A Model Comparison: Dietary (Food and Water) Exposure in DEEM/Calendex, CARES, and LifeLine

U.S. Environmental Protection Agency
Office of Pesticide Programs

FIFRA Scientific Advisory Panel Meeting
Arlington, VA

April 28-29, 2004

LIST OF ACRONYMS

AHS	American Housing Survey
aPAD	acute Population Adjusted Dose
BMI	Body Mass Index
CARES	Cumulative and Aggregate Risk Evaluation System
CEC	Critical Exposure Commodities
CSFII	Continuing Survey of Food Intakes by Individuals
CS-FF-CM	Food Form, including cooked status, food form, and cooking method
DEEM	Dietary Exposure Evaluation Model
FCID	Food Commodity Intake Database
FF	Food Form (used in this document to mean cs-ff-cm, see above)
HRI	Hampshire Research Institute
ILSI	International Life Science Institute
NCHS	National Center for Health Statistics
NHANES III	Third National Health and Nutrition Examination Survey
NHAPS	National Human Activity Pattern Survey
NHGPUS	National Home and Garden Pesticide Use Survey
PDP	Pesticide Data Program
PRZM-EXAMS	Pesticide Root Zone/Exposure Analysis Modeling System
PUMS	US Census Bureau Public-Use Microdata Samples
RAC	Raw Agricultural Commodity
REJV	Residential Exposure Joint Venture
RP	Reference Population in CARES
WIC	Woman, Infants. and Children (USDA Nutrition Program)

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I. Introduction

Over the last several years, OPP sponsored a number of presentations to the FIFRA Scientific Advisory Panel of pesticide exposure models which have aggregation capabilities: LifeLine, CARES, and DEEM/Calendex. The SAP reviewed each of these models and provided valuable feedback to the Agency. The models all permit a time-based integration of both residential and dietary (food and water) exposures to pesticides. This is performed probabilistically, such that aggregation (or combining) of residues across multiple routes is accounted for in an appropriate and realistic manner. Past SAP sessions for these models resulted in valuable feedback and suggestions and the models have been significantly upgraded and improved, in part, as a result of these SAP comments.

In contrast to previous SAPs where the model developers were invited to make presentations to the SAP, this SAP presentation will demonstrate the results of EPA's own model runs. This document provides background information to the SAP on each of the three models, compares exposure estimates and results generated by each of the three models[1] using a common data set for a hypothetical chemical, and investigates specific reasons why-- and to what extent -- exposure estimates generated by the three models might be expected to differ. Such differences are of interest to OPP in a regulatory context, particularly if the differences are large, are systematic, or span regions of regulatory interest.

Pathways considered and discussed in this document are ingestion through food and ingestion through water. Methods by which the models consider and use data will be discussed and resulting model outputs will be presented and considered. The main "quantitative" focus of the presentation will be a comparison of dietary exposures (food + water) as estimated by each of the three models. Future work by EPA will focus on the residential pathway and a comparison of exposure through all three exposure routes (food, water, and residential lawn use) in an aggregate assessment.

II. Introduction to the Models and Review of Past SAPs

[1] SHEDS is another major model which is available and was developed by EPA's Office of Research and Development. This model is being used by OPP for its assessment of the CCA wood preservative, and was taken to the FIFRA SAP in early December 2003. The focus of this earlier SAP session was exposure of children to CCA-treated wood decks by the ingestion and dermal pathways. We anticipate an examination of the SHEDS model following this SAP to compare results for all four models (Lifeline, CARES, DEEM and SHEDS).

EPA's Office of Pesticide Programs (OPP) is responsible for regulating pesticide residues in food under the Federal Food, Drug, and Cosmetic Act (FFDCA) as amended by the Food Quality Protection Act (FQPA). The FQPA amendments to the FFDCA directed OPP to consider "aggregate exposure" in its decision-making. Aggregate exposure and risk assessment involve the analysis of exposure to a single chemical by multiple pathways and routes of exposure. In general an aggregate exposure assessment considers the potential for pesticide residues in food and drinking water, as well as residues from pesticide use in residential, nonoccupational environments. Prior to the FQPA amendments to FIFRA and FFDCA, OPP generally performed its risk assessments and established the safety of pesticides by examining each pathway separately, i.e., exposures to a pesticide through the food, drinking water, and residential pathways were each assessed independently and no concerted effort was made to evaluate potential exposures through all three pathways simultaneously. As a result of FQPA, OPP has modified its exposure and risk assessment methods to assess the impact of pesticide chemicals entering the body through multiple pathways (food, drinking water, and residential uses) and routes (ingestion, dermal, and inhalation).

