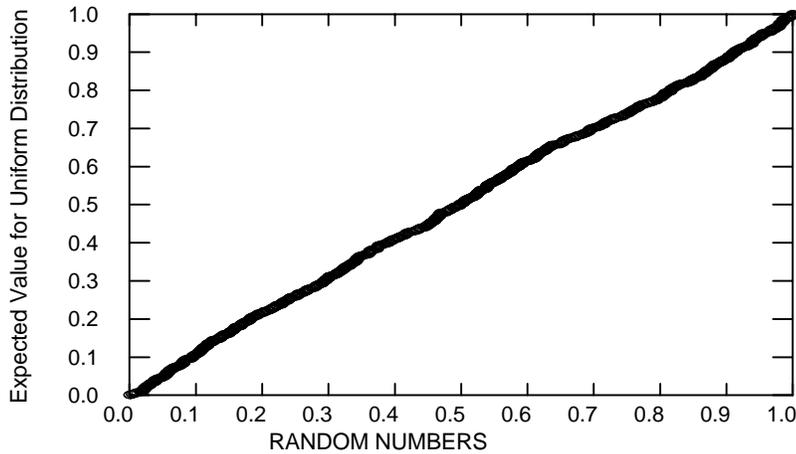
- **Data used:**

Sets of 1000 random numbers (in the order in which they were generated) used by DEEM™ were analyzed to detect any correlations or patterns likely to bias results. We present below a representative set of these analyses:

- **Results:**



P-P PLOT OF THE GENERATED RANDOM NUMBERS



Test of the goodness of fit of the uniform distribution

Test	Statistic	P-Value
Chi-Square (Crystal Ball®)	27.4640	0.4931
Kolmogorov-Smirnov (SYSTAT®)	0.025	0.534

The correlations shown in the auto-correlations plot are all negligible (close to zero). Only three of the 100 estimated coefficients are significantly different from zero (less than the 5% that would be expected by chance alone), implying that there are no significant associations between the random numbers. In addition, the P-P plot shows that the random numbers fit a uniform distribution, as expected if the randomization is functioning correctly.

6.2 DEEM™ RDFgen™ Module

6.2.1 Quality audits of the data transfers in the RDFgen™ module

The Pesticide Data Program information from 1994-1997 was thoroughly checked after it was received from USDA. This included confirming that the records count in the Novigen master PDP database matched the record count in the official PDP documentation and also spot checking the contents of the final database against the official PDP annual reports. In addition, every field in the Novigen master PDP database was queried individually and the results were scrutinized for unusual or confusing entries, such as duplicate records, residue values greater than 1000 PPM, and samples with non-zero concentrations that were less than the reported LOD. All potential inconsistencies were reported to PDP for confirmation. In every case, the Novigen master PDP database proved to be completely consistent with the database utilized by PDP.

The databases utilized by RDFgen™ are derived from the 1994-1997 Novigen master PDP database described above. In order to confirm that the data were extracted properly, detailed queries were run on the Novigen master PDP database, which generated the number of samples and the average, minimum, and maximum concentrations for every pesticide and commodity combination on a year-by-year basis. These results were compared to the statistical output generated during the RDFgen™ extraction process and in all cases the results matched exactly. In addition, all the extracted data were compared result by result to the official PDP annual reports. Again, all potential inconsistencies were reported to PDP for confirmation and once again, the Novigen master PDP database proved to be completely consistent with the database utilized by PDP.

6.2.2 Validation of the decomposing algorithm in RDFgen™

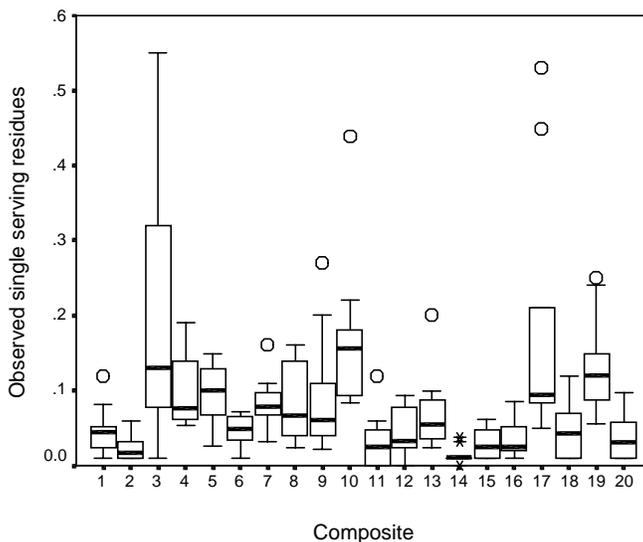
6.2.2.1 Validation of the multiple distribution assumption

- Using PDP data

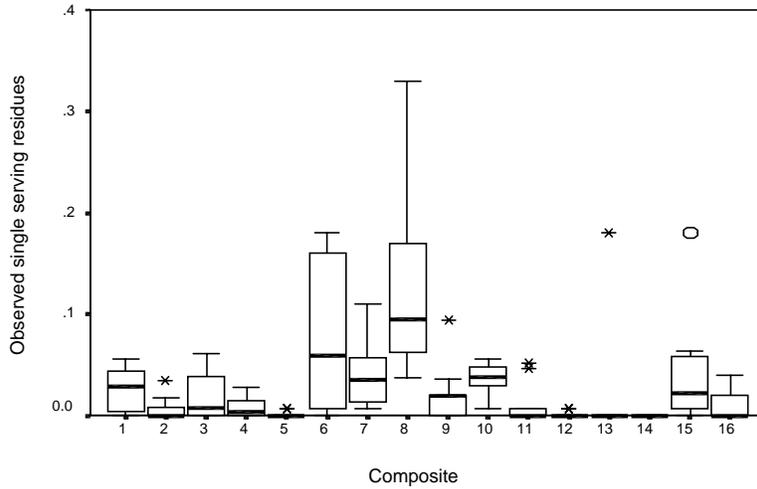
Observed single serving data from composite samples collected by PDP for two compounds (A and B) were analyzed to determine the validity of the multiple distribution assumption (Box plots and Analysis of Variance).

The box plots of the distributions of single serving residues indicate a difference between composites validating the approach of assuming multiple distributions. In addition, the analysis of variance tests conducted indicated a significant difference between the distributions of single serving residues from different composites (p-values (one-way ANOVA of the log-transformed residue values) <0.001 for each of the two compounds).

Box Plots of the PDP single serving residues from different composites (Compound A)



Box Plots of the PDP single serving residues from different composites (Compound B)

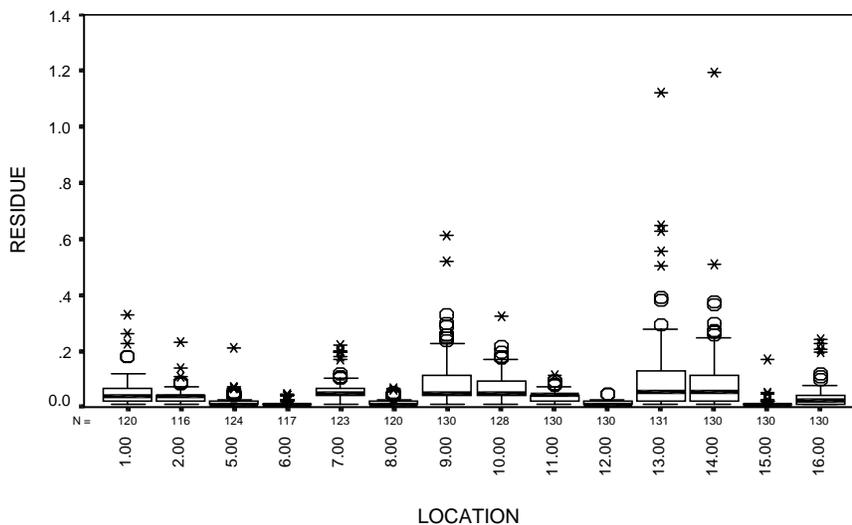


- Using field trials data

Example 1:

Data on single serving residues from field trials conducted with compound C in 14 different locations still show differences (One-way ANOVA of the log-transformed residues, p-value < 0.001), even though the trials were conducted under identical conditions.

Box Plots of the single serving residues from different locations (Compound C)



Example 2:

Data on single serving residues and corresponding composites, collected from the SAME field were available. Analysis of variance of the logarithm single serving residues failed to show a significant composite sample effect, implying that there was no significant difference between single serving residues making composites collected from the same field (One-way ANOVA, p -value = 0.477).

6.2.2.2 Validation of the estimation algorithms

Validation of the algorithms requires comparison of the single serving data generated by RDFgen™ for a given set of composite samples to the actual single serving data that made these composites. Actual residue data of this type are very limited. We used PDP data, field trial data, and simulated data.

6.2.2.2.1 Using PDP data**▪ Example 1: Compound A – Ten observed single servings per composite****▪ Data Used:**

Single serving analyses for compound A were performed on all single servings from composites with quantifiable residues (i.e., > LOQ). Twenty such composite samples and their corresponding 200 (10 per composite) single serving samples were available. Of the 200 single serving residues, 29 had trace levels, i.e., residues above the LOD but below the LOQ, and were assigned a value equal to half the LOQ, and six samples did not have any detectable residues and were assigned a value equal to half the LOD.

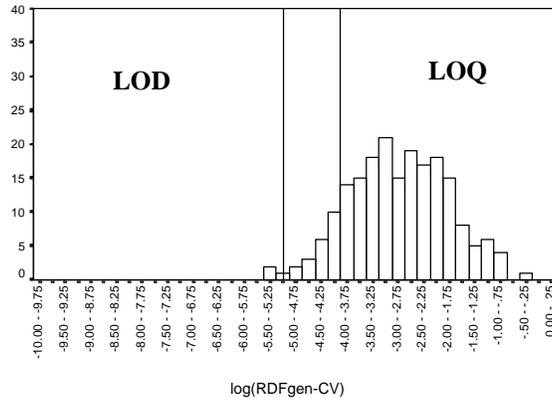
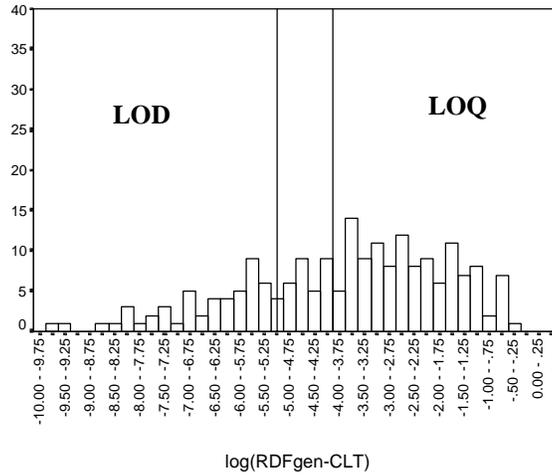
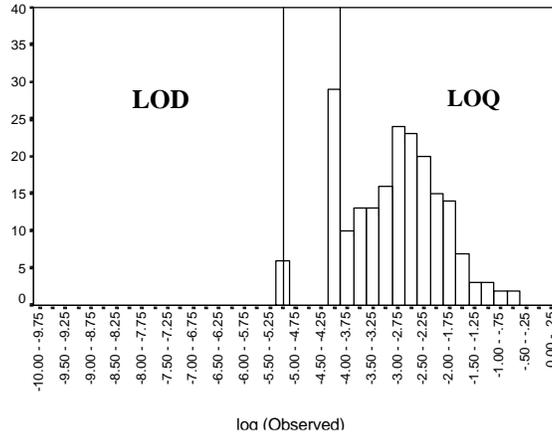
▪ Results:

Two sets of analyses were conducted. The first assumed that no additional information about the relative variability of the single serving residue distribution was available, while the second assumed a known coefficient of variation. Typically, the coefficient of variation would be estimated either from field trials or another set of single serving residues, if available. In this example, there were no such data, however, to illustrate the impact of using additional information, we estimated the coefficient of variation from each of the 20 sets of single serving residues, and used the minimum, average and maximum of these 20 estimates (42%, 71% and 120%, respectively).

The histograms and summary percentiles indicate that single serving residues generated in the absence of information (RDFGEN-CLT) show more variability than the observed single serving residues. Part of this variability is due to the fact that a large proportion of the observed single serving residues refer to censored values (either at the LOQ or the LOD), while the residues generated by the RDFgen™ approach are not “censored”. Based on the quantile-quantile plots and the results of the Kolmogorov-Smirnov tests, the generated single serving residues that best “approximate” the observed single serving residues are those generated using an average coefficient of variation with RDFgen™. However, based on the results of the Kolmogorov-

Smirnov tests, the distribution generated using coefficients of variation of 120% still provides a good fit to the observed data, while the distribution generated using coefficients of variation of 42% does not. Note, however, that the quantile-quantile plot of the distribution generated using coefficients of variation of 42% indicates a fairly good fit. This apparent contradiction is due to the fact that the Kolmogorov-Smirnov test focuses on the maximum absolute difference between the two cumulative distributions. Thus, the uncertainty or “imperfect” knowledge of the relative variability of the single serving residue distributions did not have a significant impact on the resulting generated single serving distributions.

HISTOGRAMS OF LOG (RESIDUES)
Example 1: PDP - Compound A
20 Composite Samples
10 Single Servings Per Composite Sample

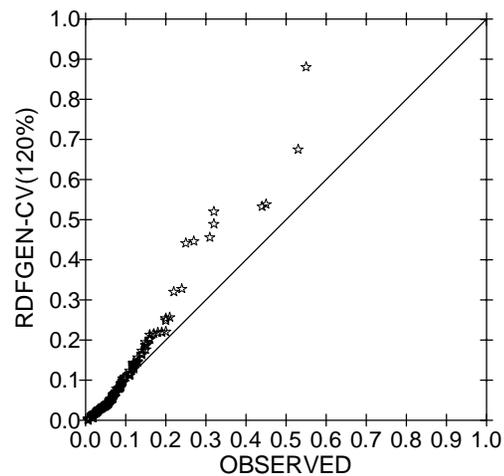
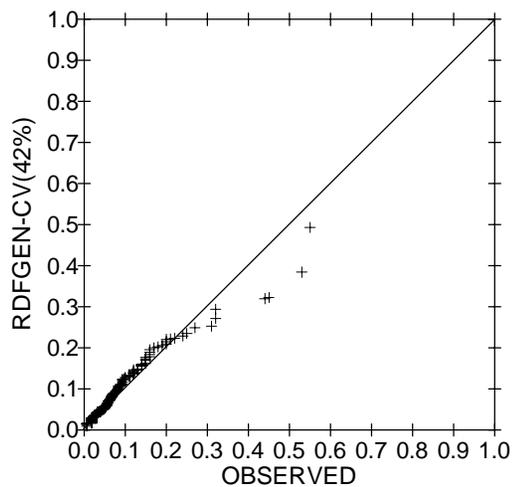
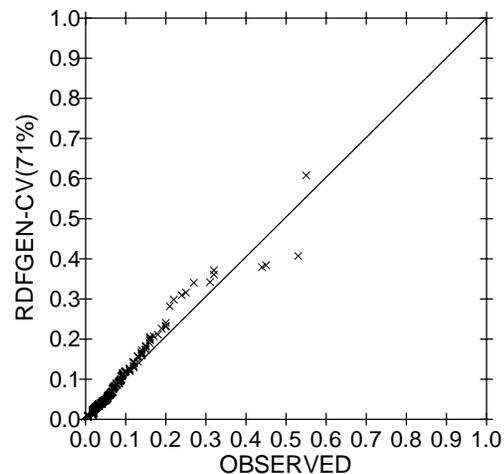
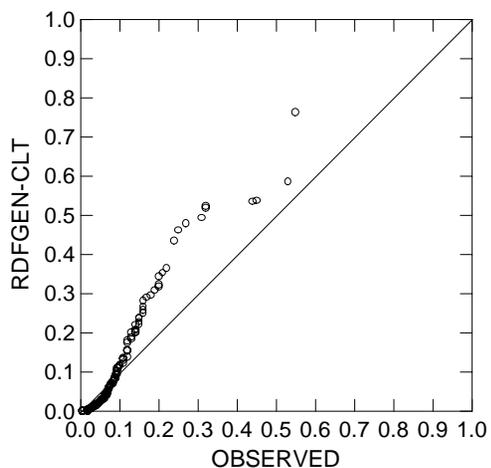


QUANTILE-QUANTILE PLOTS OF THE OBSERVED AND GENERATED DISTRIBUTIONS

Example 1: PDP - Compound A

20 Composite Samples

10 Single Servings Per Composite Sample



PERCENTILES OF THE OBSERVED AND GENERATED DISTRIBUTIONS

Example 1: PDP - Compound A
20 Composite Samples
10 Single Servings Per Composite Sample

Percentile Distributions

	OBSERVED	RDFgenCLT	RDFgenCV71	RDFgenCV42	RDFgenCV120
N	200	200	200	200	200
Mean	.0800	.0881	.0884	.0884	.0883
Std. Deviation	.0848	.1337	.0909	.0742	.1233
Minimum	.0060	.0001	.0050	.0095	.0002
Maximum	.5500	.7629	.6081	.4932	.8808
Percentiles					
10.0	.0180	.0012	.0166	.0230	.0106
20.0	.0210	.0035	.0241	.0300	.0168
30.0	.0310	.0088	.0324	.0384	.0238
40.0	.0428	.0173	.0439	.0486	.0333
50.0	.0570	.0297	.0587	.0652	.0437
60.0	.0690	.0476	.0768	.0852	.0585
70.0	.0877	.0812	.0966	.1078	.0838
80.0	.1200	.1504	.1323	.1386	.1323
90.0	.1600	.2657	.2006	.1889	.2038
95.0	.2390	.4310	.3089	.2285	.3278
97.5	.3200	.5232	.3706	.2933	.5200
99	.5292	.5846	.4064	.3837	.6744
99.5	.5499	.7620	.6071	.4926	.8798
99.9

**Kolmogorov-Smirnov Two Sample Test results
 EXAMPLE 1: PDP - COMPOUND A
 20 Composite Samples
 10 Single Servings Per Composite Sample**

Maximum differences for pairs of variables					
	OBSERVED	RDFGENCLT	RDFGENCV71	RDFGENCV42	RDFGENCV120
OBSERVED	0.000				
RDFGENCLT	0.235	0.000			
RDFGENCV71	0.070	0.310	0.000		
RDFGENCV42	0.140	0.365	0.090	0.000	
RDFGENCV120	0.110	0.250	0.140	0.215	0.000
Two-sided probabilities					
	OBSERVED	RDFGENCLT	RDFGENCV71	RDFGENCV42	RDFGENCV120
OBSERVED	.				
RDFGENCLT	0.000	.			
RDFGENCV71	0.711	0.000	.		
RDFGENCV42	0.040	0.000	0.393	.	
RDFGENCV120	0.178	0.000	0.040	0.000	.

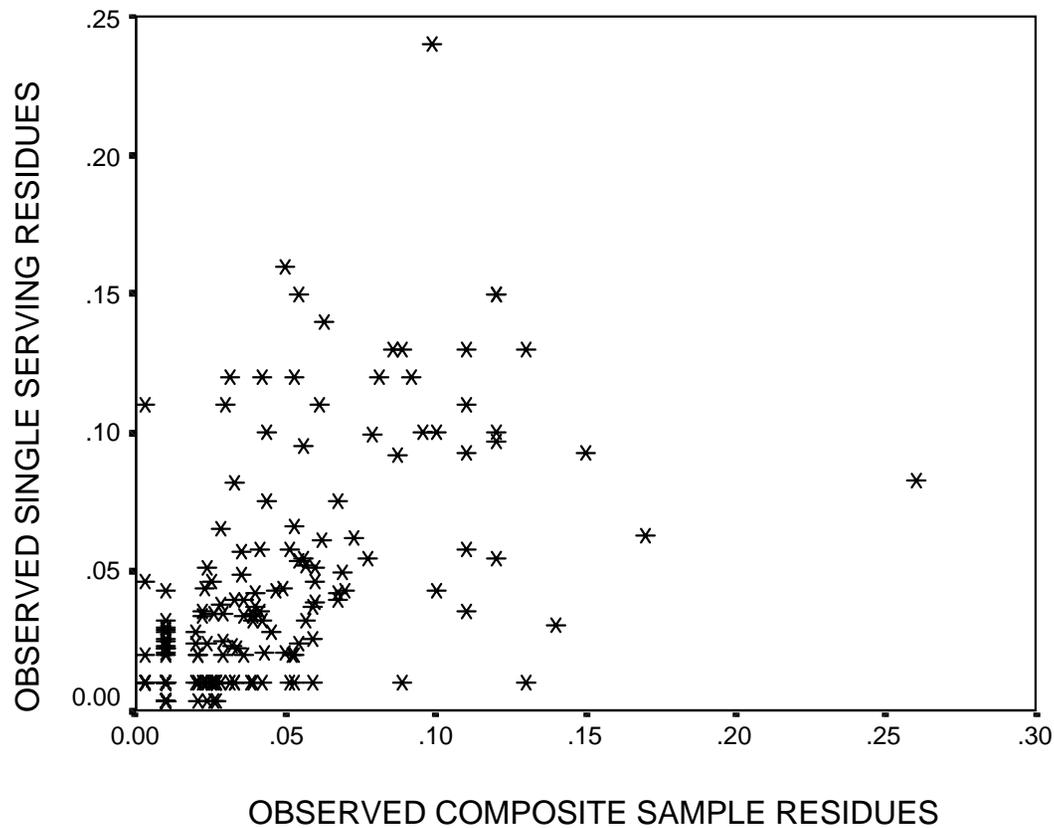
Example 2: Compound A – One Observed Single Serving per Composite

- **Data Used:**

Single serving analyses for compound A were performed on one single serving per composite for all composites. Residue values from 334 composite samples and their corresponding 342 single serving samples were available. Two single serving analyses were missing, and ten composite samples had two matching single serving residues. Based on information about the market share of the compound and the percent samples with detectable residues it was decided to assume that all samples that had both a non-detectable composite residue and a non-detectable single serving residue are not treated with the compound of interest. Thus, data from 231 composite samples and their “corresponding” 238 single serving samples were available for this analysis. Of the 238 single serving residues, 33 were below the LOD while 117 were below the LOQ. On the other hand, 11 of the composite samples had residues below the LOD and 94 had residues below the LOQ.

The scatter plot (see following Figure) of the observed composite and associated single serving residues shows a positive association between the two sets of residues. It should be noted that the mean and standard deviation of the observed single serving residues (0.0346 ppm and 0.0396 ppm) and composite residues (0.0350 ppm and 0.0364 ppm) were very similar. While it is not surprising that the two averages were similar, it is surprising that the standard deviation of the single serving residues is not much larger than that of the composite samples. If the one single serving residue available for each composite is a true random sample from the single servings making each composite then these results would imply very little variability within composite. However the standard deviation of single serving residues for the same compound, described in Example 1 varied from 0.0114 ppm to 0.174 ppm for the 20 composites (the standard deviation of the entire set of single serving residues, irrespective of composite was 0.0859 ppm).

SCATTER PLOT OF THE OBSERVED RESIDUES
Example 2: PDP - Compound A
One Observed SS Per Composite Sample

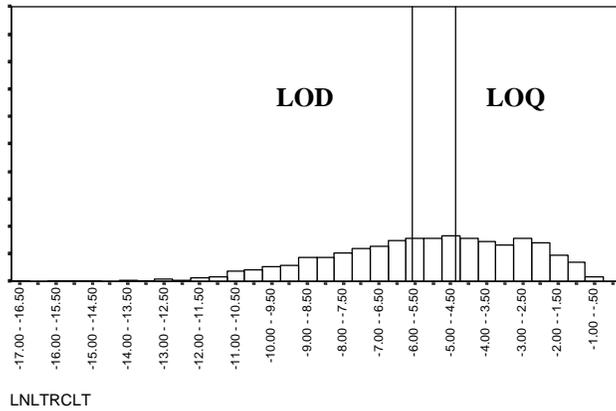
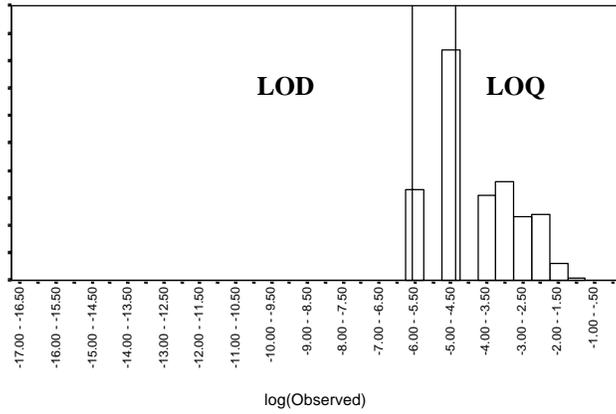


- **Results:**

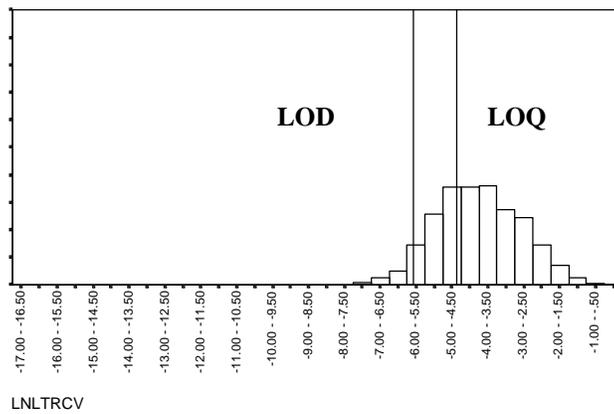
Two sets of analyses were conducted. The first assumed that no additional information about the relative variability of the single serving residue distribution was available, while the second used the average coefficient of variation from the sets of single serving residues described in Example 1.

The single serving residues generated using the average coefficient of variation from the data described in Example 1 show a better fit than those derived in the absence of additional information. However both distributions were significantly different from the observed single serving residues (Kolmogorov-Smirnov Tests). However, this result is not surprising given the fact that only one observed single serving residue out of 10 is available for each composite sample and the fact that the single serving residue distribution did not show more variability than the composite residue distribution (see above discussion).

HISTOGRAMS OF LOG (RESIDUES)
Example 2: PDP - Compound A
One Observed Single Serving Per Composite Sample
Ten Generated Single Servings Per Composite Sample

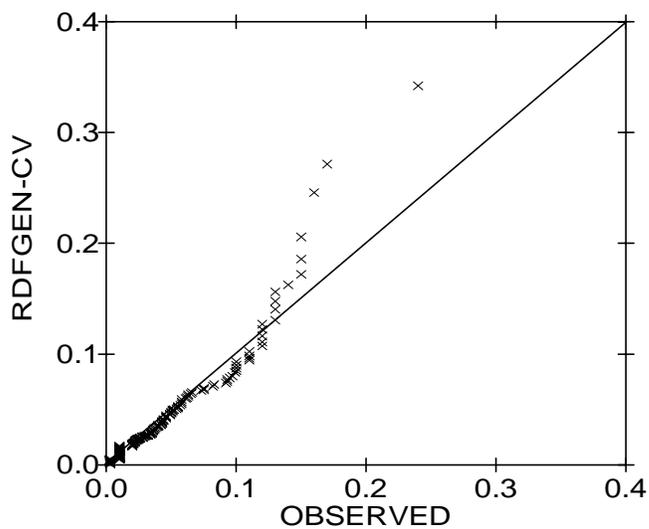
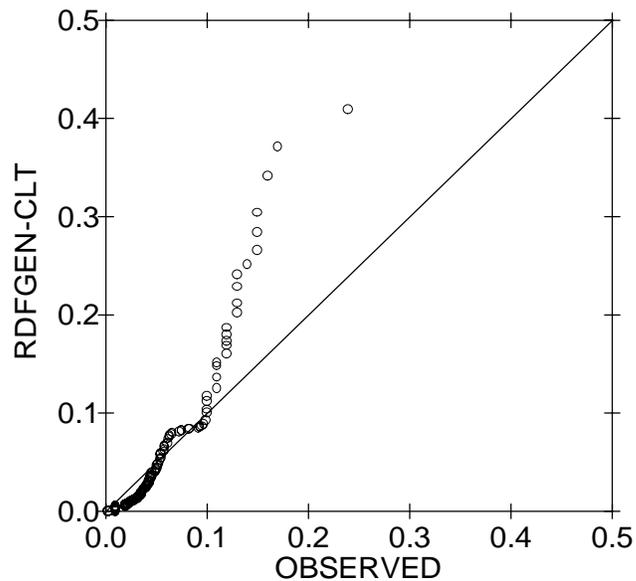


LNLTRCLT



LNLTRCV

**QUANTILE-QUANTILE PLOTS
OF THE OBSERVED AND GENERATED DISTRIBUTIONS
Example 2: PDP - Compound A
One Observed Single Serving Per Composite Sample
Ten Generated Single Servings Per Composite Sample**



PERCENTILES OF THE OBSERVED AND GENERATED DISTRIBUTIONS

Example 2: PDP - Compound A
One Observed Single Serving Per Composite Sample
Ten Generated Single Servings Per Composite Sample

Estimated Percentiles

	Observed	RDFgenCLT	RDFgen-CV
N	238	2310	2310
Mean	.0346	.0350	.0350
Std. Deviation	.0396	.0678	.0492
Minimum	.0030	.0000	.0006
Maximum	.2400	.4753	.6962
Percentiles			
10	.0030	.0001	.0041
20	.0100	.0004	.0066
30	.0100	.0011	.0091
40	.0100	.0025	.0126
60	.0280	.0106	.0247
70	.0393	.0237	.0344
80	.0550	.0539	.0515
90	.1000	.0988	.0847
95	.1205	.1836	.1262
97.5	.1500	.2583	.1697
99	.1661	.3438	.2554
99.5	.2264	.3777	.3043
99.9	.	.4496	.4494

KOLMOGOROV-SMIRNOV TWO SAMPLE TEST RESULTS

Example 2: PDP - Compound A
One Observed Single Serving Per Composite Sample
Ten Generated Single Servings Per Composite Sample

Maximum differences for pairs of groups			
	RDFCLT	RDFCV	OBSERVED
RDFCLT	0.000		
RDFCV	0.376	0.000	
OBSERVED	0.451	0.189	0.000
Two-sided probabilities			
	RDFCLT	RDFCV	OBSERVED
RDFCLT	.		
RDFCV	0.000	.	
OBSERVED	0.000	0.000	.

- **Example 3: Compound A**

- **Data Used:**

The observed composite and single serving data are the same as those used in Example 2. However, only one of the ten generated single serving samples per composite are used in this validation. Specifically, one single serving value was randomly selected from each set of 10 single servings. As in the previous example, the observed single serving values that were below the LOD and LOQ were set at half the LOD and half the LOQ in the following summaries.

- **Results:**

As in the previous example, two sets of analyses were conducted. The first assumed that no additional information about the relative variability of the single serving residue distribution was available, while the second used the average coefficient of variation from the sets of single serving residues described in Example 1.

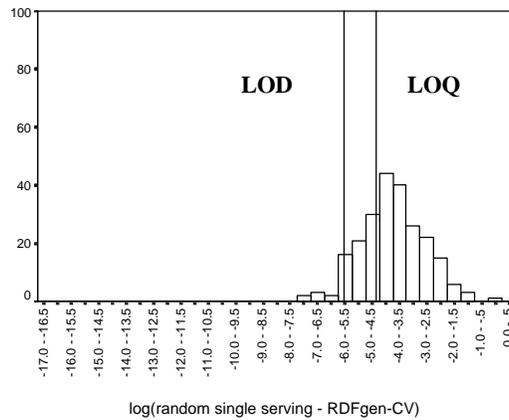
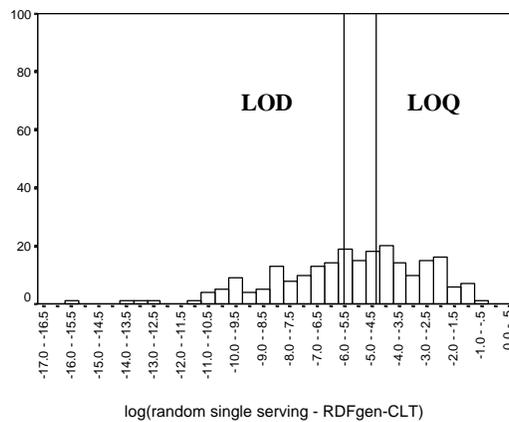
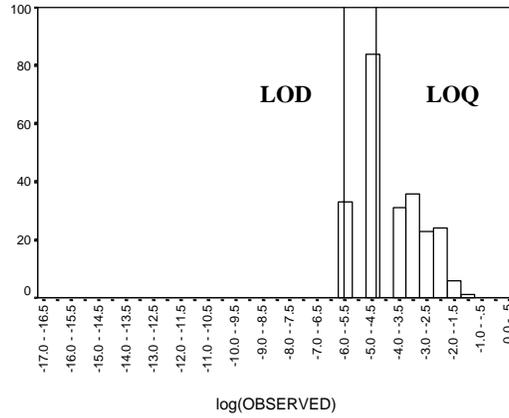
The single serving residues generated using the average coefficient of variation from the data described in Example 1 show a better fit than those derived in the absence of additional information. However both distributions were significantly different from the observed single serving residues (Kolmogorov-Smirnov Tests). However, as noted earlier, this is not surprising, considering that the observed single serving residues refer to a single observation for the 10 apples making the composite and the fact that the single serving residue distribution did not show more variability than the composite residue distribution.

HISTOGRAMS OF THE LOGARITHM OF THE SINGLE SERVING RESIDUES

Example 3: Compound A

One observed single serving per composite

One random generated single serving per composite

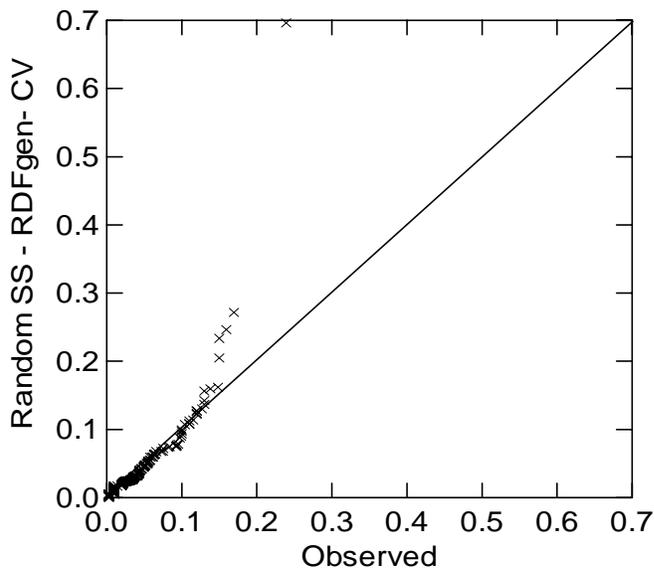
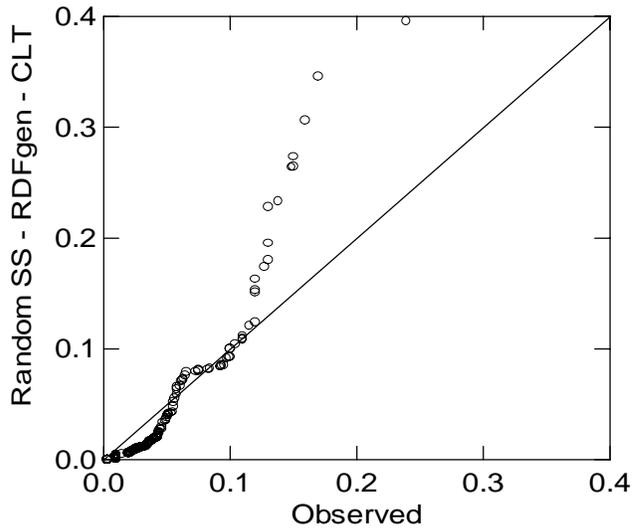


QUANTILE-QUANTILE PLOTS

Example 3: Compound A

One observed single serving per composite

One random generated single serving per composite



PERCENTILE DISTRIBUTIONS
Example 3: Compound A
One observed single serving per composite
One random generated single serving per composite

Percentile Distributions

		Observed	Random-RDFgen-CLT	Random-RDFgen-CV
N	Valid	238	231	231
Mean		.0346	.0317	.0368
Std. Deviation		.0396	.0624	.0615
Percentiles	5	.0030	.0000	.0032
	6	.0030	.0000	.0035
	10	.0030	.0001	.0041
	20	.0100	.0004	.0069
	30	.0100	.0012	.0102
	40	.0100	.0026	.0127
	70	.0393	.0180	.0316
	80	.0550	.0462	.0508
	90	.1000	.0924	.0928
	95	.1205	.1672	.1286
	97.5	.1500	.2641	.1705
	99	.1661	.3330	.2635
	99.5	.2264	.3879	.6282

KOLMOGOROV-SMIRNOV TWO SAMPLE TEST RESULTS
Example 3: Compound A
One observed single serving per composite
One random generated single serving per composite

Maximum differences for pairs of groups			
	Observed	RDFgen-CLT	RDFgen-CV
Observed	0.000		
RDFgen-CLT	0.277	0.000	
RDFgen-CV	0.197	0.394	0.000
Two-sided probabilities			
	Observed	RDFgen-CLT	RDFgen-CV
Observed	.		
RDFfwn-CLT	0.000	.	
RDFgen-CV	0.000	0.000	.

Example 4: Compound B – Ten Observed Single Servings per Composite

- **Data Used**

Data available:

Data for compound B from composite and matching single serving samples from selected composite samples analyzed by PDP were available. Specifically, 342 composite samples of 10 single servings each were available. Twenty of these composite samples had detectable compound B residues. Single serving residues were available for 16 of these samples. Four composites did not have complete data for their corresponding single serving samples. Specifically, five single serving residues were missing for one composite sample, 2 single serving residues were missing for two composite samples and one single serving residue was missing for one composite sample. Thus, the number of single serving residues available for validation was 150.

CID	Composite Value	Observed Single Serving Residues ¹
C1	0.15	0.068,0.33,0.17,0.16,0.062,0.057,0.07,0.2,0.12,0.037
C2	0.09	0.17,0.16,0.062,nd,0.016,0.09,0.007,0.18,0.055,0.007
C3	0.064	nd,nd,nd,0.18,nd,M,M,M,M,M
C4	0.054	M,M,M,M,M,M,M,M,M,M
C5	0.045	0.007,0.007,nd,nd,nd,nd,nd,nd,nd,nd
C6	0.045	0.043,0.056,0.033,0.029,0.028,0.048,0.053,0.038,0.007,0.037
C7	0.044	0.026,0.039,0.032,nd,0.048,nd,0.007,0.055,M,M
C8	0.035	0.057,0.11,0.071,0.047,0.037,0.033,0.021,0.012,0.007,0.013
C9	0.03	0.058,nd,0.056,0.007,0.064,0.015,0.007,0.028,0.18,nd
C10	0.029	nd,0.061,0.038,0.007,0.061,nd,nd,nd,0.039,M
C11	0.028	0.02,0.094,0.019,0.036,nd,nd,0.019,0.016,0.02,nd
C12	0.023	M,M,M,M,M,M,M,M,M,M
C13	0.007	nd,nd,nd,0.007,nd,nd,nd,nd,nd,0.007
C14	0.007	nd,nd,0.007,0.014,0.028,nd,0.025,0.015,nd,nd
C15	0.007	nd,0.035,nd,nd,nd,nd,nd,0.017,M,M
C16	0.007	nd,nd,0.007,nd,0.047,nd,nd,nd,0.052,0.007
C17	0.007	nd,nd,nd,0.04,0.02,0.027,nd,nd,0.007,nd
C18	0.007	nd,nd,nd,nd,nd,nd,nd,nd,nd,nd
C19	0.007	M,M,M,M,M,M,M,M,M,M
C20	0.007	M,M,M,M,M,M,M,M,M,M

¹ nd: non-detectable residue, M: missing analysis

Market share data were also used to assess the number of composite samples with non-detectable residues that are “implied treated”. In the summary tables and graphs of the observed single serving residues presented below, these samples were assumed to be at the LOD. In addition, data single serving residues from field trials were available. These data were used to estimate a coefficient of variation of the single serving residue distribution (90%).

Treatment of missing single serving data:

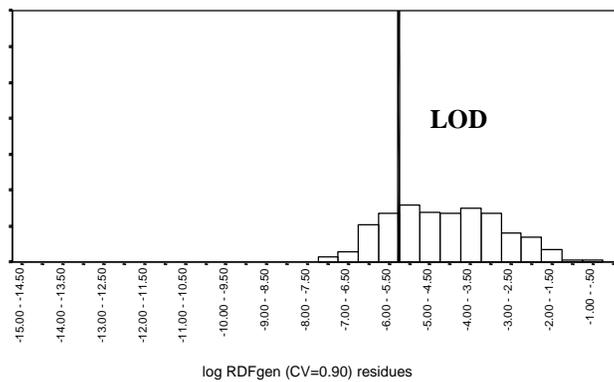
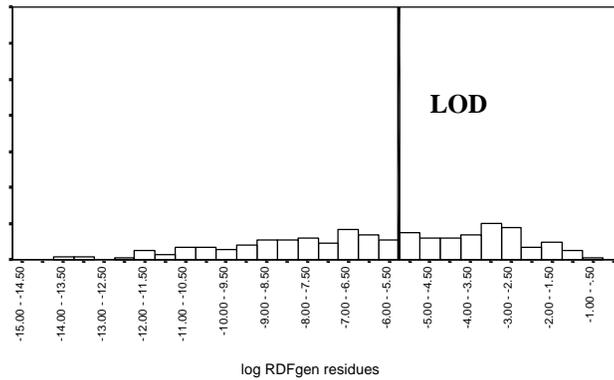
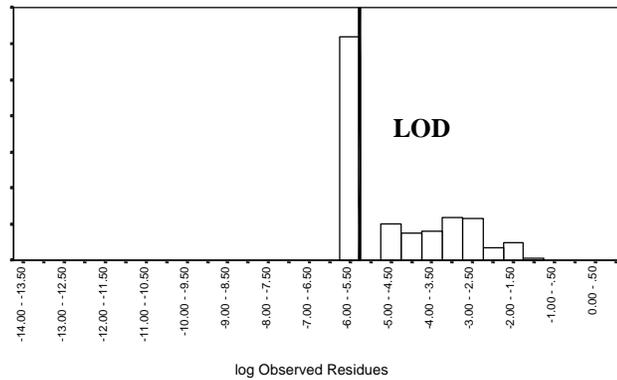
In order to compare the generated single serving residues with the observed ones, some assumptions were made regarding the missing (M) single serving residues. Specifically, the single serving residues associated with composite samples C19 (0.007 ppm) and C20 (0.007 ppm) were assumed to be similar to those associated with composite samples C17 (0.007 ppm) and C14 (0.007 ppm), respectively. The single serving residues associated with composite C6 (0.045 ppm) were multiplied by (0.054/0.045) and used to represent the missing single serving residues associated with composite C4 (0.054ppm). Similarly, the single serving residues associated with composite C11 (0.028 ppm) were multiplied by (0.023/0.028) and used to represent the single serving residues associated with composite C12 (0.023 ppm). Finally, the single serving residues missing from the single servings associated with composites C3, C7, C10 and C16 were assumed to be either non-detect or assigned values that would make the average of the single serving residues equal to the associated composite value.

- **Results:**

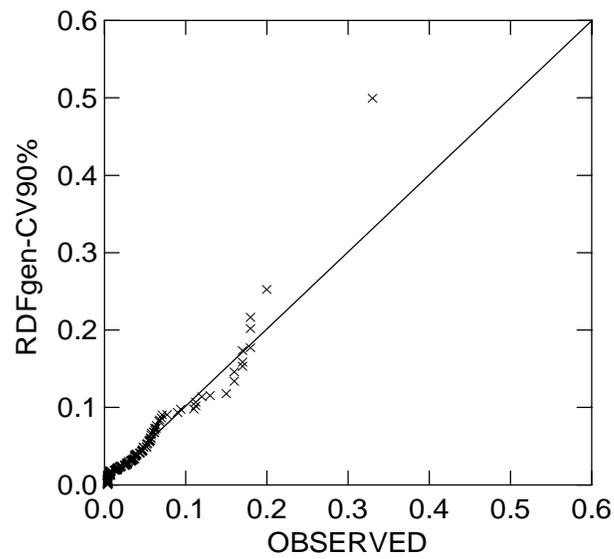
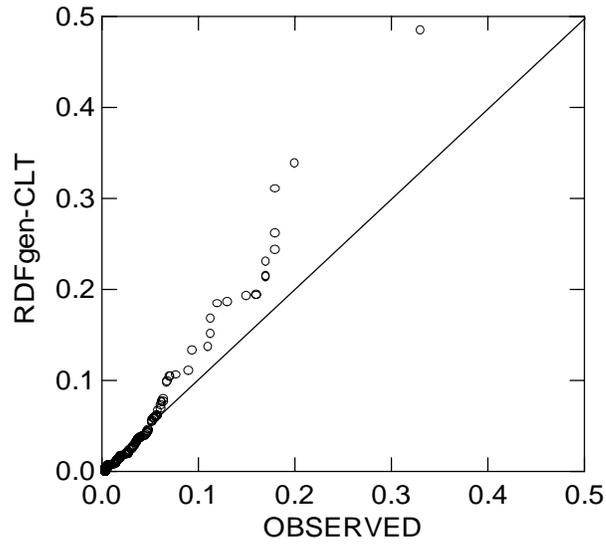
Two sets of single serving residues were generated, the first assumed that no additional information about the single serving residue distribution was available, while the second used the 90% coefficient of variation derived from field trials.

The graph summaries seem to indicate a better fit of the single serving residues generated using a CV of 90%. However, results of the Kolmogorov-Smirnov tests do not indicate a significant difference between the single serving residues generated in the absence of information and the observed single serving residues, while a significant difference between the single serving residues generated using the CV of 90% and the observed single serving residues was detected.

**HISTOGRAM OF THE LOGARITHM
OF THE OBSERVED AND GENERATED SINGLE SERVING RESIDUES**
Example 4: Compound B
10 Single Serving Residues per Composite



**QUANTILE- QUANTILE PLOTS
OF THE OBSERVED AND GENERATED SINGLE SERVING RESIDUES
Example 4: Compound B
10 Single Serving Residues per Composite**



**PERCENTILES OF THE OBSERVED AND GENERATED
SINGLE SERVING RESIDUES**

**Example 4: Compound B
10 Single Serving Residues per Composite**

Percentile Distributions

	OBSERVED	RDFCLT	RDFCV90
Mean	.0267	.0297	.0295
Std. Deviation	.0439	.0632	.0501
Minimum	.0040	.0000	.0006
Maximum	.3300	.4842	.4994
Percentiles			
10	.0040	.0000	.0022
20	.0040	.0001	.0036
30	.0040	.0005	.0053
40	.0040	.0014	.0076
50	.0040	.0034	.0116
60	.0106	.0076	.0183
70	.0267	.0192	.0260
80	.0441	.0392	.0415
90	.0640	.0794	.0764
95	.1295	.1860	.1153
97.5	.1700	.2296	.1731
99	.1918	.3268	.2377

KOLMOGOROV-SMIRNOV TWO SAMPLE TEST RESULTS

**Example 4: Compound B
10 Single Serving Residues per Composite**

Maximum differences for pairs of variables			
	OBSERVED	RDFCLT	RDFCV90
OBSERVED	0.000		
RDFCLT	0.054	0.000	
RDFCV90	0.292	0.400	0.000
Two-sided probabilities			
	OBSERVED	RDFCLT	RDFCV90
OBSERVED	.		
RDFCLT	0.873	.	
RDFCV90	0.000	0.000	.

6.2.2.2.2 Using hypothetical data

Four scenarios and sets of data were used. In each case, 10 composite samples of 20 single serving residues were generated from 10 different lognormal distributions, and single serving residues were generated for each of the 10 composites using the RDFgen™ approach. The generated and observed single serving residue distributions were compared. The scenarios differed with respect to how different the means of the original lognormal distributions (representing potential differences between field) were and how variable the distributions were (representing variability within fields). Three sets of single serving residue distributions were generated, the first used the RDFgen™ approach and assumed no additional information about the distributions, the second used the RDFgen™ approach and assumed a constant coefficient of variation, while the third used Allender’s single distribution approach.

The distributions generated using the RDFgen™ multi-distribution approach were closer to the original single serving distributions, than those generated using the single lognormal distribution assumption. In addition, upper percentiles of the single distributions generated using the RDFgen™ approach and a “known” coefficient were closer to the observed single serving residues than those generated using the RDFgen™ approach in the absence of additional information or those generated using the single distribution assumption. The largest impact of using the additional information about the relative variability of the distributions (i.e., using a known coefficient of variation) was observed for the scenarios with small within field variability, i.e., Examples 1 and 2.

Example 1: “Large variability between fields, small variability within field”

Means: random values between 0.001 and 6.000
 SD/Mean: random values between 0.5 and 1.5

Percentile	Original Data	RDFgen™ approach		Allender’s Single Distribution
	20 ss in 10 composites	Known CV = 1	CLT	
10%	0.358	0.253	0.009	0.077
20%	0.480	0.421	0.035	0.160
30%	0.735	0.616	0.094	0.270
40%	1.011	0.894	0.212	0.422
50%	1.473	1.246	0.444	0.641
60%	1.974	1.774	0.809	0.973
70%	2.781	2.423	1.489	1.522
80%	3.851	3.630	2.864	2.569
90%	6.288	6.049	6.800	5.309
95%	8.382	9.034	12.01	9.669
97.5%	11.25	12.07	19.81	16.26
99%	14.06	16.70	29.64	29.76
99.5%	16.35	19.81	32.39	44.92

Example 2: “Small variability between fields, small variability within field”

Means: random values between 0.001 and 3.000
 SD/Mean: random values between 0.5 and 1.5

Percentile	Original Data 20 ss in 10 composites	RDFgen™ approach		Allender's Single Distribution
		Known CV = 1	CLT	
10%	0.081	0.081	0.002	0.034
20%	0.175	0.176	0.009	0.073
30%	0.272	0.286	0.030	0.126
40%	0.424	0.433	0.076	0.201
50%	0.535	0.628	0.174	0.311
60%	0.891	0.906	0.372	0.481
70%	1.221	1.309	0.758	0.767
80%	1.790	1.974	1.491	1.324
90%	3.424	3.327	3.660	2.825
95%	6.013	5.032	6.918	5.284
97.5%	8.062	7.113	10.76	9.093
99%	10.69	9.92	17.35	17.09
99.5%	14.25	13.83	20.94	26.27

Example 3: “Large variability between fields, large variability within field”

Means: random values between 0.001 and 6.000
 SD/Mean: random values between 1.5 and 2.5

Percentile	Original Data 20 ss in 10 composites	RDFgen™ approach		Allender's Single Distribution
		Known CV = 2	CLT	
10%	0.220	0.149	0.025	0.165
20%	0.412	0.295	0.114	0.313
30%	0.588	0.497	0.291	0.497
40%	0.848	0.759	0.571	0.738
50%	1.149	1.125	0.958	1.068
60%	1.920	1.632	1.554	1.546
70%	2.655	2.450	2.455	2.295
80%	4.351	3.858	4.111	3.644
90%	7.338	7.302	7.880	6.922
95%	11.52	12.37	13.10	11.76
97.5%	19.97	23.40	25.33	18.61
99%	22.20	29.84	29.93	31.76
99.5%	27.42	35.32	31.18	45.69

Example 4: “Large variability between fields, large variability within field”

Means: random values between 0.001 and 3.000
 SD/Mean: random values between 1.5 and 2.5

Percentile	Original Data	RDFgen™ approach		Allender’s Single Distribution
	20 ss in 10 composites	Known CV = 2	CLT	
10%	0.080	0.070	0.011	0.049
20%	0.156	0.127	0.035	0.099
30%	0.251	0.205	0.082	0.163
40%	0.352	0.311	0.159	0.249
50%	0.501	0.444	0.289	0.371
60%	0.672	0.642	0.500	0.553
70%	1.053	0.970	0.849	0.847
80%	1.648	1.551	1.537	1.396
90%	3.158	3.079	3.415	2.789
95%	5.675	4.749	6.177	4.940
97.5%	7.697	8.978	11.33	8.109
99%	10.42	12.08	13.72	14.43
99.5%	11.77	13.49	14.46	21.37

7. Other

7.1 Water Consumption

The CSFII collected information about non-food based water consumption, that is water consumed as “water”, not mixed in foods (e.g., soup) or beverages (e.g., coffee). However, the information was collected on only one survey day, and the method used to collect the information was different from that used to collect the rest of the of the dietary intakes. Specifically, the information referred to the entire quantity of non-food based water consumed during that day. That is, no information is available about when, during the day, the water was consumed, how often it was consumed during the day, or the various amounts consumed (if it was consumed more than once).

In the absence of additional data, DEEM™ assumes that the amounts reported apply to all the survey days, and allows the incorporation of the water consumption in its exposure assessments.

7.2 Missing body weights

The body weights of some of the survey respondents were missing. DEEM™ estimates the body weights of these individuals using the reported body weights of individuals in the same age and sex group. Specifically, linear regression models relating body weight and age were derived for males and females in the following age groups:

- infants, ages 0 to 11 months,
- children ages 1 to 5 years,
- children ages 6 to 11 years,
- children ages 12 to 16 years.

These models (see Appendix 2) were used in the estimation of the missing body weights of infants and children.

For all other age groups, missing body weights were replaced by the average body weight of the individuals in the same age and sex group (see Appendix 2).

7.3 Foods with no consumption

EPA has developed a master list of RACs (Appendix 1). The master EPA list contains 458 RACs. Each of the foods reported consumed in the CSFII was translated into one or more RACs using Novigen translation factors. There was no consumption for some of these RACs in one or more of the surveys (some were reported consumed in the 1989-91 CSFII; some in the 1994-94 CSFII, some in neither survey). If the RAC was not consumed in a particular survey, DEEM™ assumes that the consumption of that RAC is insignificant for that survey period and assigns a value of zero. The user is notified that there was no consumption of the particular RAC as a part of the results' reports.

8.0 References

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United States Department of Agriculture (USDA) (1998b). Pesticide Data Program Agricultural Marketing Service. Science and Technology Division. Dataset for calendar year 1996.

Figures

**FIGURE 1
COMPONENTS OF A CUMULATIVE RISK ASSESSMENT**

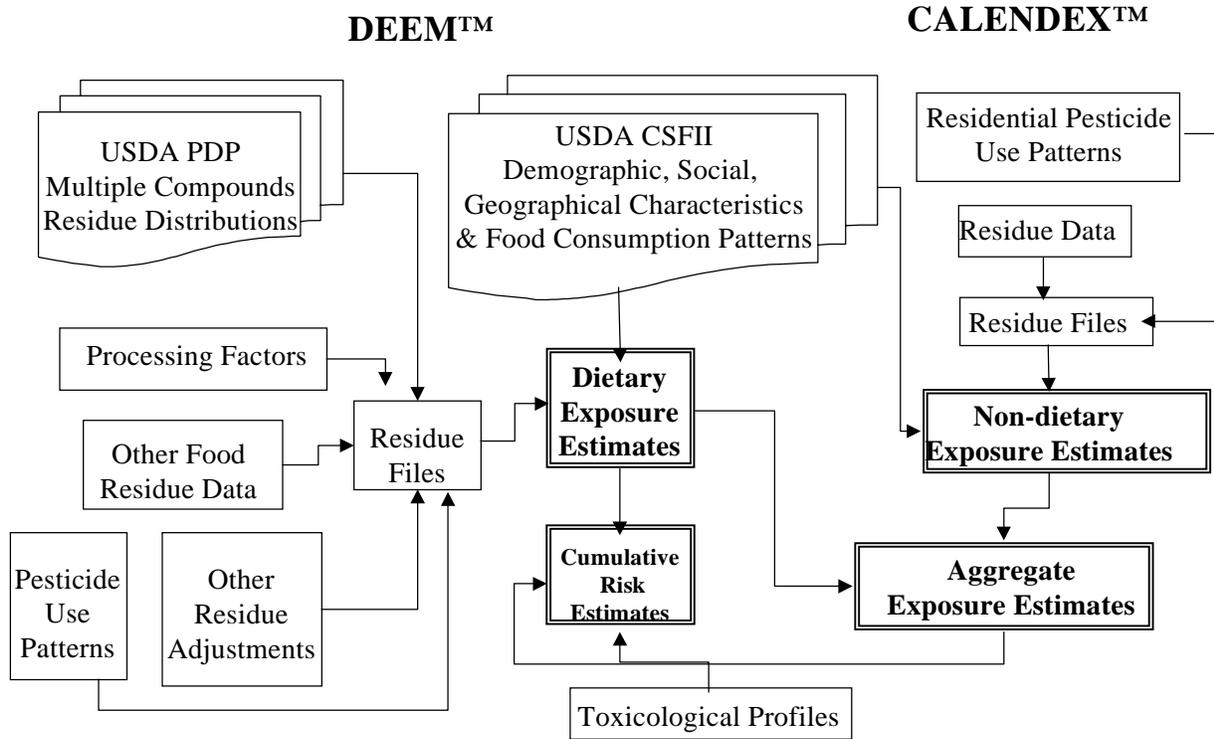


FIGURE 2
DEFAULT OUTPUT OF THE DEEM™ CHRONIC ANALYSIS MODULE
Exposures Compared to the RfD and NOEL

Novigen	Ver. 7.02
DEEM Chronic analysis for TEST CHEMICAL	(1994-96 data)
Residue file name: C:\My Documents\sample outputs\chrntest.RS7	
	Adjustment factor #2 used.
Analysis Date 01-16-2000/08:21:10	Residue file dated: 01-16-2000/08:17:17/1
Reference dose (RfD, Chronic) = .01 mg/kg bw/day	
NOEL (Chronic) = 1 mg/kg bw/day	
COMMENT 1: sample run	
=====	
Total exposure by population subgroup	

	Total Exposure

Population Subgroup	mg/kg body wt/day Margin of Exposure Percent of RfD
-----	-----
U.S. Population (total)	0.000305 3,274 3.1%
U.S. Population (spring season)	0.000298 3,353 3.0%
U.S. Population (summer season)	0.000294 3,401 2.9%
U.S. Population (autumn season)	0.000304 3,292 3.0%
U.S. Population (winter season)	0.000327 3,057 3.3%
Northeast region	0.000338 2,960 3.4%
Midwest region	0.000301 3,327 3.0%
Southern region	0.000263 3,802 2.6%
Western region	0.000349 2,866 3.5%
Hispanics	0.000335 2,988 3.3%
Non-hispanic whites	0.000315 3,174 3.2%
Non-hispanic blacks	0.000233 4,295 2.3%
Non-hisp/non-white/non-black	0.000284 3,518 2.8%
All infants (< 1 year)	0.001017 983 10.2%
Nursing infants	0.000751 1,332 7.5%
Non-nursing infants	0.001095 913 10.9%
Children 1-6 yrs	0.001033 968 10.3%
Children 7-12 yrs	0.000327 3,054 3.3%
Females 13-19 (not preg or nursing)	0.000131 7,643 1.3%
Females 20+ (not preg or nursing)	0.000233 4,301 2.3%
Females 13-50 yrs	0.000192 5,198 1.9%
Females 13+ (preg/not nursing)	0.000213 4,696 2.1%
Females 13+ (nursing)	0.000271 3,688 2.7%
Males 13-19 yrs	0.000129 7,764 1.3%
Males 20+ yrs	0.000196 5,104 2.0%
Seniors 55+	0.000278 3,597 2.8%

FIGURE 3
DEFAULT OUTPUT OF THE DEEM™ CHRONIC ANALYSIS MODULE
Exposures Compared to the Q₁*

```

Novigen
DEEM Chronic analysis for TEST CHEMICAL
Residue file name: C:\My Documents\sample outputs\chrntest.RS7
Ver. 7.02
(1994-96 data)
Adjustment factor #2 used.
Analysis Date 01-16-2000/08:19:21 Residue file dated: 01-16-2000/08:17:17/1
Q* = 0.1
COMMENT 1: sample run
=====
Total exposure by population subgroup
-----

```

Population Subgroup	Total Exposure	
	mg/kg body wt/day	Lifetime risk (Q*= .1)
U.S. Population (total)	0.000305	3.05E-05
U.S. Population (spring season)	0.000298	2.98E-05
U.S. Population (summer season)	0.000294	2.94E-05
U.S. Population (autumn season)	0.000304	3.04E-05
U.S. Population (winter season)	0.000327	3.27E-05
Northeast region	0.000338	3.38E-05
Midwest region	0.000301	3.01E-05
Southern region	0.000263	2.63E-05
Western region	0.000349	3.49E-05
Hispanics	0.000335	3.35E-05
Non-hispanic whites	0.000315	3.15E-05
Non-hispanic blacks	0.000233	2.33E-05
Non-hisp/non-white/non-black	0.000284	2.84E-05
All infants (< 1 year)	0.001017	
Nursing infants	0.000751	
Non-nursing infants	0.001095	
Children 1-6 yrs	0.001033	
Children 7-12 yrs	0.000327	
Females 13-19 (not preg or nursing)	0.000131	
Females 20+ (not preg or nursing)	0.000233	
Females 13-50 yrs	0.000192	
Females 13+ (preg/not nursing)	0.000213	
Females 13+ (nursing)	0.000271	
Males 13-19 yrs	0.000129	
Males 20+ yrs	0.000196	
Seniors 55+	0.000278	

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FIGURE 4
DEEM™ CHRONIC MODULE - COMPLETE COMMODITY CONTRIBUTION ANALYSIS
(ALL INFANTS SUBPOPULATION)

Novigen				Ver. 7.02		
DEEM Chronic analysis for TEST CHEMICAL				(1994-96 data)		
Residue file name: C:\My Documents\sample outputs\chrntest.RS7				Adjustment factor #2 used.		
Analysis Date 01-16-2000/08:21:16		Residue file dated: 01-16-2000/08:17:17/1				
Reference dose (RfD, Chronic) = .01 mg/kg bw/day						
NOEL (Chronic) = 1 mg/kg bw/day						
COMMENT 1: sample run						
=====						
Complete commodity contribution analysis for						
All infants (< 1 year)						

Crop Group = (0) Other						
Exposure Analysis						

Food name	Residue (ppm)	Adjustment Factors		mg/kg body wt/day	Margin of Exposr 1/	Perc. of RfD
-----	-----	-----		-----	-----	-----
Grapes	0.500000	1.000	0.400	0.0000000	>1000000	0.0%
Grapes-raisins	0.500000	4.300	0.400	0.0000044	229,302	0.0%
Grapes-juice	0.500000	1.200	0.400	0.0000944	10,596	0.9%
Bananas	0.500000	1.000	1.000	0.0005991	1,669	6.0%
Bananas-dried	0.500000	3.900	1.000	0.0001370	7,299	1.4%
Grapes-leaves	0.500000	1.000	0.400	no exposure		
Grapes-wine and sherry	0.500000	1.000	0.400	0.0000000	>1000000	0.0%
Bananas-juice	0.500000	1.000	1.000	0.0000232	43,036	0.2%
Grapes-juice-concentrate	0.500000	3.600	0.400	0.0001216	8,225	1.2%
Crop group subtotal				0.0009797	1,021	9.8%
Crop Group = (10) Citrus Fruits						
Exposure Analysis						

Food name	Residue (ppm)	Adjustment Factors		mg/kg body wt/day	Margin of Exposr 1/	Perc. of RfD
-----	-----	-----		-----	-----	-----
Grapefruit-peeled fruit	0.040000	1.000	0.200	no exposure		
Grapefruit-juice	0.040000	2.100	0.200	0.0000006	>1000000	0.0%
Grapefruit-juice-concentr	0.040000	8.260	0.200	no exposure		
Grapefruit peel	0.040000	1.000	0.200	no exposure		
Crop group subtotal				0.0000006	>1000000	0.0%
Crop Group = (11) Pome Fruits						
Exposure Analysis						

Food name	Residue (ppm)	Adjustment Factors		mg/kg body wt/day	Margin of Exposr 1/	Perc. of RfD
-----	-----	-----		-----	-----	-----
Apples	0.010000	1.000	0.500	0.0000099	100,805	0.1%
Apples-dried	0.010000	8.000	0.500	0.0000006	>1000000	0.0%
Apples-juice/cider	0.010000	1.300	0.500	0.0000098	102,088	0.1%
Apples-juice-concentrate	0.010000	3.900	0.500	0.0000162	61,905	0.2%
Crop group subtotal				0.0000365	27,383	0.4%
Population subgroup total				0.0010169	983	10.2%

1. Margin of Exposure = NOEL / Dietary Exposure						

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FIGURE 5
DEEM™ CHRONIC MODULE - CRITICAL COMMODITY CONTRIBUTION ANALYSIS
(ALL INFANTS SUBPOPULATION)

Novigen Ver. 7.02
 DEEM Chronic analysis for TEST CHEMICAL (1994-96 data)
 Residue file name: C:\My Documents\sample outputs\chrntest.RS7
Adjustment factor #2 used.
 Analysis Date 01-16-2000/08:21:16 Residue file dated: 01-16-2000/08:17:17/1
 NOEL (Chronic) = 1 mg/kg bw/day
 COMMENT 1: sample run

=====
 Critical Commodity Contribution Analysis for
 All infants (< 1 year)

Total Exposure = .0010169 mg/kg bw/day

Crop groups with total exposure contribution > 5%
 Foods/Foodforms with exposure contribution > 1%

Crop group	mg/kg	% of Total	Percent	Margin
Food	body wt/day	Exposure	of NOEL	of Exposr
Foodform				

Crop Group = (0) Other				
Grapes-juice	0.0000944	9.28%	0.0%	10,596
Bananas	0.0005991	58.92%	0.1%	1,669
Bananas-dried	0.0001370	13.47%	0.0%	7,299
Bananas-juice	0.0000232	2.29%	0.0%	43,036
Grapes-juice-concentrate	0.0001216	11.96%	0.0%	8,225

Total for crop group	0.0009797	96.35%	0.1%	1,021

Crop Group = (11) Pome Fruits				
Apples-juice-concentrate	0.0000162	1.59%	0.0%	61,905

Total for crop group	0.0000365	3.59%	0.0%	27,383

Total for crop groups listed above:	0.0010163	99.94%	0.1%	984

1. Margin of Exposure = NOEL / Dietary Exposure

FIGURE 6
DEEM™ CHRONIC MODULE - RESIDUE FILE SUMMARY

Novigen Ver. 7.02
 DEEM Chronic analysis for TEST CHEMICAL 1994-96 data
 Residue file: C:\My Documents\sample outputs\chrntest.RS7 Adjust. #2 used
 Analysis Date 01-16-2000 Residue file dated: 01-16-2000/08:17:17/1
 Reference dose (RfD) = 0.01 (NOEL) = 1 mg/kg bw/day
 Comment: sample run

Food Code	Crop Grp	Food Name	RESIDUE (ppm)	Adj. Factors #1	Adj. Factors #2	Comment
13	0	Grapes	0.500000	1.000	0.400	
14	0	Grapes-raisins	0.500000	4.300	0.400	
15	0	Grapes-juice	0.500000	1.200	0.400	
22	10	Grapefruit-peeled fruit	0.040000	1.000	0.200	
23	10	Grapefruit-juice	0.040000	2.100	0.200	
52	11	Apples	0.010000	1.000	0.500	
53	11	Apples-dried	0.010000	8.000	0.500	
54	11	Apples-juice/cider	0.010000	1.300	0.500	
72	0	Bananas	0.500000	1.000	1.000	
73	0	Bananas-dried	0.500000	3.900	1.000	
195	0	Grapes-leaves	0.500000	1.000	0.400	
315	0	Grapes-wine and sherry	0.500000	1.000	0.400	
377	11	Apples-juice-concentrate	0.010000	3.900	0.500	
378	0	Bananas-juice	0.500000	1.000	1.000	
392	0	Grapes-juice-concentrate	0.500000	3.600	0.400	
441	10	Grapefruit-juice-concentrate	0.040000	8.260	0.200	
448	10	Grapefruit peel	0.040000	1.000	0.200	

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**FIGURE 7
DEFAULT OUTPUT OF THE DEEM™ ACUTE MODULE**

```

Novigen Sciences, Incorporated                               Ver. 7.02
DEEM ACUTE analysis for NOVICHEM                         (1994-96 data)
Residue file: acmctest.RS7                               Adjustment factor #2 NOT used.
Analysis Date: 01-16-2000/21:01:54   Residue file dated: 10-06-1999/11:17:05/1
NOEL (Acute) = 0.250000 mg/kg body-wt/day
Daily totals for food and foodform consumption used.
MC iterations = 100      MC list in residue file      MC seed = 1
Run Comment: TEST SERIES FOR DEEM ACUTE MODULES
=====
  
```

All infants -----	Daily Exposure Analysis 1/ (mg/kg body-weight/day)	
	per Capita	per User

Mean	0.000066	0.000086
Standard Deviation	0.000168	0.000187
Margin of Exposure 2/	3,783	2,890

Percent of Person-Days that are User-Days = 76.39%

Estimated percentile of user-days falling below calculated exposure
in mg/kg body-wt/day with Margin of Exposure (MOE)

Percentile	Exposure	MOE	Percentile	Exposure	MOE

10.00	0.000000	797,317	90.00	0.000192	1,298
20.00	0.000003	74,684	95.00	0.000390	641
30.00	0.000013	19,789	97.50	0.000573	436
40.00	0.000033	7,559	99.00	0.000872	286
50.00	0.000049	5,142	99.50	0.001003	249
60.00	0.000061	4,119	99.75	0.001027	243
70.00	0.000073	3,440	99.90	0.001068	234
80.00	0.000092	2,703			

Estimated percentile of per-capita days falling below calculated exposure
in mg/kg body-wt/day with Margin of Exposure (MOE)

Percentile	Exposure	MOE	Percentile	Exposure	MOE

10.00	0.000000	>1,000,000	90.00	0.000139	1,792
20.00	0.000000	>1,000,000	95.00	0.000324	772
30.00	0.000000	>1,000,000	97.50	0.000453	551
40.00	0.000005	49,400	99.00	0.000686	364
50.00	0.000023	11,014	99.50	0.000888	281
60.00	0.000043	5,831	99.75	0.001010	247
70.00	0.000061	4,075	99.90	0.001056	236
80.00	0.000078	3,186			

1/ Analysis based on all two-day participant records in CSFII 1994-96 survey.
2/ Margin of Exposure = NOEL/ Dietary Exposure.

**FIGURE 8
DEEM™ ACUTE MODULE PLOT FILE**

```

Novigen Sciences, Incorporated                               Ver. 7.02
DEEM ACUTE PLOT FILE for NOVICHEM                         (1994-96 data)
Residue file: acmctest.RS7                               Adjustment factor #2 NOT used.
Analysis Date: 01-16-2000/21:01:54   Residue file dated: 10-06-1999/11:17:05/1
NOEL (Acute) = 0.250000 mg/kg body-wt/day
Daily totals for food and foodform consumption used.
MC iterations = 100      MC list in residue file      MC seed = 1
Run Comment: TEST SERIES FOR DEEM ACUTE MODULES

```

```

=====
Number of populations included in this file: 1
Populations:

```

1 = All infants

```

Pops: ,      1,
Means: ,      0.000086,
PCTLS
90.00,      0.000000,
80.00,      0.000003,
.
.
2.50,      0.000573,
1.00,      0.000872,
0.50,      0.001003,
0.25,      0.001027,
0.10,      0.001068,
0.00,      0.010247,

```

```

All infants
Total person days (weighted & unweighted) =,      7544592,      718
Total user days (weighted & unweighted) =,      5763691,      521
Bin totals based on 100 iterations.

```

BIN TOTALS:

```

Users , -----Exposure Bin-----
, Low Bound, High bound
47151610, 0.0 , 0.00000000
44419194, 0.00000000, 0.00000133
19277563, 0.00000133, 0.00000266
8509380, 0.00000266, 0.00000398
5353774, 0.00000398, 0.00000531
.
.
9494, 0.00511968, 0.00517087
43516, 0.00554388, 0.00559932
6376, 0.00565531, 0.00571186
6490, 0.00650063, 0.00656564
11713, 0.00669761, 0.00676458
24969, 0.00747231, 0.00754703
5727, 0.00841998, 0.00850418
13959, 0.00987309, 0.00997183
9591, 0.01017226, 0.01024721

```

FIGURE 9
DEEM™ ACUTE MODULE CRITICAL EXPOSRE CONTRIBUTION ANALYSIS

```

Novigen Sciences, Incorporated
DEEM Acute Critical Exposure Contribution Analysis (Ver 7.02)
CSFII 1994-96
Residue file = C:\My Documents\sample outputs\acmctest.RS7
Acute report = C:\My Documents\sample outputs\acmctest.AC7
Date and time of analysis: 01-16-2000 21:00:48
Minimum exposure contribution = 1%
Monte Carlo Iterations = 100 Seed = 1
Exposures divided by body weight
Subpopulations:
  1 All infants

All infants
Low percentile for CEC records: 95 Exposure (mg/day) = 0.000390
High percentile for CEC records: 100 Exposure (mg/day) = 0.010247
Number of actual records in this interval: 3191

Critical foods/foodforms for this population (as derived from these records):
  N=number of appearances in all records (including duplicates)
  %=percent of total exposure for all records (including duplicates)
Food FF N % Name
398, 16, 2780, 67.11, Milk-based water-Pasteurized
65, 31, 99, 7.89, Peaches-Canned: NFS
398, 31, 303, 5.42, Milk-based water-Canned: NFS
320, 16, 2775, 2.86, Milk sugar (lactose)-Pasteurized
318, 16, 2775, 2.27, Milk-nonfat solids-Pasteurized
319, 16, 2768, 1.69, Milk-fat solids-Pasteurized
54, 11, 79, 1.49, Apples-juice/cider-Uncooked
320, 31, 436, 1.46, Milk sugar (lactose)-Canned: NFS
159, 34, 622, 1.15, Tomatoes-whole-Canned: Boiled
65, 11, 11, 1.14, Peaches-Uncooked
.
.
53, 14, 10, 0.00, Apples-dried-Boiled
65, 14, 6, 0.00, Peaches-Boiled
53, 18, 1, 0.00, Apples-dried-Dried
320, 12, 3, 0.00, Milk sugar (lactose)-Cooked: NFS
318, 12, 3, 0.00, Milk-nonfat solids-Cooked: NFS
52, 31, 5, 0.00, Apples-Canned: NFS
159, 33, 1, 0.00, Tomatoes-whole-Canned: Baked
17, 14, 84, 0.00, Strawberries-Boiled
52, 14, 4, 0.00, Apples-Boiled
398, 12, 100, 0.00, Milk-based water-Cooked: NFS
392, 31, 2, 0.00, Grapes-juice-concentrate-Canned: NFS
398, 32, 97, 0.00, Milk-based water-Canned: Cooked
398, 45, 100, 0.00, Milk-based water-Frozen: Fried
14, 14, 7, 0.00, Grapes-raisins-Boiled

```

FIGURE 9 (CONT'D)

Number of printed records = 500

Number of records represented = 1791

(nf = number of foods/ff reported for this daily exposure amount (exceeding minimum contribution)

(nx = number of times this exposure amount was computed for the same person on the same day.)

Demographic data for each record:

Demographic data for each record:

Exposure contribution data by food/ff consumed (nf lines):

Pid	day	sex	age	bw-kg	nf	nx	Tot expos	samplwt	Line	food	ff	amt(g)	residue	adj#1	adj#2	Cntrbtn	Percent
63	2	M	7M	8.18	1	1	0.010247	9591	1	65	31	139.4	0.6	1	1	0.010223	99.76
71	1	F	9M	9.55	1	1	0.009938	13959	1	65	11	157	0.6	1	1	0.009869	99.3
12	1	M	5M	6.82	1	1	0.008473	5727	1	65	31	96.2	0.6	1	1	0.008466	99.91
54	1	M	7M	7.73	1	3	0.007485	8323	1	65	31	96.4	0.6	1	1	0.007485	100
27	2	M	8M	7.27	1	1	0.006755	11713	1	65	31	81.6	0.6	1	1	0.006732	99.65
68	1	M	8M	10	1	1	0.006539	6490	1	65	31	108.8	0.6	1	1	0.006528	99.83
32	2	F	10M	8.64	1	1	0.00569	6376	1	65	31	81.6	0.6	1	1	0.005669	99.63
55	1	M	9M	10.45	1	1	0.005567	21758	1	65	31	96.4	0.6	1	1	0.005533	99.39
55	1	M	9M	10.45	1	1	0.00557	21758	1	65	31	96.4	0.6	1	1	0.00553	99.4
67	2	F	11M	9.55	2	1	0.00515	9494	1	65	11	78.5	0.6	1	1	0.00493	95.73
67	2	F	11M	9.55	2	1	0.00515	9494	2	398	16	348.9	0.005	1	1	0.00018	3.55
15	1	M	6M	7.27	1	1	0.00499	8834	1	65	31	60.4	0.6	1	1	0.00498	99.94
29	2	M	6M	6.82	1	1	0.00483	4161	1	65	31	54.4	0.6	1	1	0.00479	99.19
34	1	M	7M	6.82	1	1	0.00423	2978	1	65	31	48	0.6	1	1	0.00422	99.97
22	2	M	8M	8.18	1	1	0.00416	4532	1	54	11	542.3	0.06274	1	1	0.00416	99.92

etc.

**FIGURE 10
DEEM™ RESIDUE FILE SUMMARY**

Novigen Sciences, Incorporated Ver. 7.02
 DEEM Acute analysis for NOVICHEM
 Residue file name: C:\My Documents\sample outputs\acmctest.RS7
 Analysis Date 01-16-2000 Residue file dated: 10-06-1999/11:17:05/1
 Reference dose (NOEL) = 0.25 mg/kg bw/day
 Comment: TEST SERIES FOR DEEM ACUTE MODULES

 RDL indices and parameters for Monte Carlo Analysis:

Index #	Dist Code	Parameter #1	Param #2	Param #3	Comment
1	6	Apple.rdf			
2	6	Celery.rdf			
3	6	Grape.rdf			
4	6	Lettuce.rdf			
5	6	Peach.rdf			
6	6	Straw.rdf			
7	6	Tomato.rdf			
8	5	0.004	0.01	0.5	lognormal(0.004,0.01), max:0.5
9	0	0			

Food Code	Crop Grp	Food Name	Def Res (ppm)	Adj.Factors #1	Adj.Factors #2	-RDL I#1	Indices Ratio#1	and I#2	Ratios- Ratio#2
13	0	Grapes							
			0.025000	1.000	1.000	3	1.0000		
14	0	Grapes-raisins							
			0.003000	1.000	1.000	3	1.0000		
15	0	Grapes-juice							
			0.003000	0.060	1.000	3	1.0000		
17	0	Strawberries							
			0.014000	1.000	1.000	6	1.0000		
52	11	Apples							
		11-Uncooked							
			0.020000	0.200	1.000	1	1.0000		
		12-Cooked: NFS							
			0.020000	0.050	1.000	1	1.0000		
		13-Baked							
			0.020000	0.050	1.000	1	1.0000		
		14-Boiled							
			0.020000	0.050	1.000	1	1.0000		
		15-Fried							
			0.020000	0.050	1.000	1	1.0000		
		18-Dried							
			0.020000	0.200	1.000	1	1.0000		
		31-Canned: NFS							
			0.020000	0.050	1.000	1	1.0000		
		32-Canned: Cooked							
			0.020000	0.050	1.000	1	1.0000		
		33-Canned: Baked							
			0.020000	0.050	1.000	1	1.0000		
		34-Canned: Boiled							
			0.020000	0.050	1.000	1	1.0000		
		42-Frozen: Cooked							
			0.020000	0.050	1.000	1	1.0000		

FIGURE 10 (CONT'D)

Food Code	Crop Grp	Food Name	Def Res (ppm)	Adj.Factors #1	Adj.Factors #2	-RDL I#1	Indices Ratio#1	Indices I#2	Ratios Ratio#2
53	11	Apples-dried	0.020000	8.000	1.000	1	1.0000		
54	11	Apples-juice/cider	0.004000	1.000	1.000	8	0.1000	9	0.9000
64	12	Nectarines	0.600000	1.000	1.000	5	1.0000		
65	12	Peaches	0.060000	1.000	1.000	5	1.0000		
66	12	Peaches-dried	0.060000	7.000	1.000	5	1.0000		
159	8	Tomatoes-whole	0.011000	1.000	1.000	7	1.0000		
160	8	Tomatoes-juice	0.004000	0.020	1.000	7	1.0000		
161	8	Tomatoes-puree	0.004000	0.020	1.000	7	1.0000		
162	8	Tomatoes-paste	0.004000	0.500	1.000	7	1.0000		
163	8	Tomatoes-catsup	0.004000	0.020	1.000	7	1.0000		
166	4B	Celery	0.070000	1.000	1.000	2	1.0000		
176	4A	Lettuce-leafy varieties	0.100000	1.000	1.000	4	1.0000		
182	4A	Lettuce-unspecified	0.100000	1.000	1.000	4	1.0000		
192	4A	Lettuce-head varieties	0.100000	1.000	1.000	4	1.0000		
290	O	Cottonseed-oil	0.005000	0.010	1.000				
291	O	Cottonseed-meal	0.005000	0.020	1.000				
315	O	Grapes-wine and sherry	0.003000	1.000	1.000	3	1.0000		
318	D	Milk-nonfat solids	0.005000	1.000	1.000				
319	D	Milk-fat solids	0.005000	1.000	1.000				
320	D	Milk sugar (lactose)	0.005000	1.000	1.000				
377	11	Apples-juice-concentrate	0.004000	1.000	1.000	8	0.1000	9	0.9000
384	4B	Celery juice	0.012000	1.000	1.000	2	1.0000		
392	O	Grapes-juice-concentrate	0.003000	0.180	1.000	3	1.0000		
398	D	Milk-based water	0.005000	1.000	1.000				
402	12	Peaches-juice	0.040000	1.000	1.000	5	1.0000		
416	O	Strawberries-juice	0.007000	1.000	1.000	6	1.0000		
423	8	Tomatoes-dried	0.004000	14.300	1.000	7	1.0000		

Appendix 1

Listing of Foods, Food Forms, and Crop Groups

APPENDIX 1
LISTING OF FOODS, FOOD FORMS, AND CROP GROUPS

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
1	13A	Blackberries	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
2	13A	Boysenberries	1.00		
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
3	13A	Dewberries	1.00		
4	13A	Loganberries	1.00		
5	13A	Raspberries	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled			X
		41 Frozen: NFS		X	X
6	13A	Youngberries	1.00		
7	13B	Blueberries	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
8	0	Cranberries	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
		42 Frozen: Cooked		X	X
9	0	Cranberries-juice	1.10		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
10	13B	Currants	1.00		
		11 Uncooked		X	X
11	13B	Elderberries	1.00		
12	13B	Gooseberries	1.00		
13	0	Grapes	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
14	0	41 Frozen: NFS Grapes-raisins	4.30	X	X
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		18 Dried		X	X
		42 Frozen: Cooked		X	X
15	0	Grapes-juice	1.20		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	
16	13B	Huckleberries	1.00		
17	0	Strawberries	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
18	0	Juneberry	1.00		
19	0	Mulberries	1.00		
		11 Uncooked		X	X
20	10	Citrus citron	1.00		
		13 Baked		X	X
		14 Boiled		X	X
22	10	Grapefruit-peeled fruit	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	
		31 Canned: NFS		X	X
23	10	Grapefruit-juice	2.10		
		11 Uncooked		X	X
		31 Canned: NFS		X	X
24	10	Kumquats	1.00		
26	10	Lemons-peeled fruit	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
27	10	Lemons-peel	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
28	10	Lemons-juice	2.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
30	10	Limes-peeled fruit	1.00		
		11 Uncooked		X	X
31	10	Limes-peel	1.00		
		13 Baked		X	X
		14 Boiled		X	X
32	10	Limes-juice	2.00		
		11 Uncooked		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
33	10	Oranges-juice-concentrate	6.70		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	
		14 Boiled		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
34	10	Oranges-peeled fruit	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
35	10	Oranges-peel	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
36	10	Oranges-juice	1.80		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
37	10	Tangelos	1.00		
38	10	Tangerines	1.00		
		11 Uncooked		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	
39	10	Tangerines-juice	2.30		
		11 Uncooked			X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	
40	14	Almonds	1.00		
		11 Uncooked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		18 Dried		X	X
		41 Frozen: NFS		X	X
41	14	Brazil nuts	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
		16 Pasteurized		X	X
42	14	Cashews	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
43	14	Chestnuts	1.00		
		12 Cooked: NFS		X	
		13 Baked			X
44	14	Filberts (hazelnuts)	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
45	14	Hickory nuts	1.00		
		11 Uncooked		X	
46	14	Macadamia nuts (bush nuts)	1.00		
		13 Baked		X	X
47	14	Pecans	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
48	14	Walnuts	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
49	14	Butter nuts	1.00		
50	0	Pistachio nuts	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
51	14	Beechnuts	1.00		
52	11	Apples	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
53	11	Apples-dried	8.00		
		13 Baked		X	X
		14 Boiled		X	X
		18 Dried		X	X
		42 Frozen: Cooked		X	
54	11	Apples-juice/cider	1.30		
		11 Uncooked		X	X
		12 Cooked: NFS			X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	
55	11	Crabapples	1.00		
		31 Canned: NFS			X
56	11	Pears	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	
		14 Boiled		X	X
		31 Canned: NFS		X	X
57	11	Pears-dried	6.25		
		13 Baked		X	X
		14 Boiled		X	
		18 Dried		X	X
58	11	Quinces	1.00		
59	12	Apricots	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
60	12	Apricots-dried	6.00		
		13 Baked		X	X
		14 Boiled		X	X
		18 Dried		X	X
61	12	Cherries	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		33 Canned: Baked		X	X
		41 Frozen: NFS		X	X
62	12	Cherries-dried	4.00		
63	12	Cherries-juice	1.50		
		13 Baked		X	
		14 Boiled		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	
64	12	Nectarines	1.00		
		11 Uncooked		X	X
65	12	Peaches	1.00		
		11 Uncooked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
66	12	Peaches-dried	7.00		
		14 Boiled		X	
		18 Dried		X	X
67	12	Plums (damsons)	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	
68	12	Plums-prunes (dried)	5.00		
		13 Baked		X	X
		14 Boiled		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
69	12	Plums/prune-juice	1.40		
		11 Uncooked		X	X
		31 Canned: NFS		X	X
70	0	Avocados	1.00		
		11 Uncooked		X	X
72	0	Bananas	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
73	0	Bananas-dried	3.90		
		13 Baked		X	X
		15 Fried		X	X
		18 Dried		X	X
		32 Canned: Cooked			X
74	0	Coconut	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
75	0	Coconut-dried (copra)	2.10		
		12 Cooked: NFS			X
		13 Baked		X	X
		14 Boiled		X	X
		18 Dried		X	X
76	0	Coconut-water	1.00		
		11 Uncooked		X	
		14 Boiled		X	X
77	0	Dates	1.00		
		13 Baked		X	X
		14 Boiled		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
78	0	18 Dried Figs	1.00	X	X
		11 Uncooked		X	X
		13 Baked		X	X
79	0	Guava	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
80	0	Mangoes	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
81	11	Loquats	1.00		
82	0	Olives	1.00		
		60 Canned: Cured		X	X
84	0	Papayas-pulp	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
85	0	Papayas-dried	1.80		
		18 Dried		X	
86	0	Papayas-juice	1.50		
		11 Uncooked		X	X
87	0	Pawpaws	1.00		
88	0	Persimmons	1.00		
		11 Uncooked		X	X
89	0	Pineapples-peeled fruit	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		33 Canned: Baked		X	X
		41 Frozen: NFS		X	X
90	0	Pineapples-dried	5.00		
		18 Dried		X	X
91	0	Pineapples-juice	1.70		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
		42 Frozen: Cooked		X	X
92	0	Passion fruit (granadilla)	1.00		
		31 Canned: NFS		X	X
93	0	Pomegranates	1.00		
		11 Uncooked		X	X
94	0	Plantains-ripe	1.00		
		11 Uncooked		X	X
		14 Boiled		X	X
		15 Fried		X	X
95	0	Lychees (litchi)/fresh	1.00		
96	0	Lychee-dried	1.85		
97	0	Kiwi fruit	1.00		
		11 Uncooked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		31 Canned: NFS			X
98	O	Acerola	1.00		
99	O	Ginkgo nuts	1.00		
100	O	Maney (mammee apple)	1.00		
		11 Uncooked		X	
101	O	Pitanga (surinam cherry)	1.00		
102	O	Soursop (annona muricata)	1.00		
		11 Uncooked		X	
103	O	Sugar apples (sweetsop)	1.00		
104	O	Bread fruit	1.00		
		14 Boiled			X
105	O	Bread nuts	1.00		
106	O	Carambola (starfruit)	1.00		
		11 Uncooked			X
107	O	Cherimoya	1.00		
108	O	Longan fruit	1.00		
109	O	Genip (spanish lime)	1.00		
110	O	Chocolate-cocoa butter	1.00		
		12 Cooked: NFS		X	X
111	O	Chocolate	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		41 Frozen: NFS		X	X
112	O	Coffee	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
113	O	Tea	1.00		
		12 Cooked: NFS		X	X
114	1AB	Chicory	1.00		
115	19B	Anise	1.00		
		14 Boiled		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
116	19A	Basil	1.00		
		13 Baked		X	X
		14 Boiled		X	X
117	19B	Caraway	1.00		
		13 Baked		X	X
118	19B	Cassia	1.00		
119	19B	Cinnamon	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
120	19B	Clove	1.00		
		12 Cooked: NFS		X	X
121	19B	Coriander	1.00		
		12 Cooked: NFS		X	X
122	19B	Cumin	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96	
		14 Boiled		X	X	
		42 Frozen: Cooked		X		52 Cured:
Cooked(smokd/pickl/saltd)			X	X		
123	19A	Dill	1.00			
		13 Baked			X	
		14 Boiled		X	X	
124	1CD	Ginger	1.00			
		11 Uncooked		X	X	
		12 Cooked: NFS		X	X	
		13 Baked		X	X	
		14 Boiled		X	X	
125	O	Hops	1.00			
		99 Alcohol/Fermented/Distilled		X	X	
126	1AB	Horseradish	1.00			
		12 Cooked: NFS		X	X	
		14 Boiled		X	X	
		34 Canned: Boiled		X	X	
		51 Cured: NFS (smoked/pickled/saltd)		X	X	
127	19A	Rosemary	1.00			
		12 Cooked: NFS		X	X	
128	19A	Marjoram	1.00			
		12 Cooked: NFS		X	X	
		18 Dried		X		
129	19A	Oregano	1.00			
		11 Uncooked		X	X	
		12 Cooked: NFS		X	X	
		42 Frozen: Cooked		X		
130	19B	Mustard seed	1.00			
		11 Uncooked		X	X	
		12 Cooked: NFS		X	X	
		42 Frozen: Cooked		X		
131	19B	Nutmeg	1.00			
		12 Cooked: NFS		X	X	
132	19B	Mace	1.00			
		13 Baked		X	X	
133	19A	Sage	1.00			
		12 Cooked: NFS		X	X	
134	19A	Savory	1.00			
135	19A	Bay	1.00			
		12 Cooked: NFS		X	X	
136	19A	Thyme	1.00			
		12 Cooked: NFS		X	X	
137	1CD	Turmeric	1.00			
		12 Cooked: NFS		X	X	
138	19B	Allspice	1.00			
		12 Cooked: NFS		X	X	
139	8	Paprika	1.00			
		12 Cooked: NFS		X	X	
140	19B	Poppy	1.00			
		12 Cooked: NFS		X	X	
141	9A	Melons-cantaloupes-juice	1.00			
142	9A	Melons-cantaloupes-pulp	1.00			

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		11 Uncooked		X	X
143	9A	Casabas	1.00		
		11 Uncooked		X	X
144	9A	Crenshaws	1.00		
145	9A	Melons-honeydew	1.00		
		11 Uncooked		X	X
146	9A	Melons-persian	1.00		
147	9A	Watermelon	1.00		
		11 Uncooked		X	X
148	9B	Cucumbers	1.00		
		11 Uncooked		X	X
		34 Canned: Boiled		X	X
		60 Canned: Cured		X	X
149	9B	Pumpkin	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
150	9B	Squash-summer	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	
151	9B	Squash-winter	1.00		
		11 Uncooked		X	
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
152	9B	Bitter melon	1.00		
		12 Cooked: NFS		X	X
153	O	Towelgourd	1.00		
154	8	Eggplant	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
155	8	Peppers-sweet (garden)	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
156	8	Peppers-chilli incl jalapeno	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		60 Canned: Cured		X	X
157	8	Peppers-other	1.00		
		11 Uncooked			X
158	8	Pimientos	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	
		31 Canned: NFS		X	X
		60 Canned: Cured		X	X
159	8	Tomatoes-whole	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
160	8	Tomatoes-juice	1.50		
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked			X
161	8	Tomatoes-puree	3.30		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
162	8	Tomatoes-paste	5.40		
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
163	8	Tomatoes-catsup	2.50		
		34 Canned: Boiled		X	X
164	8	Groundcherries	1.00		
165	2	Beets-garden-tops(greens)	1.00		
		11 Uncooked			X
		14 Boiled		X	X
166	4B	Celery	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
167	4A	Chicory(french/belgian endive)	1.00		
		11 Uncooked		X	X
168	5A	Broccoli	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		32 Canned: Cooked		X	X
		42 Frozen: Cooked		X	X
		44 Frozen: Boiled		X	X
169	5A	Brussels sprouts	1.00		
		14 Boiled		X	X
		42 Frozen: Cooked			X
170	5A	Cabbage-green and red	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
171	5A	Cauliflower	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		15 Fried		X	X
		42 Frozen: Cooked		X	X
172	5B	Collards	1.00		
		14 Boiled		X	X
		32 Canned: Cooked			X
		42 Frozen: Cooked			X
174	5B	Kale	1.00		
		12 Cooked: NFS			X
		14 Boiled		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		32 Canned: Cooked			X
175	5A	Kohlrabi	1.00		
		14 Boiled		X	
176	4A	Lettuce-leafy varieties	1.00		
		11 Uncooked		X	X
177	4A	Dandelion-greens	1.00		
		11 Uncooked		X	X
178	4A	Endive-curley and escarole	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
179	19B	Fennel	1.00		
		12 Cooked: NFS		X	X
180	4A	Cress-garden/field	1.00		
		11 Uncooked		X	
		14 Boiled		X	
181	O	Artichokes-globe	1.00		
		14 Boiled		X	X
182	4A	Lettuce-unspecified	1.00		
		31 Canned: NFS		X	X
183	5B	Mustard greens	1.00		
		14 Boiled		X	X
184	4A	Parsley	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	
		34 Canned: Boiled		X	X
185	4B	Rhubarb	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	
		43 Frozen: Baked		X	X
186	4A	Spinach	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled			X
		42 Frozen: Cooked		X	X
		44 Frozen: Boiled			X
187	4A	Swiss chard	1.00		
		11 Uncooked		X	
		14 Boiled		X	X
188	2	Turnips-tops	1.00		
		14 Boiled		X	X
		32 Canned: Cooked			X
		44 Frozen: Boiled			X
189	O	Watercress	1.00		
		11 Uncooked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		14 Boiled		X	
		31 Canned: NFS		X	X
190	2	Taro-greens	1.00		
		14 Boiled			X
191	4A	Cress-upland	1.00		
192	4A	Lettuce-head varieties	1.00		
		11 Uncooked		X	X
193	O	Lambsquarter	1.00		
		12 Cooked: NFS			X
194	O	Cactus pads (nopal)	1.00		
195	O	Grapes-leaves	1.00		
		14 Boiled		X	X
196	O	Oriental vegetables/leafy	1.00		
197	1AB	Beets-garden-roots	1.00		
		11 Uncooked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
198	1AB	Carrots	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		44 Frozen: Boiled		X	X
199	1AB	Celeriac	1.00		
200	19A	Chives	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		18 Dried		X	
201	1CD	Taro-root	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
202	3	Garlic	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
203	1CD	Artichokes-jerusalem	1.00		
		11 Uncooked			X
204	3	Leeks	1.00		
		11 Uncooked			X
		12 Cooked: NFS		X	X
205	3	Onions-dry-bulb (cipollini)	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		43 Frozen: Baked			X
		44 Frozen: Boiled		X	X
		60 Canned: Cured		X	X
206	3	Onions-dehydrated or dried	9.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
207	1C	Potatoes/white-whole	1.00		
		11 Uncooked		X	
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
208	1C	Potatoes/white-unspecified	1.00		
		31 Canned: NFS			X
209	1C	Potatoes/white-peeled	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		43 Frozen: Baked		X	X
		45 Frozen: Fried		X	X
210	1C	Potatoes/white-dry	6.50		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
211	1C	42 Frozen: Cooked Potatoes/white-peel only	1.00	X	X
		13 Baked		X	X
		15 Fried		X	X
212	1AB	Radishes-roots	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
213	2	Radishes-tops	1.00		
214	1AB	Rutabagas-roots	1.00		
215	2	Rutabagas-tops	1.00		
		12 Cooked: NFS		X	X
216	1AB	Salsify(oyster plant)	1.00		
217	3	Shallots	1.00		
218	1CD	Sweet potatoes (incl yams)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	
219	1AB	Turnips-roots	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
220	1AB	Parsnips	1.00		
		14 Boiled		X	X
221	1CD	Yambean tuber (jicama)	1.00		
		11 Uncooked		X	X
222	1CD	Cassava (yuca blanca)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
224	1CD	Yautia (tannier)	1.00		
225	1AB	Parsley roots	1.00		
226	O	Water chestnuts	1.00		
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
227	6C	Beans-dry-great northern	1.00		
		32 Canned: Cooked			X
228	6C	Beans-dry-kidney	1.00		
		12 Cooked: NFS			X
		13 Baked		X	X
		14 Boiled		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
229	6C	42 Frozen: Cooked Beans-dry-lima	1.00	X	X
		14 Boiled		X	X
		32 Canned: Cooked		X	X
230	6C	Beans-dry-navy (pea)	1.00		
		32 Canned: Cooked		X	
		34 Canned: Boiled		X	X
231	6C	Beans-dry-other	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		34 Canned: Boiled		X	X
232	6C	Beans-dry-pinto	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		32 Canned: Cooked		X	X
		42 Frozen: Cooked		X	X
233	6B	Beans-succulent-lima	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		32 Canned: Cooked		X	X
		42 Frozen: Cooked		X	X
		44 Frozen: Boiled		X	X
234	6A	Beans-succulent-green	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		31 Canned: NFS			X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		44 Frozen: Boiled		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	
235	6A	Beans-succulent-other	1.00		
		34 Canned: Boiled		X	X
236	6A	Beans-succulent-yellow/wax	1.00		
		14 Boiled		X	X
		32 Canned: Cooked		X	X
		42 Frozen: Cooked			X
237	15	Corn/pop	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
238	15	Corn/sweet	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		32 Canned: Cooked		X	X

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		34 Canned: Boiled		X	X
		35 Canned: Fried		X	X
		42 Frozen: Cooked		X	X
240	6C	Peas (garden)-dry	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
241	6AB	Peas (garden)-green	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		44 Frozen: Boiled		X	X
		45 Frozen: Fried		X	X
243	6C	Lentils	1.00		
		14 Boiled		X	X
244	6C	Mung beans (sprouts)	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		15 Fried		X	X
245	0	Okra	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		15 Fried		X	X
		32 Canned: Cooked		X	X
		42 Frozen: Cooked		X	X
		44 Frozen: Boiled		X	X
247	0	Carob	1.00		
		13 Baked		X	X
248	0	Alfalfa sprouts	1.00		
		11 Uncooked		X	X
249	6C	Beans-dry-broadbeans	1.00		
		14 Boiled		X	X
250	6B	Beans-succulent-broadbeans	1.00		
251	6C	Beans-dry-pigeon beans	1.00		
252	0	Sesame seeds	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
		42 Frozen: Cooked		X	
253	6	Beans-unspecified	1.00		
254	0	Pinenuts	1.00		
		11 Uncooked		X	X
		14 Boiled		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
255	6A	Soybeans-sprouted seeds 14 Boiled	0.33	X	X
256	6C	Beans-dry-hyacinth	1.00		
257	6	Beans-succulent-hyacinth	1.00		
258	6C	Beans-dry-blackeye peas/cowpea 14 Boiled	1.00	X	X
259	6C	Beans-dry-garbanzo/chick pea 12 Cooked: NFS 14 Boiled 15 Fried 32 Canned: Cooked	1.00		X X X X
260	0	Asparagus 11 Uncooked 14 Boiled 32 Canned: Cooked 42 Frozen: Cooked	1.00	X X X	X X X X
261	0	Mushrooms 11 Uncooked 12 Cooked: NFS 13 Baked 14 Boiled 15 Fried 31 Canned: NFS 32 Canned: Cooked 33 Canned: Baked 34 Canned: Boiled 42 Frozen: Cooked	1.00	X X X X X X X X X X	X X X X X X X X X
262	3	Onions-green 11 Uncooked 12 Cooked: NFS 13 Baked 14 Boiled 15 Fried 31 Canned: NFS 32 Canned: Cooked	1.00	X X X X X X X	X X X X X X X
263	0	Poke greens 14 Boiled	1.00	X	X
264	0	Bamboo shoots 11 Uncooked 12 Cooked: NFS 14 Boiled	1.00	X X X	X X X
265	15	Barley 11 Uncooked 12 Cooked: NFS 13 Baked 14 Boiled 15 Fried 31 Canned: NFS 32 Canned: Cooked 34 Canned: Boiled 99 Alcohol/Fermented/Distilled	1.00	X X X X X X X X X X	X X X X X X X X X

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
266	15	Corn grain-endosperm	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		43 Frozen: Baked		X	X
		45 Frozen: Fried		X	X
		99 Alcohol/Fermented/Distilled		X	X
267	15	Corn grain-bran	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
268	15	Corn grain/sugar/hfcs	1.50		
		98 Refined		X	X
269	15	Oats	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
270	15	Rice-rough (brown)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		99 Alcohol/Fermented/Distilled		X	X
271	15	Rice-milled (white)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		99 Alcohol/Fermented/Distilled		X	X
272	15	Rye-rough	1.00		
		12 Cooked: NFS		X	
		13 Baked		X	X
273	15	Rye-germ	1.00		
		13 Baked			X
274	15	Rye-flour	1.00		
		13 Baked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
275	15	Sorghum (including milo)	1.00		
		14 Boiled			X
276	15	Wheat-rough	1.00		
		11 Uncooked		X	
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
277	15	Wheat-germ	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
278	15	Wheat-bran	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
279	15	Wheat-flour	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		43 Frozen: Baked		X	X
		45 Frozen: Fried		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
280	15	Millet	1.00		
		13 Baked		X	X
281	0	Honey	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		34 Canned: Boiled		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	
282	1A	Sugar-beet	1.00		
		98 Refined		X	X
283	0	Sugar-cane	1.00		
		98 Refined		X	X
284	0	Sugar-cane/molasses	1.00		
		13 Baked		X	X
285	0	Maple sugar	1.00		
		14 Boiled		X	X
286	15	Buckwheat	1.00		
		12 Cooked: NFS		X	X
287	6C	Guar beans	1.00		
		13 Baked		X	X
288	0	Castor beans	1.00		

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
289	15	Corn grain-oil	1.00		
		98 Refined		X	X
290	O	Cottonseed-oil	1.00		
		98 Refined		X	X
291	O	Cottonseed-meal	1.00		
		13 Baked		X	X
292	O	Flax seed	1.00		
		98 Refined		X	X
293	O	Peanuts-oil	1.00		
		98 Refined		X	X
294	O	Safflower-seed	1.00		
295	O	Safflower-oil	1.00		
		98 Refined		X	X
296	O	Sesame-oil	1.00		
		98 Refined		X	X
297	6A	Soybeans-oil	1.00		
		98 Refined		X	X
298	O	Sunflower-oil	1.00		
		98 Refined		X	X
299	O	Coconut-oil	1.00		
		98 Refined		X	X
300	O	Olive oil	1.00		
		98 Refined		X	X
301	O	Canola oil (rape seed oil)	1.00		
		98 Refined		X	X
302	O	Palm oil	1.00		
		98 Refined		X	X
303	6A	Soybean-other	1.00		
304	6A	Soybeans-mature seeds dry	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		41 Frozen: NFS		X	X
305	6A	Soybeans-flour (full fat)	1.00		
		12 Cooked: NFS		X	X
		13 Baked			X
		14 Boiled		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
306	6A	Soybeans-flour (low fat)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
307	6A	Soybeans-flour (defatted)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		42 Frozen: Cooked		X	X
		98 Refined		X	X
308	O	Oriental vegetables/non-leafy	1.00		
309	O	Seeds (misc.)	1.00		
		11 Uncooked			X
		13 Baked		X	X
		14 Boiled		X	X
310	O	Peppermint	1.00		
311	O	Peppermint-oil	1.00		
		14 Boiled		X	X
312	O	Spearmint	1.00		
313	O	Spearmint-oil	1.00		
314	O	Vinegar	1.00		
		99 Alcohol/Fermented/Distilled		X	X
315	O	Grapes-wine and sherry	1.00		
		99 Alcohol/Fermented/Distilled		X	X
316	O	Alcohol-distilled	1.00		
		99 Alcohol/Fermented/Distilled		X	X
317	O	Gelatin	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		41 Frozen: NFS		X	X
318	D	Milk-nonfat solids	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		16 Pasteurized		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		43 Frozen: Baked		X	X
		45 Frozen: Fried		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		98 Refined		X	
319	D	Milk-fat solids	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		16 Pasteurized		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		45 Frozen: Fried		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
320	D	Milk sugar (lactose)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		16 Pasteurized		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		45 Frozen: Fried		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
321	M	Beef-meat byproducts	1.00		
		12 Cooked: NFS		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
322	M	Beef-other organ meats	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
323	M	Beef-dried	1.92		
324	M	Beef-fat w/o bones	1.00		
		11 Uncooked			X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		45 Frozen: Fried		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		59 Cured: Dried (smokd/pickld/saltd)		X	X
325	M	Beef-kidney	1.00		
		12 Cooked: NFS			X
		15 Fried		X	
326	M	Beef-liver	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		15 Fried		X	X
327	M	Beef-lean (fat/free) w/o bones	1.00		
		11 Uncooked			X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		59 Cured: Dried (smokd/pickld/saltd)		X	X
328	M	Goat-meat byproducts	1.00		
329	M	Goat-other organ meats	1.00		
330	M	Goat-fat w/o bone	1.00		
		13 Baked		X	X
		14 Boiled		X	X
331	M	Goat-kidney	1.00		
332	M	Goat-liver	1.00		
333	M	Goat-lean (fat/free) w/o bone	1.00		
		13 Baked		X	X
		14 Boiled		X	X
334	M	Horsemeat	1.00		
335	M	Rabbit	1.00		
		12 Cooked: NFS		X	X
336	M	Sheep-meat byproducts	1.00		
337	M	Sheep-other organ meats	1.00		
338	M	Sheep-fat w/o bone	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
339	M	Sheep-kidney	1.00		
340	M	Sheep-liver	1.00		
341	M	Sheep-lean (fat free) w/o bone	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
342	M	Pork-meat byproducts	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		15 Fried		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
343	M	Pork-other organ meats	1.00		
		12 Cooked: NFS		X	X
		15 Fried		X	X
344	M	Pork-fat w/o bone	1.00		
		11 Uncooked		X	
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		60 Canned: Cured		X	X
345	M	Pork-kidney	1.00		
346	M	Pork-liver	1.00		
		12 Cooked: NFS		X	X
		15 Fried		X	X
347	M	Pork-lean (fat free) w/o bone	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		60 Canned: Cured		X	X
349	F	Fish-shellfish	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		35 Canned: Fried		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
350	O	Meat-game	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		59 Cured: Dried (smokd/pickld/saltd)		X	X
351	F	Fish-roe/caviar	1.00		
		11 Uncooked		X	X
352	F	Fish-finfish/freshwater	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
353	F	Fish-finfish/saltwater (incl. tuna)	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		35 Canned: Fried		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		59 Cured: Dried (smokd/pickld/saltd)		X	
354	F	Fish-finfish-saltwater-dried	1.60		
		18 Dried			X
		59 Cured: Dried (smokd/pickld/saltd)		X	
355	P	Turkey-byproducts	1.00		
		12 Cooked: NFS		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
356	P	Turkey-giblets (liver)	1.00		
		12 Cooked: NFS		X	X
357	P	Turkey--fat w/o bones	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
358	P	Turkey- lean/fat free w/o bones	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
360	P	Poultry-other-lean (fat free) w/o bone	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
361	P	Poultry-other-giblets(liver)	1.00		
362	P	Poultry-other-fat w/o bones	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
363	P	Eggs-whole	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		45 Frozen: Fried		X	X
364	P	Eggs-white only	1.00		
		11 Uncooked			X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
365	P	Eggs-yolk only	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
366	P	Chicken-byproducts	1.00		
		12 Cooked: NFS		X	X
		34 Canned: Boiled		X	X
367	P	Chicken-giblets(liver)	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	
		15 Fried		X	X
		42 Frozen: Cooked		X	
368	P	Chicken-fat w/o bones	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
369	P	Chicken-lean/fat free w/o bones	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	X
376	O	Aloe vera-juice	1.00		
		11 Uncooked			X
377	11	Apples-juice-concentrate	3.90		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
378	O	Bananas-juice	1.00		
		11 Uncooked		X	X
		31 Canned: NFS		X	X
379	1A	Sugar-beet-molasses	1.00		
		98 Refined			X
380	13A	Blackberries-juice	1.00		
		11 Uncooked		X	X
		31 Canned: NFS		X	X
381	19B	Pepper/black	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		42 Frozen: Cooked		X	X
		52 Cured: Cooked(smokd/pickl/saltd)		X	X
382	1AB	Burdock	1.00		
		12 Cooked: NFS		X	
383	5B	Cabbage-savoy	1.00		
		12 Cooked: NFS			X
384	4B	Celery juice	1.00		
		31 Canned: NFS		X	X
385	P	Chicken-giblets (excl. liver)	1.00		
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		34 Canned: Boiled		X	X
		42 Frozen: Cooked		X	
386	9B	Christophine	1.00		
387	O	Coconut-milk	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
388	15	Corn grain/sugar-molasses	1.50		
		12 Cooked: NFS		X	X
		41 Frozen: NFS		X	X
389	O	Cranberries-juice-concentrate	3.30		
		31 Canned: NFS		X	X
390	O	Fern shoots (fiddleheads)	1.00		
392	O	Grapes-juice-concentrate	3.60		
		12 Cooked: NFS		X	X
		13 Baked		X	X

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APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		14 Boiled		X	X
		31 Canned: NFS		X	X
		41 Frozen: NFS		X	X
393	O	Guava-juice	1.00		
		31 Canned: NFS			X
394	O	Jackfruit	1.00		
395	O	Jobo	1.00		
396	O	Lotus root	1.00		
		14 Boiled		X	X
397	9B	Okra/chinese (luffa)	1.00		
398	D	Milk-based water	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		16 Pasteurized		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		43 Frozen: Baked		X	X
		45 Frozen: Fried		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
399	15	Oats-bran	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	
400	O	Palm hearts	1.00		
		14 Boiled		X	X
401	O	Passion fruit-juice	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
402	12	Peaches-juice	1.00		
		11 Uncooked		X	X
		31 Canned: NFS		X	X
403	O	Peanuts-butter	1.89		
		13 Baked		X	X
		14 Boiled		X	X
404	11	Pears-juice	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		31 Canned: NFS		X	X
		33 Canned: Baked		X	X
		41 Frozen: NFS		X	

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
405	6B	42 Frozen: Cooked Peas-succulent/blackeye/cowpea	1.00	X	X
		12 Cooked: NFS			X
		14 Boiled		X	X
		32 Canned: Cooked			X
		42 Frozen: Cooked			X
406	O	Pineapples-juice-concentrate	6.30		
		12 Cooked: NFS		X	X
		31 Canned: NFS		X	X
		33 Canned: Baked		X	X
		41 Frozen: NFS		X	X
407	1AB	Radishes-japanese (daiken)	1.00		
		12 Cooked: NFS			X
408	15	Rice-bran	1.00		
		11 Uncooked		X	
		12 Cooked: NFS		X	X
		13 Baked		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
409	15	Rice-wild	1.00		
		14 Boiled		X	X
		42 Frozen: Cooked		X	X
410	12	Apricot juice	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS			X
		31 Canned: NFS		X	X
		42 Frozen: Cooked		X	X
411	O	Seaweed	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
412	O	Sequin (portuguese squash)	1.00		
413	6A	Snowpeas	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		15 Fried		X	X
		42 Frozen: Cooked		X	X
414	O	Soursop-juice	1.00		
415	9B	Squash-spaghetti	1.00		
		14 Boiled			X
416	O	Strawberries-juice	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
417	O	Sunflower-seeds	1.00		
		11 Uncooked		X	X
		13 Baked		X	X
418	2	Sweet potatos-leaves	1.00		
419	O	Tamarind	1.00		
		11 Uncooked			X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
420	10	Tangerines-juice-concentrate	7.35		
422	O	Thistle leaves	1.00		
423	8	Tomatoes-dried	14.30		
		12 Cooked: NFS			X
		15 Fried		X	
424	M	Veal-fat w/o bones	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	
425	M	Veal-lean (fat free) w/o bones	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	
426	M	Veal-kidney	1.00		
		15 Fried			X
427	M	Veal-liver	1.00		
		14 Boiled			X
428	M	Veal-other organ meats	1.00		
429	M	Veal-dried	1.92		
430	M	Veal-meat byproducts	1.00		
431	14	Walnut oil	1.00		
432	O	Water-bottled	1.00		
433	O	Water-tap	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
434	O	Water-commercial processing	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		16 Pasteurized		X	X
		18 Dried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		35 Canned: Fried		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		43 Frozen: Baked		X	X
		44 Frozen: Boiled			X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		60 Canned: Cured		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		98 Refined		X	X
435	O	Water-non-food based	1.00		
436	9A	Watermelon-juice	1.00		
437	15	Wheat-germ oil	1.00		
		13 Baked		X	X
438	O	Wi-apple	1.00		
439	9B	Wintermelon	1.00		
		14 Boiled			X
440	O	Yeast	1.00		
		12 Cooked: NFS		X	X
		99 Alcohol/Fermented/Distilled		X	X
441	10	Grapefruit-juice-concentrate	8.26		
		41 Frozen: NFS		X	X
442	10	Lemons-juice-concentrate	11.40		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
443	10	Limes-juice-concentrate	6.00		
		12 Cooked: NFS		X	X
		41 Frozen: NFS		X	X
447	4A	Chervil	1.00		
		14 Boiled		X	X
448	10	Grapefruit peel	1.00		
449	P	Turkey-other organ meats	1.00		
		12 Cooked: NFS		X	X
450	1AB	Ginseng	1.00		
		11 Uncooked			X
451	5A	Broccoli-chinese	1.00		
		14 Boiled		X	X
452	5B	Bok choy	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		14 Boiled		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
460	O	Seafood-misc(turtle/frog)	1.00		
		12 Cooked: NFS			X
		14 Boiled		X	X
467	19B	Celery seed	1.00		
		11 Uncooked		X	X
		14 Boiled		X	X
		31 Canned: NFS		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
473	O	Sapodilla	1.00		
480	O	Plantains-green	1.00		
		15 Fried			X
481	O	Plantains-dried	3.90		
482	O	Soybeans-protein isolate	1.00		
		12 Cooked: NFS		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \ Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)			X
483	O	Chayote	1.00		
484	O	Radishes-oriental	1.00		
485	O	Leaves (misc)	1.00		
		11 Uncooked		X	
		14 Boiled		X	X
		31 Canned: NFS		X	X
		34 Canned: Boiled		X	X
489	O	Vanilla	1.00		
		99 Alcohol/Fermented/Distilled		X	X
491	O	Arugula	1.00		
		11 Uncooked			X
492	O	Radicchio	1.00		
		11 Uncooked			X
493	O	Tarragon	1.00		
		14 Boiled		X	X
494	O	Saffron	1.00		
		14 Boiled		X	X
495	O	Cilantro	1.00		
		11 Uncooked			X
		12 Cooked: NFS			X
496	O	Nopales	1.00		
		11 Uncooked			X
		14 Boiled		X	X
497	9B	Balsam pear	1.00		
498	4A	Amaranth	1.00		
		13 Baked		X	X
890	O	Miscellaneous/nfs	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		33 Canned: Baked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
		51 Cured: NFS (smoked/pickled/saltd)		X	X
		52 Cured: Cooked(smokd/pickld/saltd)		X	X
		60 Canned: Cured		X	X

APPENDIX 1 (CONT'D)

Food Code	Crop Grp	Food Name \Food Form	Adjust Factor	CSFII 89-92	CSFII 94-96
891	0	Jute	1.00		
892	0	Chrysanthemum	1.00		
893	0	Salt	1.00		
		98 Refined		X	X
894	0	Leavening agents	1.00		
		12 Cooked: NFS		X	X
895	0	Psyllium	1.00		
		13 Baked		X	X
896	0	Sweeteners-artificial	1.00		
		12 Cooked: NFS		X	X
897	0	Gums/gels	1.00		
		11 Uncooked		X	X
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		31 Canned: NFS		X	X
		32 Canned: Cooked		X	X
		34 Canned: Boiled		X	X
		41 Frozen: NFS		X	X
		42 Frozen: Cooked		X	X
911	0	Molasses-nfs	1.00		
		98 Refined		X	X
940	0	Peanuts-hulled	1.00		
		12 Cooked: NFS		X	X
		13 Baked		X	X
		14 Boiled		X	X
		15 Fried		X	X
		41 Frozen: NFS		X	X
950	0	Beer	1.00		
		99 Alcohol/Fermented/Distilled		X	X

Appendix 2

Algorithm Documentation for the DEEM™ Acute and Chronic Program Modules

Algorithm Documentation for the DEEM™ Acute and Chronic Program Modules*

By:
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Presented to:
The Advanced DEEM™ Users Workshop
Washington, DC

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Algorithm Documentation for the DEEM™ Acute and Chronic Program Modules

By Stephen R. Petersen, Durango Software, LLC

The Novigen Sciences Dietary Exposure and Evaluation Model (DEEM™), written in Visual Basic for IBM-compatible personal computers by Durango Software LLC, consists of four executable modules: The main DEEM™ module, the Acute analysis module, the Chronic analysis module, and the RDFgen™ module. The main DEEM™ module is used by the exposure analyst to create and edit residue files for specific chemical application, to launch the separate DEEM™ Acute, Chronic and RDFgen™ modules, and to specify file directories and certain report formatting options. This documentation focuses on the computational algorithms in the two analytical modules. User-created DEEM™ residue files are self-documenting. That is, both the residue file itself and an annotated version of the file (for inclusion with a completed DEEM™ analysis) can be printed or displayed to the screen for visual inspection and verification. The RDFgen™ module also produces self documented files.

Before undertaking either a DEEM™ Acute or DEEM™ Chronic analysis, the user must prepare a chemical-specific residue file, using the DEEM™ residue file editor, in which default chemical residue amounts, residue distribution functions, and adjustment factors are set up for each food or food/foodform of interest, along with the toxicology endpoints (separately for chronic and acute analyses) to be used in the analyses. The same DEEM™ residue file can be used by both the DEEM™ Chronic and DEEM™ Acute modules for the analysis of a given chemical, as well as by the Novigen Sciences Calendex™ program for computing dietary exposure in an aggregate or cumulative exposure. (Toxicology endpoints can be changed at the time that the analyses are launched.) The validity of the Acute and/or Chronic analyses for a given chemical is largely determined by the quality of the data in the residue file used in the analysis. (The GIGO principle.) The Acute and Chronic modules apply the residue data in the residue files (and in supporting residue distribution files) to food consumption data derived from the USDA's Continuing Survey of Food Intakes by Individuals (CSFII) to determine acute and chronic exposure amounts in the U.S. Population and specified subsets of that population. The validity of the DEEM™ Acute and Chronic analyses for a given chemical is largely determined by the quality of the data in the residue file used in those analyses. (The GIGO principle.)

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A. The Acute Exposure Module

1. Variables used in the Acute analysis module

User specifies the following variables to be used in an Acute analysis:

	<u>Variable</u>	<u>Type</u>
Residue file name (*.R96 or *.RS7)		
Divide Exposure by Body Weight	bw	Boolean (0,1)
Use second adjustment factor	usesecond	Boolean (0,1)
Use Monte Carlo Analysis (MCA)	flagmc	Boolean (0,1)
Generate CEC file	CEC	Boolean (0,1)
Evaluate foods by eating occasion	lineitem	Boolean (0,1)
Number of Standard Pops to be evaluated	npops	integer 1-27
Standard populations to be evaluated	popx (1 to 27)	Boolean (0,1)
Number of Custom Pops to be evaluated	nsubpops	integer 1-6
List of custom populations	isubpop (1 to 6)	Boolean (0,1)
NFCS survey to be used	survey	1 = 1989-91; 2 = 1994-96

If MCA is used:

number of iterations	nsims	integer 1 to 5000
random number seed	seed	integer 1 to 32,000

If CEC file is to be generated:

Number of printed records	nrecordstosave	integer 1 0 500
Minimum exposure contribution by food/foodform	cecminperc!	Real 1 to 100
Excel format	ExcelOption	Boolean (0,1)
Low percentile boundary	LowPctl!	Real .95 to .999
High percentile boundary	HighPctl!	Real .95 to 1.0

The current residue file defines the list of residue distribution functions in general and specific default residue values, adjustment factors, and (optionally) residue distribution pointers and ratios for each food/foodform to be include in the current analysis.

All valid food (RAC) and Foodform codes are shown in the DEEM™ residue file editor with their corresponding names. RAC codes are assigned to all foods (integer 1-950, but not all numbers in this series are used.)

Foodform codes are assigned to all foods which are actually consumed in either CSFII survey (integer 11-99, but not all numbers are used.)

Active foodforms for any consumed food (RAC) were predetermined at the time that Novigen recipe translation factors were initially applied to the CSFII foods “as-eaten” for all participants in preparing the Acute food consumption data base; only those food/foodform combinations that are derived from the foods “as eaten” either survey (CSFII 1989-91 or 1994-96) are considered “active”. Note that food/foodform consumption records in the Acute data base were calculated for each individual separately, and that the total daily consumption amount for each food/foodform for each individual was rounded to the nearest 0.1g before it was saved to the Acute data base. (By multiplying the daily consumption amount for each food/foodform by 10 the resulting amount could be saved as an integer instead of a real number, which halved the data storage requirement for this large data base. The conversion of the food consumption values in the data base back to 0.1 g is performed as part of the Acute analysis.) Note that in the “line item” data base of individual food consumption for Acute analysis by eating occasion, each occurrence of food/foodform consumption is rounded to 0.1 g, multiplied by 10, and saved separately as an integer amount rather than combining them into a daily total. In both the daily total food consumption data base and the line-item food consumption data base used in the Acute analysis module, food/foodform consumption amounts represent intake amounts by individuals unadjusted for body weight.

If survey = 1 (CSFII 89-91) then

nregions = 9 (CSFII 89-91 uses 9 census regions)
 ndays = 3 (Number of days in survey)
 k1 = 458 (Number of foods (RACs))
 k2 = 1264 (Number of food/food form combinations, plus nfb water)
 k4 = 27 (Number of standard populations, including pacific census region)

If survey = 2 (CSFII 94-96)

nregions = 4 (CSFII 94-96 uses 4 census regions)
 ndays = 2 (Number of days in survey)
 k1 = 458 (Number of foods (RACs))
 k2 = 1270 (Number of food/food form combinations, plus nfb water)
 k4 = 26 (Number of standard populations, (Pacific is not available due to limitation on census regions))

Other variables and arrays needed in the analysis:

RacIndex(rac) = array with RAC indices as function of RACs (k1 indices)
 NSI(rac index) = array with RACs as function of rac indices (reverse of RacIndex array)
 Ffcd(1-k2) is array with active foodform codes for each RAC
 FFF(1-k1) is array with location in Ffcd() of first foodform available for each RAC (as indexed)
 NFF(1-k1) is array with number of food forms in Ffcd() available for each RAC (as indexed)
 waterindex = 415 (the rac index for nfb water, which is not included directly in the CSFII food consumption records)
 k7 = number of standard populations (npops) + number of custom populations (nsubpops) selected for analysis in the current run.

Programming conventions:

All variable and array names ending with “!” are real numbers (7 significant digits).

All variable and array names ending with “&” are long integers.

All variable and array names ending with “#” are double-precision real numbers (14 significant digits).

All variables and array names ending with “\$” are strings. All variable names ending without a special character are integers (0-32,767).

2. Important constants used in the acute analysis module:

Percentile markers:

pctl!(0) = 100 pctl!(1) = 90
 pctl!(2) = 80 pctl!(3) = 70
 pctl!(4) = 60 pctl!(5) = 50
 pctl!(6) = 40 pctl!(7) = 30
 pctl!(8) = 20 pctl!(9) = 10
 pctl!(10) = 5 pctl!(11) = 2.5
 pctl!(12) = 1 pctl!(13) = 0.5
 pctl!(14) = 0.25 pctl!(15) = 0.1

Standard Populations:

1 U.S. Pop - 48 states - all seasons
 2 U.S. Population - spring season
 3 U.S. Population - summer season
 4 U.S. Population - autumn season
 5 U.S. Population - winter season
 6 Northeast region
 7 Midwest region
 8 Southern region
 9 Western region
 10 Hispanics
 11 Non-hispanic whites

- 12 Non-hispanic blacks
- 13 Non-hispanic other than black or white
- 14 All infants (<1 year)
- 15 Nursing infants (<1 year)
- 16 Non-nursing infants (<1 year)
- 17 Children (1-6 years)
- 18 Children (7-12 years)
- 19 Females (13+/pregnant/not nursing)
- 20 Females (13+/nursing)
- 21 Females (13-19 yrs/not preg. or nursing)
- 22 Females (20+ years/not preg. or nursing)
- 23 Females (13-50 years)
- 24 Males (13-19 years)
- 25 Males (20+ years)
- 26 Seniors (55+)
- 27 Pacific Region (Used only in CSFII 1989-91 analyses)

3. Ten steps in the Acute Analysis:

Step 1: Read in the residue file to be used in this analysis

- (1) Read in distribution functions ($i = 1$ to N_{indices})
 - ResDistType(i) = residue distribution type (0-6) of i th function (see list of distribution types and parameters)
 - ResParam!(i, j) = j th residue parameter for i th residue distribution function ($j = 1$ to 3)
 - McFl\$(i) = name of RDF file if i th residue distribution type = 6
- (2) Read in residue amounts, conversion factors, distribution pointers and probabilities ratios
 - Tol!(i) = residue amount for i th Rac in residue file ($i = 1$ to totalfoods)
 - Cf!(i) = conversion factor #1 for i th food
 - Cf2!(i) = conversion factor #2 for i th food
 - Rff(i) = number of food forms included in the residue file for this RAC
 - DistPointer(i, j) = j th distribution index for i th RAC ($j = 1$ to 5)
 - DistRatio!(i, j) = j th distribution probability ratio for i th RAC ($j = 1$ to 5) (must add to 1.0)
 - FFTol!(l) = residue amount for food form FFF(l)
 - FFCf!(l) = conversion factor #1 for food form FFF(l)
 - FFCf2!(l) = conversion factor #2 for food form FFF(l)
 - FFDistPointer(l, j) = j th distribution index for l th food form ($j = 1$ to 5)
 - FFDistRatio!(l, j) = j th distribution probability ratio for l th food form ($j = 1$ to 5) (must add to 1.0)

Step 2: For any RAC without foodforms, convert RACs to its constituent food forms (analysis is never performed at RAC level because all food consumption amounts in the Acute food consumption data base are stored at the foodform level.

See code segment #1

Step 3: (MCA with RDFs only) Preprocess all residue distribution file (RDF) declared in the current residue file and save results to two temporary files. (1) The first contains summary statistics for each RDF file, including the number of declared zeros/, the number of declared LODs (limit of detection), the LOD residue value, the number of specified residue values, and a location variable showing the starting address of its corresponding list of specified residue values in the second file. (2) The second file contains a vector of the individually specified residue values for all of the RDF files declared in the residue file.

Step 4: (MCA only) Compute fmcmean!, CumProb!, and wtdmeanff! Arrays for use in MCA.

The fmcmean! array is the approximate mean value that will be returned from any given residue distribution function (not including the declared zeros in the case of an RDF file). It is computed in subroutine rdfmeans. Note that the approximate mean for distribution types 2-5 is found by sampling the referenced distribution with random sampling values of 0.05, 0.15, ...0.95, summing these values and then dividing by 10 (an exact value is not needed; these means

will be used to estimate the mean exposure amount for each population which in turn will be used to calibrate the bins for capturing the exposure distribution.

See code segment #2

The CumProb! array is the cumulative probability of use (real, 0 to 1) for each of up to 5 different residue distribution functions specified for a given food/foodform in the current residue file. The cumulative probability is based on the individual probabilities assigned to each function (which must add up to 1.0) and the order in which they are included in the residue file for that food/foodform. See code segment #3.

The wtdmeanff! array is the weighted mean for each food/foodform based on the 1 to 5 RDF's specified for that using one or more residue distribution functions and cumulative probability of each rdf used with each foodform). See code segment #3.

Step 5: Compute FFFactor! array of preliminary exposure calculations for each food/foodform having a defined residue in the current residue file. If MCA is not used, or there is no RDL pointer for the lth food/food form, then FFFactor!(l) (l here is lower case letter L) is the residue amount, multiplied by the adjustment factors, that can be multiplied by individual food/foodform consumption amounts to yield individual exposure for that food/foodform. If MCA is used and one or more RDL pointers are used for any given food/foodform, then FFFactor!(l) represents the adjustment factors only; the residue amount must be determined probabilistically from the appropriate residue distribution function. If a food/foodform is not included in the residue file, then FFFactor!(l) = 0.

See code segment #4.

Step 6: First pass through entire food consumption data base to compute the approximate mean daily exposure for users (participants who consume at least one of the food/foodforms in the residue file) in each population group specified when setting up the analysis. These means will be used to set up the exposure bins needed for distribution analysis.

Residue selection: If this is not an MCA, the default (deterministic) residues amounts for each food/foodform in the residue file are used in computing individual exposure amounts. If this is an MCA, then the mean residue amounts for each food/foodform, as derived from the residue distribution functions (wtdmeanff!(1 to k2)) in the residue file, are used. However, in the first pass only a single iteration is performed and no stochastic processes (using random numbers) are employed.

Set testmean = 1.

Then call the computeexpos subroutine to compute mean daily exposure for the users in each population
Return with array cmeans!(i), i = 1 to number of populations to be evaluated (including both standard populations (npops) and custom populations (nsubpops)). Set scalar! array = Cmeans! array. ComputeExpos subroutine shown below.

Step 7: (only used when generating CEC file): Make a pass through the entire food consumption data base with 10 iterations (if MCA) or 1 iteration (if no MCA) to determine the approximate user exposure at the 95th percentile for each population selected.

Set CEC = 1, testmean = 0, and Nsims (number of MC iterations) = 10

Call subroutine computeexpos

Return with distribution array, ex#():

Call distribution subroutine with Ex# array to find daily exposure at 95th percentile for each selected population (1-k7) and place in Array cecvalue!(k7).

Step 8: Call ComputeExpos to determine the total daily exposure for each individual on each day in the survey and place this exposure amount into the bin vector, bin&(), for each population. Also generate the summation variables needed to compute mean, standard deviation, and standard error of mean for each population.

If this total daily exposure exceeds the preliminary exposure estimate at the 95th percentile, as determined in step 7, save a record of this individual's demographic variables (age, sex, body weight) and daily exposure amount, along with a list of the food/foodforms eaten that contribute to this exposure amount, including their consumption amount, residue amount, and adjustment factors. Individual foods/foodforms are only included in this list if their percentage contribution to the total daily exposure exceeds the percentage level specified by the user ("minimum exposure contribution by food"). These CEC records are saved to a temporary disk file which is post-processed after the final acute exposure analysis report is generated.

Step 9: Call the report subroutine to generate the acute analysis report, which contains user and per capita means, standard deviation, and standard error or mean, as well as exposure distributions for users and per capita, for all designated populations.

For each population of interest, i (1 to $k7$), compute the percent of total person-days in the survey that are user days (i.e., at least one of the food/foodform combinations in the residue file were eaten)

See code segment #14

For both users and per capita, compute:

- (1) the mean exposure: See code segment #15
- (2) standard deviation and standard error of mean: code segment #16
- (3) MOE: code segment #17
- (4) exposure distribution statistics (exposure at predefined percentiles with toxicology endpoint calculations): code segment #18 (users) and code segment #19 (per capita)

Step 10: (CEC only) Generate the CEC file, refining and sort the list of CEC records saved during the current analysis. Read the temporary CEC records file generated during the last pass through the food consumption data. For each population of interest, find all records in the file and save these to a second file sorted by population type (some records may be included in more than one population). Then read the records for each population individually from second file; for each record for which total daily exposure falls within the low and high percentile bounds specified by the user in this run, save this subset in a third file. Count the number of times each food/foodform is found in the records in this subset and sum the exposures for each food/foodform. Then divide the sum of exposures for each food/foodform by the sum of total daily exposures in this subset to get the percent contribution by each food/foodform toward the total exposure in the referenced percentile interval. Sort the individual records in the subset in decreasing order of total daily exposure and print the number of individual records specified by the user to the final CEC report, starting with the individual with the highest exposure. (This is repeated for each population of interest; summaries and record listings for each population of interest are included in the same CEC report).

4. Subroutine ComputeExpos

This is the "computational engine" of the acute program, in which the individual exposure amounts are calculated for each individual, summed and binned for later post-processing and reporting.

Step C1. Seed the random number generator with the seed specified by the user. See code segment #5.

Step C2. Initialize arrays with bins for each population, Array $\text{bin}\#(j, i)$, $j = 0$ to 1200, $i = 1$ to $k7$, and upper boundary of each bin, Array $\text{ubex}\!(i, j)$ ($i = 1$ to $k7$, $j = 1$ to 1201)

For each standard population and for each custom population ($k = 1$ to $k7$), compute the upper boundary of each bin ($\text{ubex}\!(k7, \text{nbinsx} + 1)$) as follows:

For the first 100 bins (1 to 100), the upper boundary of the bin for a given population is the mean daily exposure for users divided by 100, where the mean is established in the first iteration through subroutine ComputeExpos.

For bins $j = 101$ through 1200, the upper boundary is computed as $\text{mean}\!(i) \times 1.01^{(j-100)}$. An exposure amount x is placed in bin j if $\text{ubex}\!(j-1) \leq x < \text{ubex}\!(j)$. Note that if an exposure amount exactly equals the upper boundary of a

bin, it is added to the next higher bin. See code segment #6 for the code used to compute the upper boundaries. The code used to place exposure amounts into the appropriate bin is discussed below in step

Step C3. Initialize arrays used in exposure analysis

Array $cmeans!(1 \text{ to } k7)$ = mean daily exposure for each population
 Array $max!(1 \text{ to } k7)$ = maximum daily exposure for each population
 Array $subtotal0\#(i)$ = sum of daily exposure for each indiv in population i (1 to $k7$) x their statistical wt
 Array $subtotal3\#(i)$ = sum of square of daily exposure for each indiv in population i (1 to $k7$) x their statistical wt
 Array $total0\#(i)$ = sum of all individual daily exposures for entire 3-year survey, weighted (populations 1 to $k7$)
 Array $total3\#(i)$ = sum squares of all individual daily exposures for entire 3-year survey, weighted (populations 1 to $k7$)
 Note: $subtotal0\#(i)$ and $subtotal3\#(i)$ are reinitialized at start of each file of food consumption records processed in Acute module, then summed into $total0\#(i)$ and $total3\#(i)$ at end of each file.
 Array $total1\#(i)$ = total number of persons in population i (1 to $k7$) in the survey (weighted)
 Array $total1u\#(i)$ = total number of persons in population i (1 to $k7$) in the survey (unweighted)
 Array $total1\#(i)$ = total number of persons in population i (1 to $k7$) in the survey (weighted)
 Array $total1u\#(i)$ = total number of persons in population i (1 to $k7$) in the survey (unweighted)
weighted
 Array $total2u\#(i)$ = number of persons in population i (1 to $k7$) that consume one or more foods in the residue file (“users”),unweighted

Step C4. For each file (1 to 9) of food consumption data in the data base for the designated survey, get household and individual records.

Get the next household demographic record.
 For each individual in household get the individual’s demographic record.
 If this individual passes the demographic test (i.e., matches designated sex, age, region, race, pregnant/nursing status) then proceed with this individual, otherwise skip this individual.

If this individual passes the demographics test (to match to designated populations for analysis), then for each day in survey ($d = 1$ to $ndays$), read the food code and consumption amounts for each of the $nf(d)$ foods eaten by that individual on that day ($j = 1$ to $nf(d)$) into the following arrays:
 Array $ffindex(j)$, where this index is the RAC/foodform code used in the DEEM™ consumption data base to identify specific RACs and foodforms.
 Array $amount!(j)$, the total daily amount consumed in grams.
 Also compute $totamount!$ as the total amount of food consumption on this day in grams (this will be used to determine whether or not the individual is a user, not the exposure amount, which could be zero if the residue amounts are zero).

Step C5. Now for each person-day in the survey, perform the designated number of MCA iterations (or 1 iteration only if MCA is not used), recomputing total daily exposure for this individual at each iteration.

Individual daily exposure is computed as the sum of exposures from each food/foodform, then the exposure amount is “binned” into each appropriate population vector in the bin array. (Any given individual can belong to two or more standard populations and custom populations.) The summation variables for each appropriate population are accumulated with the exposure amount, population count, user count, etc.

Step C5a.

For each food/foodform eaten ($j = 1$ to $nf(d)$)
 If MCA is not used, multiply the $FFFactor!()$ corresponding to $ffindex(j)$ (in ppm) by the consumption amount (in grams) and divide by 1000 to compute exposure for that food/foodform in mg/day. (The $FFFactor!$ already contains the deterministic residue amount for that food/foodform.)

If MCA is used, then a residue amount must be drawn at random from the appropriate residue distribution function(s) assigned to that food/foodform. If there is only one residue distribution function assigned, then this function is used in this iteration. If there are 2 or more functions assigned, each with its own probability ratio, then draw a random number

(p!) between 0 and 1 to determine which function will be used in this iteration. (Use the function designated for the current food/foodform for which its CumProb value first exceeds p!.)

Given the RDF to be used as the source for the residue for this food/foodform for this iteration, use one of the following methods to choose a residue, based on its distribution type.

(1) Distribution type = 0 (constant):

Use the constant as the residue.

(2) Distribution type = 1 through 5 (distribution functions with parameters)

Choose a random number, p!, between 0 and 1. Call the associated subroutine with p! and the parameters for that function and return with a distribution. (These distribution subroutines are documented below.)

(3) Distribution type = 6 (RDF file)

RDF files can have a specified number of zero residues (Totalz), a specified number of LOD residues (TotalLOD, all having the same value), and other (usually non-zero) specified residues, with the latter residues entered into a vector of residue values. Let totobs& = the total number of residue values (if all were enumerated separately, i.e., zeros + LOD's + individually specified residues) that are enumerated in the RDF file. Let rx& = the integer value of totobs& x p! + 1. If rx& <= the number of individually specified residues, then the residue amount is the value in cell rx& of the residue vector of specified residues for that RDF file. If rx& is greater than the number of individually specified residues, then if rx& <= the sum of the individually specified residues + the number of LODs, then the residue amount equals the LOD amount. Otherwise the residue amount is zero (i.e., rx& lies within the specified zeros zone).

Note: if the total number of individually specified residues < 32,000 for all of the RDF files used in a single analysis, then a named vector (array) is established. Otherwise the individual residue values are written to a random access file saved to the disk and retrieved using rx& as a record number in order to reduce the memory requirements of the program. (The 32,000 limit on the vector size is a carry over from an earlier version of the program when memory was more limited. This limit is subject to be raised in the future as memory capabilities are increased.)

See code segment #8

For MCA analyses, the daily exposure amount for the food/foodform for this individual and MC iteration on day d is calculated as the product of the FFFactor! for that food/foodform, the residue amount, and the consumption amount. The resulting exposure for each food/foodform is accumulated for this individual/day/iteration.

See code segment #9

Step C5b. After the exposure is calculated for all foods/foodforms for this person/day/iteration, divide it by the individual's body weight to compute exposure in mg/kg-body weight - day.

See code segment #10

Step C5c: Insert the individual's statistical weight into the distribution vector for each population for which this individual is member.

Use the resulting total daily exposure for this individual to determine where in the binning vector to insert the individual's statistical weighting (sw). The sw is added to the bin#(i, j) array for each population i, where j is computed as follows: Scalar!(i) is the mean user consumption (= cmeans!(i)) for each population i (1 to k7), computed in the first pass through the entire survey using mean residue amounts. Wght& is the individuals sampling weight; nbinsx = the number of bins available, 1200 to start. If 1200 is not large enough, then one additional superbin is added so that the program will not crash. However, the user is warned that the largest available bin is not sufficient, implying that a computed residue amount was probably unrealistically high. The 1200 bins used in the Acute module allows for a maximum bin size 56,690 times the mean user exposure amount.

See code segment #11

Step C5d: Keep track of maximum exposure for each population (max(i), i = 1 to k7:

See code segment #12

Step C5e: Aggregate the summation statistics for the individuals in each population:

See code segment #13

5. Acute module code segments (taken directly from the source code, with additional remarks):

Code segment #1:

Purpose: to expand residue amounts, adjustment factors, and distribution pointers and ratios defined at the food level to the foodform level for foods which were not declared at the foodform level in the residue file. (The same parameters used for the foods are transferred to the foodforms. Note that acute analysis is always performed at the foodform level.) From step 1.

```
For i = 1 To k1
  If TOL!(i) > 0 And nff(i) = 0 Then
    TOL!(i) = 0 (foods without foodforms are not used)
  ElseIf TOL!(i) > 0 And rff(i) = 0 Then 'expand to ff
    For k = fff(i) To fff(i) + nff(i) - 1
      fftol!(k) = TOL!(i)
      ffcf!(k) = CF!(i)
      ffcf2!(k) = CF2!(i)
      If flagmc Then 'monte carlo analysis will be performed in this run
        For l = 1 To NIndices
          ffdistpointer(k, l) = DistPointer(i, l)
          ffdistperc!(k, l) = DistPerc!(i, l)
        Next
      End If
    Next
    rff(i) = nff(i)
  End If
Next
```

Code segment #2:

Subroutine rdfmeans (used to calculate the mean of all non-zero residues in each residue function (including RDF files) referenced in the current residue file). From step 4.

Variables:

Nrdfiles is number of residue distribution functions in the current residue file

Resdistype(i) is the distribution type (0-6) for the ith residue distribution function. (Note: The "0" distribution type (constant) is handled as "-1" so as not to confuse with the null.

Rdfpointer&(i) (distribution type 6 (RDF file) only) is the address of the first specified residue value for the ith RDF file in the vector (array mcres!) containing all specified residue values from all referenced RDF files in the current residue file.

Rdfarray is a flag indicating that the vector of residue values is in a random access file rather than the mcres! array.

totobs&(i) is the total number of specified residue values in the ith RDF file.

totmld&(i) is the number of declared LOD values in the ith RDF file

mld!(i) is the declared LOD value in the ith RDF file

totobsml d&(i) = totobs&(i) + totmld&(i)

```

For i = 1 To nrdfiles
  If resdistype(i) = 6 Then
    rec& = rdfpointer&(i)
    sum! = 0
    For j& = 1 To totobs&(i)
      ran& = rec& + j& - 1
      If rdfarray Then
        sum! = sum! + mcres!(ran&)
      Else
        Get #6, ran&, r
        sum! = sum! + r.res
      End If
    Next
    sum! = sum! + totmld&(i) * mld!(i)
    'note that zero residues are not included in this mean
    'totobsml d& is number of all individually specified residues + number of mlds
    'mlds are assumed to be non-zero
    If totobsml d&(i) Then
      ffmcm ean!(i) = sum! / (totobsml d&(i))
    Else
      ffmcm ean!(i) = 0
    End If

    ElseIf resdistype(i) = -1 Then
      ffmcm ean!(i) = resparam!(i, 1)
    ElseIf resdistype(i) = 1 Then
      p! = 0.5
      Call uniform(p!, resparam!(i, 1), resparam!(i, 2), ffmcm ean!(i))
    ElseIf resdistype(i) = 2 Then
      meantotal! = 0
      For k = 0 To 9
        p! = k / 10 + 0.05
        Call pareto(p!, resparam!(i, 1), resparam!(i, 2), resparam!(i, 3), ffmcm eanx!)
        meantotal! = meantotal! + ffmcm eanx!
      Next
      ffmcm ean!(i) = meantotal! / 10
    ElseIf resdistype(i) = 3 Then
      meantotal! = 0
      For k = 0 To 9
        p! = k / 10 + 0.05
        Call triangular(p!, resparam!(i, 1), resparam!(i, 2), resparam!(i, 3), ffmcm eanx!)
        meantotal! = meantotal! + ffmcm eanx!
      Next
      ffmcm ean!(i) = meantotal! / 10
    ElseIf resdistype(i) = 4 Then
      meantotal! = 0
      For k = 0 To 9
        p! = k / 10 + 0.05
        Call normal(p!, resparam!(i, 1), resparam!(i, 2), resparam!(i, 3), ffmcm ean!(i))
        meantotal! = meantotal! + ffmcm eanx!
      Next
      ffmcm ean!(i) = meantotal! / 10
    ElseIf resdistype(i) = 5 Then
      meantotal! = 0

```

```

For k = 0 To 9
  Call lognormal(p!, resparam!(i, 1), resparam!(i, 2), resparam!(i, 3), ffmtcmean!(i))
  meantotal! = meantotal! + ffmtcmeanx!
Next
ffmtcmean!(i) = meantotal! / 10
Else
  'error in resdistype
  Stop
End If
If ffmtcmean!(i) < 0 Then ffmtcmean!(i) = 0 'do not allow negative residue values that might be generated by some
distributions
Next

```

Code segment #3:

Compute cumprob! and wtdmeanff! arrays used in estimating the mean exposure in the first pass through the food consumption data and which of (up to) 5 residue distributions for a given food/foodform will be used in MCA. From step 4.

(All variables, except indices) have been defined above)

```

ReDim cumprob!(k2, NIndices), wtdmeanff!(k2)
For i = 1 To k1
  If TOL!(i) > 0 And nff(i) > 0 Then
    For k = fff(i) To fff(i) + nff(i) - 1
      For l = 1 To NIndices
        cumprob!(k, l) = cumprob!(k, l - 1) + ffdistperc!(k, l)
      Next
      If cumprob!(k, NIndices) Then
        sumperc! = 0
        For l = 1 To NIndices
          If ffmtcmean!(ffdistpointer(k, l)) Then
            wtdmeanff!(k) = wtdmeanff!(k) + ffmtcmean!(ffdistpointer(k, l)) * ffdistperc!(k, l)
            sumperc! = sumperc! + ffdistperc!(k, l)
          End If
        Next l
        If sumperc! > 0 And sumperc! < 1 Then wtdmeanff!(k) = wtdmeanff!(k) / sumperc!
        'we only want to include non-zero rdl means in the wtdmean calc here
      End If
    Next k
    'note: cumprob!(k, nindices) > 0 means that this ff has at least one valid rdl pointer
  End If
Next i

```

Code segment #4:

Compute fffactor! array with partial exposure calculations before starting through the food consumption records. This includes the first adjustment factor, second adjustment factor (if use is specified) and a conversion factor of 1000 needed eventually to convert the product of residue amount (in ppm) and the food consumption amount (in grams) to mg units. From step 5.

```

ReDim fffactor!(k2) 'initialize array
nfbwater = 0 'initialize
For i = 1 To k1
  If rff(i) Then

```

```

If i = waterindex Then nfbwater = 1 (flag to indicate that nfbwater is to be evaluated, which is not in food
consumption array)
For l = fff(i) To fff(i) + nff(i) - 1
  If fftol!(l) > 0 Or cumprob!(l, NIndices) > 0 Then
    fffactor!(l) = ffcf!(l) / 1000 'first conversion factor
    If UseSecond Then fffactor!(l) = fffactor!(l) * ffcf2!(l) 'include second conversion factor if specified
    If cumprob!(l, NIndices) = 0 Then fffactor!(l) = fffactor!(l) * fftol!(l) 'include residue from RES file if MCA is
not used
                                for this food/foodform
  End If
Next l
End If
Next i

```

Code segment #5:

Random number seeding (Step 1 in ComputeExpos subroutine)

```

p! = Rnd(-1) 'forces the same sequence of random numbers each time a new analysis is started
If seed = 0 Then
  Randomize Timer
Else
  Randomize seed
End If

```

Code segment #6:

Compute upper boundary of each bin, ubex!(i, j) (from Step 2 in ComputeExpos Subroutine)

```

Nbinsx = 1200 'number of bins available for each population to use in the calculation of exposure distributions
For i = 1 to k7
  ubex!(i, 0) = 0
  For j = 1 To 100
    ubex!(i, j) = scalar!(i) * j / 100
  Next
  For j = 101 To nbinsx
    ubex!(i, j) = scalar!(i) * 1.01 ^ (j - 100)
  Next
End If
Next

```

Code segment #7:

Retrieve a residue value from a residue distribution file (resdistype = 6) or a residue distribution function and compute exposure amount for each food and sum for all food/foodforms

Array totobsz&(ii) = total number of all residue values referenced in the iiith RDF file, where ii is the RDF file from which the residue value is to be drawn.

Array totobs&(ii) = total number of all individually specified residue values referenced in the iiith RDF file.

Array totobsmdl&(ii) = total number of all individually specified residue values + LOD values referenced in the iiith RDF file.

Variable rdfarray = 1 if values are stored in a vector, 0 if stored in a random access file (open file #6)

```

For j = 1 To nracs 'the number of food/foodform combinations the individual has consumed on this day
  jj = ffindex(j)
  ii = 0

```

```

If flagmc Then
If cumprob!(jj, NIndices) Then 'this ff uses residue from rdl
If testmean Then
  expos! = expos! + fffactor!(jj) * amount!(j) * wtdmeanff!(jj)
  GoTo skiptohere2
Else 'generate an ii index
If NIndices = 1 Then
  ii = ffdistpointer(jj, 1)
Else
  p! = Rnd(1)
  For m = 1 To NIndices
    If p! < cumprob!(jj, m) Then ii = ffdistpointer(jj, m): Exit For
  Next
  If ii = 0 Then MsgBox "Error selecting ii": End 'temporary check
End If
End If
End If
End If

If ii > 0 And flagmc = 1 Then 'use MC analysis to select residue from RDL
  p! = Rnd(1)
  If resdistype(ii) = 6 Then
    rx& = Int(totobsz&(ii) * p!) + 1
    If rx& <= totobs&(ii) Then
      If rdfarray Then
        resc!(j) = mcres!(rdfpoiner&(ii) + rx& - 1)
      Else
        rec& = rdfpointer&(ii)
        Get #6, rec& + rx& - 1, r
        resc!(j) = r.res
      End If

    ElseIf rx& <= totobsmlld&(ii) Then
      resc!(j) = mld!(ii)
    Else
      resc!(j) = 0
    End If

  ElseIf resdistype(ii) = -1 Then
    resc!(j) = resparam!(ii, 1)
  ElseIf resdistype(ii) = 1 Then
    Call uniform(p!, resparam!(ii, 1), resparam!(ii, 2), resc!(j))
  ElseIf resdistype(ii) = 2 Then
    Call pareto(p!, resparam!(ii, 1), resparam!(ii, 2), resparam!(ii, 3), resc!(j))
  ElseIf resdistype(ii) = 3 Then
    Call triangular(p!, resparam!(ii, 1), resparam!(ii, 2), resparam!(ii, 3), resc!(j))
  ElseIf resdistype(ii) = 4 Then
    Call normal(p!, resparam!(ii, 1), resparam!(ii, 2), resparam!(ii, 3), resc!(j))
  ElseIf resdistype(ii) = 5 Then
    Call lognormal(p!, resparam!(ii, 1), resparam!(ii, 2), resparam!(ii, 3), resc!(j))
  Else
    Stop 'error
  End If
  If resc!(j) < 0 Then resc!(j) = 0 'do not allow negative residue values that might be generated by some
distributions
  expos! = expos! + fffactor!(jj) * amount!(j) * resc!(j)

```

```

Else 'use residue from residue file
  expos! = expos! + fffactor!(ffindex(j)) * amount!(j)
  'where fffactor!(j) = ffcf!(j) / 1000 * ffcf2!(j) * fftol!(j)
  resccl!(j) = fftol!(ffindex(j))
End If

```

Code segment #9:

jj = ffindex(j), where j is the jth food eaten on this day
 expos! = expos! + fffactor!(jj) * amount!(j) * resccl!(j)
 where expos! is the variable used to cumulate exposure amounts over all of the foods/foodforms eaten
 by this person/day/iteration

Code segment #10:

Adjust exposure in mg/day to mg/kg-bw-day by dividing exposure by bodyweight in kilograms

expos! = total daily exposure in mg.
 wtbls = individuals weight in pounds, as included in his/her demographic record

```

  expos! = expos! * 2.2 / wtbls

```

Code segment #11:

Place the individual's statistical weight into the appropriate distribution bin, based on the total daily exposure amount for that individual.

```

If expos! = 0 Then
  bin#(i, 0) = bin#(i, 0) + wght&
Else
  If expos! / scalar!(i) < 1 Then
    j = Int(expos! / scalar!(i) * 100) + 1
  Else
    j = Int(Log(expos! / scalar!(i)) / Log(1.01)) + 101
  End If

  If j > nbinsx Then j = nbinsx + 1
  bin#(i, j) = bin#(i, j) + wght&
End If

```

Code segment #12:

Keep track of the maximum exposure amount in each population group, i

```

If expos! > max!(i) Then max!(i) = expos!

```

Code segment #13:

Aggregate the summation statistics for the individuals in each population:

Code executed at end of each individual/day/iteration:

```

subtotal0#(i) = subtotal0#(i) + expos! * wght&
subtotal3#(i) = subtotal3#(i) + (expos! ^ 2) * wght&

```

Code executed at end of each of the nine food consumption data base files:

```
total0#(i) = total0#(i) + subtotal0#(i)
total3#(i) = total3#(i) + subtotal3#(i)
```

Code executed for each individual passing population screen for the designated population, before looking at specific days (1-3) and iterations:

Where wght& = individuals sample weight
 Ndays = number of days in CSFII survey (3 for 1989-91, 2 for 1994-96)
 Nsims = number of MCA simulations in this run

```
total1x# = wght& * ndays 'note that this 3-part construction is needed to maintain accuracy at high iteration levels
total1x# = total1x# * nsims
total1#(1) = total1#(1) + total1x#
total1u#(1) = total1u#(1) + nsims * ndays
```

Code executed during specific day and iteration when at least one food/foodform in the residue file is consumed on that day, regardless of the residue level on that food (that is, even if the residue is zero, the individual is still a user if he/she ate the specified food/foodform on that day):

```
total2#(i) = total2#(i) + wght&
total2u#(i) = total2u#(i) + 1
```

Code segment #14:

the percent of person-days that are user days

```
If total1#(i) Then
  userpratio! = total2#(i) / total1#(i) * 100 'percent of person-days that are users
Else
  userpratio! = 0
End If
```

Code segment #15:

Compute the mean exposure both per user and per capita:

Per user means:

```
If total2#(i) > 0 Then
  cmeans!(i) = total0#(i) / total2#(i)
Else
  cmeans!(i) = 0
End If
```

Per capita means = cmeans!(i) * userpratio! / 100, mask\$)

Code segment #16:

standard deviation per user and per capita
 standard error of mean per user and per capita

```
If total2#(i) > 1 Then
```

```
varu# = (total3#(i) - (total0#(i) ^ 2) / total2#(i)) / (total2#(i) - 1)
If varu# < 0 Then varu# = 0
sdu# = varu# ^ 0.5 'standard deviation (user)
```

```
semu# = sdu# / total2u#(i) ^ 0.5 'standard error of mean (user)
varpc# = (total3#(i) - (total0#(i) ^ 2) / total1#(i)) / (total1#(i) - 1)
If varpc# < 0 Then varpc# = 0
```

```
sdpc# = varpc# ^ 0.5 'standard deviation (per capita)
If total1u#(i) > 0 Then
  sempc# = sdpc# / total1u#(i) ^ 0.5 'standard error of mean (per capita)
Else
  sempc# = 0
End If
End if
```

Code segment #17:

Compute statistics related to toxicology endpoints:

Compare\$ = N used to force computation of margin of exposure only
Compare\$ = R used to force computation of percent of RfD only
Compare\$ = P used to force computation of percent of PAD only
Compare\$ = NR used to force computation of margin of exposure and percent of RfD
Compare\$ = NP used to force computation of margin of exposure and percent of PAD

mosun! = margin of exposure, user
mospcnx! = margin of exposure, per capita
mosur! = percent of RfD or percent of PAD (user)
mospcrx! = percent of RfD or percent of PAD (per capita)
userpratio! = percent of the sample population that are users (consumers) of one or more foods on this day.
RfD! = reference dose (same for all populations).
PAD!(i) = population-adjusted dose for the ith population (Note: if this is not explicitly specified, then the RfD! is used for this population).

```
If compare$ = "N" Then
  mosun! = Noel! / cmeans!(i)
  mospcnx! = Int(mosun! / (userpratio! / 100))
  mosun! = Int(mosun!)
ElseIf compare$ = "R" Then
  mosur! = cmeans!(i) / Rfd! * 100
  mospcrx! = mosur! * (userpratio! / 100)
ElseIf compare$ = "NR" Then
  mosun! = Noel! / cmeans!(i)
  mospcnx! = Int(mosun! / (userpratio! / 100))
  mosun! = Int(mosun!)
  mosur! = cmeans!(i) / Rfd! * 100
  mospcrx! = mosur! * (userpratio! / 100)
ElseIf compare$ = "P" Then
  mosur! = cmeans!(i) / PAD!(i) * 100
  mospcrx! = mosur! * (userpratio! / 100)
ElseIf compare$ = "NP" Then
  mosun! = Noel! / cmeans!(i)
  mospcnx! = Int(mosun! / (userpratio! / 100))
  mosun! = Int(mosun!)
  mosur! = cmeans!(i) / PAD! (i) * 100
```

```

    mospcrx! = mosur! * (userpcratio! / 100)
Else
    mosun! = 0
    mospcnx! = 0
    mosur! = 0
    mospcrx! = 0
End If
Else
    mosun! = 0
    mospcnx! = 0
    mosur! = 0
    mospcrx! = 0
End If

```

Code segment #18:

Percentile calculations for users

For each population of interest, i = 1 to k7

'provide an extra bin at 1201 (nbinsx) if the maximum exposure observation is larger than the upper boundary of the 1200th bin and set the upper value of this bin to the maximum exposure value (separately for each population)

```

If max!(i) > ubex!(i, nbinsx) Then
    ubex!(i, nbinsx + 1) = max!(i)
    nbins(i) = nbinsx + 1
Else: nbins(i) = nbinsx
End If

```

'Remove all unused bins above the highest bin actually used (separately for each population)

```

Dim tempnbins
tempnbins = nbins(i)
For j = nbins(i) To 1 Step -1
    If bin#(i, j) Then Exit For
    tempnbins = tempnbins - 1
Next
nbins(i) = tempnbins
If ubex!(i, nbins(i)) > max!(i) Then ubex!(i, nbins(i)) = max!(i) 'replace upper boundary of last bin having user days
with max exposure

```

'compute the daily exposure at each of the prescribed reporting percentiles (10, 20, ...95, 97.5, 99, 99.5, 99.9) for users

```

cumperc#(i, 0) = 100 - bin#(i, 0) / total2#(i) * 100
For j = 1 To nbins(i)
    cumperc#(i, j) = cumperc#(i, j - 1) - bin#(i, j) / total2#(i) * 100
    If cumperc#(i, j) < 0 Then cumperc#(i, j) = 0
Next

```

```

k = 0
For j = 1 To npctls
    While cumperc#(i, k) > pct!(j) And k < nbins(i)
        k = k + 1
    Wend

```

```

If k = 0 Then
    aratio# = (100 - pct!(j)) / (100 - cumperc#(i, k))
    ex#(i, j) = aratio# * ubex!(i, k)

```

```

Else
  aratio# = (cumperc#(i, k - 1) - pct!(j)) / (cumperc#(i, k - 1) - cumperc#(i, k))
  ex#(i, j) = ubex!(i, k - 1) + aratio# * (ubex!(i, k) - ubex!(i, k - 1))
End If

```

‘Compute the corresponding margin of exposure, percent of RfD, etc, as specified in the run

‘mosn&(j) is the margin of exposure

‘mosr!(j) is the percent of RfD or percent of PAD as specified in the run

```

If compare$ = "N" Or compare$ = "NR" Or compare$ = "NP" Then

```

```

  If ex#(i, j) > 0 Then

```

```

    If Noel! / ex#(i, j) > 1000000 Then

```

```

      mosn&(j) = 1000000

```

```

    Else

```

```

      mosn&(j) = Int(Noel! / ex#(i, j))

```

```

    End If

```

```

  Else

```

```

    mosn&(j) = 1000000

```

```

  End If

```

```

End If

```

```

If compare$ = "R" Or compare$ = "NR" Then

```

```

  mosr!(j) = ex#(i, j) / Rfd! * 100

```

```

ElseIf compare$ = "P" Or compare$ = "NP" Then

```

```

  mosr!(j) = ex#(i, j) / PAD! * 100

```

```

End If

```

```

Next j

```

```

j = npctls + 1

```

```

pct!(j) = 0

```

```

ex#(i, j) = max!(i)

```

```

If compare$ = "N" Or compare$ = "NR" Or compare$ = "NP" Then

```

```

  If ex#(i, j) > 0 Then

```

```

    If Noel! / ex#(i, j) > 1000000 Then

```

```

      mosn&(j) = 1000000

```

```

    Else

```

```

      mosn&(j) = Int(Noel! / ex#(i, j))

```

```

    End If

```

```

  Else

```

```

    mosn&(j) = 1000000

```

```

  End If

```

```

End If

```

```

If (compare$ = "R" Or compare$ = "NR") And Rfd! > 0 Then

```

```

  mosr!(j) = ex#(i, j) / Rfd! * 100

```

```

ElseIf (compare$ = "P" Or compare$ = "NP") And PAD! > 0 Then

```

```

  mosr!(j) = ex#(i, j) / PAD! * 100

```

```

End If

```

Code segment #19:

Percentile calculations per capita

For each population of interest, i = 1 to k7 ‘compute cumulative percentage through bins, starting with bin 0 which now contains all non-users

```

cumpercpc#(i, 0) = 100 - (bin#(i, 0) + (total1#(i) - total2#(i))) / total1#(i) * 100 'add all non-users to zero bin
For j = 1 To nbins(i)
  cumpercpc#(i, j) = cumpercpc#(i, j - 1) - bin#(i, j) / total1#(i) * 100
  If cumpercpc#(i, j) < 0 Then cumpercpc#(i, j) = 0
Next

```

```

k = 0
For j = 1 To npctls
  While cumpercpc#(i, k) > pctl!(j) And k < nbins(i)
    k = k + 1
  Wend

  If k = 0 Then
    aratio# = (100 - pctl!(j)) / (100 - cumpercpc#(i, k))
    expc#(i, j) = aratio# * ubex!(i, k)
  Else
    aratio# = (cumpercpc#(i, k - 1) - pctl!(j)) / (cumpercpc#(i, k - 1) - cumpercpc#(i, k))
    expc#(i, j) = ubex!(i, k - 1) + aratio# * (ubex!(i, k) - ubex!(i, k - 1))
  End If
Next

```

'Compute the corresponding margin of exposure, percent of RfD, etc, as specified in the run
'mospcn&(j) is the margin of exposure
'mospcr!(j) is the percent of RfD or percent of PAD as specified in the run

```

ReDim mospcr!(npctls + 1), mospcn&(npctls + 1)
If bw Then
  For j = 1 To npctls
    If compare$ = "N" Or compare$ = "NR" Or compare$ = "NP" Then
      If expc#(i, j) > 0 Then
        If Noel! / expc#(i, j) > 1000000 Then
          mospcn&(j) = 1000000
        Else
          mospcn&(j) = Int(Noel! / expc#(i, j))
        End If
      Else
        mospcn&(j) = 1000000
      End If
    End If
    If (compare$ = "R" Or compare$ = "NR") And Rfd! > 0 Then
      mospcr!(j) = expc#(i, j) / Rfd! * 100
    ElseIf (compare$ = "P" Or compare$ = "NP") And PAD! > 0 Then
      mospcr!(j) = expc#(i, j) / PAD! * 100
    End If
  Next j
  mospcn&(npctls + 1) = mosn&(npctls + 1)
  mospcr!(npctls + 1) = mosr!(npctls + 1)
End If

```

6. Subroutines used to compute distributions from distribution parameters

p! is always a random number ≥ 0 and < 1 .

Code segment #20:

```
Sub lognormal (p!, m!, sd!, max!, c!)
```

m! is the mean

sd! is the standard deviation

max! is the highest value that the subroutine can return

c! is the residue amount returned

```
Dim mx!, sdx!
```

```
If m! > 0 Then
```

```
  mx! = Log((m! ^ 2) / ((m! ^ 2 + sd! ^ 2) ^ 0.5))
```

```
  sdx! = (Log(1 + (sd! / m!) ^ 2)) ^ 0.5
```

```
  Call normal(p!, mx!, sdx!, 0, c!) 'don't sent max to normal
```

```
  c! = Exp(c!)
```

```
  If c! < 0 Then c! = 0
```

```
  If max! Then
```

```
    If c! > max! Then c! = max!
```

```
  End If
```

```
Else
```

```
  c! = 0
```

```
End If
```

Code segment #21:

```
Sub normal(p!, m!, sd!, max!, c!)
```

m! is the mean

sd! is the standard deviation

max! is the highest value that the subroutine can return

c! is the residue amount returned

```
Dim Y!, top!, bottom!, quot!
```

```
If p! = 0 Then p! = 0.0000001
```

```
If p! = 1 Then p! = 0.9999999
```

```
If p! <= 0.5 Then
```

```
  Y! = -Log(2 * p!)
```

```
Else
```

```
  Y! = -Log(2 * (1 - p!))
```

```
End If
```

```
If Y! <> 0 Then
```

```
  top! = 4 * Y! ^ 4 + 100 * Y! ^ 3 + 205 * Y! ^ 2
```

```
  bottom! = 2 * Y! ^ 3 + 56 * Y! ^ 2 + 192 * Y! + 131
```

```
If bottom! Then
```

```
  quot! = top! / bottom!
```

```
Else
```

```
  quot! = 0
```

```
End If
```

```
c! = (quot! ^ 0.5)
```

```
If p! <= 0.5 Then c! = -c!
```

```
Else
```

```
  c! = 0
```

```
End If
```

```
c! = c! * sd! + m!
```

```
If max! Then
```

```
  If c! > max! Then c! = max!
```

```
End If
```

End Sub

Code segment #22:

Sub pareto(p!, a!, k!, max!, c!)

a! is the location variable

k! is the shape variable

max! is the highest value that the subroutine can return

c! is the residue value returned

If p! < 1 Then

c! = k! / (1 - p!) ^ (1/a!)

If c! < 0 Then c! = 0

If max! Then If c! > max! Then c! = max!

Else

c! = 0

End If

Code segment #23:

Sub triangular(p!, l!, m!, u!, c!)

l! is the low bound

m! is the most likely value

u! is the high bound

c! is the residue value returned

Dim h!

If u! = l! Then

c! = u!

Else

h! = (m! - l!) / (u! - l!)

If p! <= h! Then

c! = l! + (u! - l!) * (p! * h!) ^ 0.5

Else

c! = l! + (u! - l!) * (1 - (1 - h! - p! + p! * h!) ^ 0.5)

End If

End If

If c! < 0 Then c! = 0

Code segment #24:

Sub uniform(p!, l!, u!, c!)

l! is the low bound

u! is the high bound

c! is the residue value returned

c! = l! + p! * (u! - l!)

If c! < 0 Then c! = 0

B. The Chronic Exposure Module

The Chronic module uses a data base of pre-calculated per-capita mean food consumption data (g/kg-bw-day) for each food (RAC) and food/foodform used in the CSFII surveys and residue data from a DEEM™ residue file to determine

the mean residue intake (in mg/kg-bw-day) for all individuals in the standard populations. The mean food consumption data base has been pre-calculated using the same algorithms used to generate the DEEM™ data base, except that individual food consumption amounts (after conversion from foods “as eaten” to constituent food-foodform amounts and summed by food-foodform type for the day) are rounded to the nearest 0.1 g in the DEEM™ Acute data base. The population-specific average daily food-foodform consumption amounts have not been rounded in the Chronic data base, but instead saved in real number format (seven significant digits). In addition, food/foodform consumption amounts for each individual were divided by the individual’s body weight before being summed into the accumulation variables used to calculate the per-capita population-specific means. (The rationale for the rounding of individual food consumption records in the Acute program is discussed in the section addressing the Acute data base preparation.)

Mean per capita food consumption for estimating Chronic exposure can be calculated at either the food (RAC) or food/foodform level, using residue data specified at either of the levels in the DEEM™ residue file. A DEEM™ residue file can contain mixed residue data; that is, some foods can be specified at the food level and others at the food/foodform level. The residues specified at the food level will be processed using daily food consumption data at the food level; while any residues specified at the food/foodform level will be processed using daily food consumption data at the food/foodform level. (In the Acute module, all calculations are performed at the food/foodform level, even if the residues are specified at the food level.)

Note that the same DEEM™ residue file can be used for both Acute and Chronic analysis. However, any residue distribution functions and pointers in the residue file are ignored in the Chronic analysis; only the default residue amounts are used in a Chronic analysis. The residue file contains separate toxicology endpoints (NOEL and RfD) for chronic and acute analysis.

The Chronic analysis module calculates per capita daily mean, $tmrc!(j)$, for each of the standard populations $j = 1$ to $k4$, by adding up exposure from each food in residue file and multiplying by the residue amount for that food, then applying adjusting factors and normalizing the exposure amounts to mg/kg-bw-day units. $K4 = 27$ when using the CSFII 1989-91 survey (which includes the Pacific zone) and $k4 = 26$ when using the CSFII 1994-96 survey. These means are reported directly, along with the margin of exposure estimates based on the chronic toxicology endpoints included in the residue file (or as modified when setting up the Chronic analysis).

1. Steps in a Chronic Analysis

Step 1: Read in the residue file specific to the analysis

- (1) Read the toxicology endpoints
- (2) Read past the list of residue distribution functions (not used in Chronic)
- (3) Read the default residue amounts and conversion factors for each food/foodform in the residue file (ignore the distribution pointers and ratios) as set up arrays as follows:

$Tol!(i)$ = residue amount for i th Rac in residue file ($i = 1$ to totalfoods)
 $Cf!(i)$ = conversion factor #1 for i th food
 $Cf2!(i)$ = conversion factor #2 for i th food
 $Rff(i)$ = number of food forms included in the residue file for this RAC
 $FFTol!(l)$ = residue amount for food form FFF(l)
 $FFCf!(l)$ = conversion factor #1 for food form FFF(l)
 $FFCf2!(l)$ = conversion factor #2 for food form FFF(l)

Step 2. Read the NFB water consumption means for each standard population from supporting file. (See the list of NFB water means above.) $Meanw!(j)$ is per capita NFB water consumption from CSFII survey for each standard population, as computed in DEEM™ Acute. RAC(435) is NFB water. Note that NFB water consumption is not reported for each drinking occasion, as are other foods, but rather reported as a total daily amount by the individual and included with the demographic records for that individual.

Step 3. Open the two files of per capita food consumption means for the appropriate CSFII survey (1989-91 or 1994-96). (See the note on preparation of these means above.)

Mean!(j) is per-capita mean food consumption amounts (g/kg-bw-day) derived from the CSFII surveys for each standard population (j = 1 to k4), as retrieved from the Chronic food consumption data base.

K4 is the number of standard populations. (See the list of standard populations and their code above. Custom populations cannot be used in the DEEM™ Chronic module. Note that the Pacific population group is not available in the 94-96 survey because only four regions are available)

Index(rac(i)) is the NSI index number for each of the 950 RACs (same as in the Acute module)

The following variables are taken from the residue file used in the analysis:

Nfx is number of RACs with residue amounts in the residue file.

UseSecond is the Boolean operator used to determine if second adjustment factor is to be used.

Step 4. For each food or food/foodform in the residue file (all of which have a default residue amount), retrieve the food consumption record for that food or food/foodform from the Chronic data base. Multiply the residue amount by the food consumption amount for each of the k4 populations and sum for this exposure amount separately for each population. The resulting sums are reported as the total daily exposure for each population.

Step 5. Calculate the margin of exposure for each population using the toxicology endpoints and report.

See Code segment #26.

Step 6. If a critical commodity analysis and/or complete commodity analysis is desired, the same algorithms are used as shown above, but consumption and residue amounts for individual foods/foodforms are reported as well as the sum or those amounts.

Code segment #25:

Chronic module per capita daily exposure for each standard population

```

For i = 1 To nfx 'For each food in residue file (1 to nfx)
  If index(rac(i)) Then
    If rff(i) = 0 Then
      If rac(i) = 435 Then
        For j = 1 To k4
          mean!(j) = meanw!(survey, j)
        Next
      Else
        Get #1, index(rac(i)), mn94
        For j = 1 To k4
          mean!(j) = mn94.mean(j) 'read in means for the k4 standard populations from data file
        Next j
      End If
      For j = 1 To k4 'these are not computed in display order
        tmrcx! = mean!(j) * tol!(i) * cf!(i) / 1000
        If usesecond Then tmrcx! = tmrcx! * cf2!(i)
        tmrc!(j) = tmrc!(j) + tmrcx!
      Next j
    Else
      For l = kff(i) To kff(i) + rff(i) - 1
        If rac(i) = 435 Then 'assumes that there is only one foodform for nfb water which is same as food
          For j = 1 To k4
            mean!(j) = meanw!(survey, j)
          Next
        Else
          If nsiff(l) Then 'this is a valid ff
            Get #2, nsiff(l), mn94

```

```

ff = mn94.ff
For j = 1 To k4
  mean!(j) = mn94.mean(j) 'read in means for the k4 standard populations from data file
Next
Else 'this ff is not available in fformxxn.fil, set means to 0
For j = 1 To k4
  mean!(j) = 0
Next
End If
End If
For j = 1 To k4
  If mean!(j) Then
    tmrcx! = mean!(j) * fftol!(l) * ffcf!(l) / 1000
    If usesecond Then tmrcx! = tmrcx! * ffcf2!(l)
    tmrc!(j) = tmrc!(j) + tmrcx!
  End If
Next j
Next l
End If
End If
Next i

```

Code segment #26:

Computation of percent of RfD or percent of PAD

rfdchronic! = RfD or PAD to be used in the analysis
prfd! = percent RfD or % PAD as output
meanindex(survey, j) is used to reorder the order in which the k4 populations are reported
noelchronic! = chronic NOEL measure
pnoelfx! = exposure as percent of Noel
mos! = margin of exposure
qstar! = Q star
q! = lifetime risk

```

If compare$ = "R" Or compare$ = "P" Then
  For j = 1 To k4 'display order now
    o = meanindex(survey, j) 'the corresponding mean and pop$(o) location
    If tmrc!(o) Then
      prfd! = tmrc!(o) * 100 / rfdchronic!
    End If
  Next j
ElseIf compare$ = "N" Then 'noel
  For j = 1 To k4
    o = meanindex(survey, j) 'the order we want to display them
    pnoelfx! = tmrc!(o) * 100 / noelchronic!
    If tmrc!(o) Then mos! = noelchronic! / tmrc!(o) Else mos! = 0
  Next
Else
  For j = 1 To k4
    o = meanindex(survey, j) 'the order we want to display them
    If tmrc!(o) Then
      q! = tmrc!(o) * qstar!
    End If
  Next
End If

```

2. **Non-Food-Based (NFB) Water consumption means** (mg/kg-bw-day) by population (calculated in the acute module, used in Chronic module) (See population definitions corresponding to indices below.)

CSFII 89-91:

meanw!(1) = 14.09
meanw!(2) = 14.26
meanw!(3) = 14.98
meanw!(4) = 13.66
meanw!(5) = 13.48
meanw!(6) = 12.47
meanw!(7) = 13.99
meanw!(8) = 14.07
meanw!(9) = 14.86
meanw!(10) = 16.77
meanw!(11) = 13.4
meanw!(12) = 16.35
meanw!(13) = 15.19
meanw!(14) = 25.41
meanw!(15) = 9.45
meanw!(16) = 28.28
meanw!(17) = 25.66
meanw!(18) = 17.06
meanw!(19) = 14.54
meanw!(20) = 18.57
meanw!(21) = 11.39
meanw!(22) = 13.24
meanw!(23) = 12.79
meanw!(24) = 12.14
meanw!(25) = 10.98
meanw!(26) = 12.98
meanw!(27) = 14.86

CSFII 94-96:

meanw!(1) = 13.077
meanw!(2) = 13.433
meanw!(3) = 13.607
meanw!(4) = 12.562
meanw!(5) = 12.68
meanw!(6) = 11.308
meanw!(7) = 13.471
meanw!(8) = 12.487
meanw!(9) = 15.201
meanw!(10) = 15.799
meanw!(11) = 12.704
meanw!(12) = 13.836
meanw!(13) = 14.128
meanw!(14) = 12.674
meanw!(15) = 6.29
meanw!(16) = 14.965
meanw!(17) = 19.039
meanw!(18) = 13.353
meanw!(19) = 14.442
meanw!(20) = 21.098
meanw!(21) = 10.645
meanw!(22) = 12.239

meanw!(23) = 12.237
meanw!(24) = 10.848
meanw!(25) = 12.809
meanw!(26) = 11.7

3. Subroutine to calculate body weight for CSFII participants who do not have a recorded bodyweight

Infant weights are computed by age in month (0-11) and by sex (1 = male, 2 = female)
All others are computed by age in years (0-90) and by sex (1 = male, 2 = female); body weights for participants above 90 are assumed to be the same as for age 90. These body weights were derived from those individuals in the same CSFII survey for which body weight is provided (1989-91 or 1994-96), using average body weight within age intervals in which weight does not vary significantly by age, and using simple straight-line curve fitting techniques for intervals in which a straight line characterizes the weight distribution.

Note that these body weights were computed for individuals without body weights at the time that the acute and chronic data bases were developed for use with DEEM™. Body weight computations are not made during the acute or chronic analyses.

(1) Subroutine compbw for 1994-96 CSFII survey participants

Sub compbw(infwt(), agewt())

Dim m

For m = 0 To 11

infwt(1, m) = 10 + 1.24 * m

infwt(2, m) = 9 + 1.3 * m

Next

Dim y

For y = 1 To 5

agewt(1, y) = 22.1 + 4.7 * y

agewt(2, y) = 19.7 + 4.7 * y

Next

For y = 6 To 11

agewt(1, y) = -1 + 8.5 * y

agewt(2, y) = -3.4 + 8.66 * y

Next

For y = 12 To 16

agewt(1, y) = -51 + 13.6 * y

agewt(2, y) = 6.6 + 8.4 * y

Next

For y = 16 To 18

agewt(1, y) = 160

agewt(2, y) = 132

Next

For y = 19 To 21

agewt(1, y) = 171

agewt(2, y) = 137

Next

For y = 22 To 25

agewt(1, y) = 176

agewt(2, y) = 143

Next

For y = 26 To 30

agewt(1, y) = 184

agewt(2, y) = 146

```

Next
For y = 31 To 40
  agewt(1, y) = 184
  agewt(2, y) = 150
Next
For y = 41 To 50
  agewt(1, y) = 190
  agewt(2, y) = 155
Next
For y = 51 To 60
  agewt(1, y) = 187
  agewt(2, y) = 161
Next
For y = 61 To 70
  agewt(1, y) = 182
  agewt(2, y) = 154
Next
For y = 71 To 80
  agewt(1, y) = 175
  agewt(2, y) = 147
Next
For y = 81 To 90
  agewt(1, y) = 161
  agewt(2, y) = 131
Next

End Sub

```

(2) Subroutine compbw for 1989-91 CSFII survey participants

```

Sub compbw(infwt(), agewt())
Dim m, y
For m = 0 To 11
  infwt(1, m) = 10 + 1.3 * m
  infwt(2, m) = 9 + 1.3 * m
Next
For y = 1 To 5
  agewt(1, y) = 21 + 4.8 * y
  agewt(2, y) = 21 + 4.8 * y
Next
For y = 6 To 11
  agewt(1, y) = -4 + 9.36 * y
  agewt(2, y) = -4 + 9.36 * y
Next
For y = 12 To 15
  agewt(1, y) = -4 + 9.36 * y
  agewt(2, y) = 30 + 6.44 * y
Next
For y = 16 To 18
  agewt(1, y) = 155
  agewt(2, y) = 130
Next
For y = 19 To 21
  agewt(1, y) = 165
  agewt(2, y) = 134

```

```
Next
For y = 22 To 25
  agewt(1, y) = 171
  agewt(2, y) = 138
Next
For y = 26 To 30
  agewt(1, y) = 177
  agewt(2, y) = 139
Next
For y = 31 To 40
  agewt(1, y) = 181
  agewt(2, y) = 146
Next
For y = 41 To 50
  agewt(1, y) = 187
  agewt(2, y) = 151
Next
For y = 51 To 60
  agewt(1, y) = 180
  agewt(2, y) = 157
Next
For y = 61 To 70
  agewt(1, y) = 179
  agewt(2, y) = 151
Next
For y = 71 To 80
  agewt(1, y) = 174
  agewt(2, y) = 144
Next
For y = 81 To 90
  agewt(1, y) = 155
  agewt(2, y) = 129
Next
For y = 91 To 100
  agewt(1, y) = 144
  agewt(2, y) = 130
Next

End Sub
```

C. The RDFgen™ Module

RDFgen™ uses QA'ed sets of spreadsheets containing up-to-date monitoring data from the most widely used source, the Pesticide Data Program (PDP) of the U.S. Department of Agriculture (USDA). These sets of spreadsheets are ready for immediate use with RDFgen™, and are referred to by the following titles: "RDFgen™ pre-extracted PDP data set formatted for RDFgen™ Individual Analyte Mode" and "RDFgen™ pre-extracted PDP data set formatted for RDFgen™ Cumulative Mode."

Additionally, to allow creation of RDFgen™ Cumulative Mode or Individual Analyte Mode PDP residue input spreadsheets filtered for specific sample attributes (such as origin or date collected), Novigen maintains a pre-extracted data set integrating all PDP sample database and residue database information, plus the following helpful standardized fields:

- COMMOD_NAM (Translated version of the two-character COMMOD field, including separation of processed commodities that share COMMOD code with unprocessed commodities, such as green beans/processed green beans and peaches/canned peaches).
- FULL_PESTN (Standardized version of two-character PEST_NAME field).
- BOOKYEAR (PDP data annual report year to which the record belongs).
- YEARY2K (Ensures continued ability to correctly sort and query based on sample date).
- DETECT (Y/N field indicating whether sample is a detect or non-detect sample).
- ORIGINSTD (Standardized version of ORIGIN field, facilitating separation of domestic samples, imported samples, and samples of unknown origin).

This series of spreadsheets is referred to as the RDFgen™ full Pre-extracted PDP data set. Creation of RDFgen™ Cumulative or Individual Analyte Mode PDP residue input spreadsheets or user-defined subsets of the RDFgen™ full Pre-extracted PDP data set is automated by the RDFgen™ Input Generator™ Excel add-in.

RDFgen™ can operate in two primary modes: Individual Analyte Mode and Cumulative Mode. The Individual Analyte mode allows the user to perform the following residue adjustments on any single analyte residue distribution:

- Percent Crop Treated
- Decompositing

The Cumulative mode allows the user to perform the following residue adjustments on any combination of compounds, provided those individual samples have been tested for co-incident residues:

- Percent Crop Treated
- Estimation of concentrations in individual fruits/vegetables based on values in a composite sample (referred to through this document as “decompositing”)
- Relative Potency
- Processing Factors

RDFgen™ may be launched from within DEEM™ or used independently.

The RDFgen™ module of DEEM™ accepts as input any residue data spreadsheet that has been formatted according to a specified format. The user is responsible for the quality and representativeness of the data contained in user developed or modified spreadsheets. In general, Individual Analyte Mode input spreadsheets contain distributions for various commodities tested for a particular chemical, while Cumulative Mode input spreadsheets generally contain distributions for various chemicals tested on a particular commodity. Cumulative Mode should be used when it is desired to combine residue data from multiple analytes into a single distribution. Note that RDFgen™ Cumulative Mode will only use samples from the Cumulative Mode input spreadsheets that have been tested for all of the analytes that are selected for inclusion. Individual analyte mode should be employed when residue distribution adjustments are going to be performed on single analyte’s residue data.