A first step in this process was to develop guidelines. The second step was to support and encourage the development of freely available models and software tools that could be used to conduct such assessments. LifeLine was developed by Hampshire Research Institute (HRI) under a cooperative agreement with EPA and USDA and is now managed by The LifeLine Group. CARES was developed by the member companies of Crop Life America and is now being maintained by International Life Science Institute's Risk Sciences Institute (ILSI). DEEM/Calendex was developed by Durango Software and is available for a nominal annual licensing fee from Exponent, Inc. All three models are available to the public. CARES can be obtained free of charge from ILSI; LifeLine is available from The LifeLine Group for a small one-time handling fee; and DEEM can be obtained from Exponent, Inc. for a nominal annual licensing fee.

A. The LifeLine Model

1) Past SAP Reviews

There have been three previous sessions with the SAP that were devoted to the LifeLine software. The first session was held on September 22, 1999, and considered the fundamental design and principles of the LifeLine™ software. Another session held on September 28, 2000 focused on the LifeLine™ architecture and application options in conducting aggregate and cumulative exposure/risk assessment. Finally, a session held on March 16, 2001 was devoted to an HRI LifeLine v. 1.0 System Operation Review. Copies of the presentation materials, Panel discussions, and final reports from these three SAP meetings have been provided to this Panel as have the latest technical manual and users manual. In this section we will briefly summarize some of the features and operation of Lifeline. Extensive additional detail is provided in the source documents.

2) Model Background

Lifeline was developed by Hampshire Research under a Cooperative Agreement with EPA and USDA, with the primary purpose being to develop publicly accessible risk assessment software for a wide range of anticipated users. The current release of Lifeline (Version 2.0) is available from The Lifeline Group. Additional information about the model can be obtained from the following website: http://www.thelifelinegroup.org.

Overview of Lifeline Software and Data Sources

The Lifeline Software provides a probabilistic (Monte Carlo) model of aggregate exposure to pesticides (or other environmental contaminants) that occurs for each member of a simulated population of individuals over that individual's lifetime.

The model begins by selecting an individual's fixed characteristics, and then, based on these characteristics, progresses through each day of that individual's life. The route-specific doses received from diet, residential use of pesticides, and tapwater are calculated for each day and stored. Along with each day's doses, the model calculates rolling averages of dose for user-specified periods of time. When modeling of one individual's entire life is complete, the software saves the measures of dose that are of interest to the user and moves to the next individual. This process is repeated for as many individuals as desired. At the end of the modeling of individuals, the program provides the distribution of the measures of dose across the entire modeled population.

LifeLine uses data from a variety of sources to model each individual's daily exposures (magnitude, likelihood, and frequency) These include:

- Natality data (Birth records) from National Center for Health Statistics (NCHS)
- Residential mobility patterns from Current Population Statistics, US Census, and the American Housing Survey
- Anthropometric data from the Third National Health and Nutrition Examination Survey (NHANES III)
- Pesticide use data from the National Home and Garden Pesticide Use Survey
- Activity data from the National Human Activity Pattern Survey (NHAPS)
- Dietary consumption data from the Continuing Survey of Food Intake by Individuals (CSFII), US Department of Agriculture (USDA)
- Computational algorithms from Residential Exposure SOPs

- Various miscellaneous data from Exposure Factors Handbook

These combined data sets allow the model to define the exposure for each day of an individual's life. The model does this by modeling where people are born, how individuals grow and age, how they move from home to home and region to region, how they use or do not use pesticides, and their daily activity and dietary patterns. The changes that occur within the lifetime of a simulated individual must be kept internally consistent. That is, the software uses rules such that previous characteristics or actions influence future characteristics or actions so nonsensical or unlikely events are appropriately discounted. This is done in two ways. First, wherever possible, records are maintained in which multiple inputs for an individual are collected at the same time. In this way, the correlations among the various inputs are preserved. The second way consistency is maintained is via contingency tables that guide selection of input values relative to age, height, weight, sex, race, and ethnicity. More specifically, Lifeline defines the simulated individuals using "transition rules" that provide for characterization of differences in exposure related behavior among individuals, assign individual characteristics in a consistent manner, and incorporate demographic and temporo-spatial changes that may occur during each simulated individual’s lifetime.

The modeling inputs that are used to define individuals and retain consistency generally fall into three categories:

- Fixed characteristics include sex, race, ethnicity, birth date, body type, maternal socioeconomic status, etc.

- Characteristics that vary slowly over time include long term trends (weight, height, residence location), episodic changes (room sizes, pest pressures, etc.), and cyclic, or periodic changes (weekday vs. weekend, dietary residues, residential pesticide use, etc.)

- Characteristics that vary from day to day (ephemeral) include activity patterns, food consumption, and levels of pesticide residues (e.g., in food, in water, etc.)

The characteristics that are defined for each individual include:

- Permanent characteristics

- Length of the individual's life

- Physical characteristics including:

    - the height and weight of the person throughout life

    - the total surface area of the person throughout life

- the surface area of portions of the person's body (hands, arms, torso, etc.)

- the resting breathing rates for the person throughout life.

- the characteristics of the home and family into which the person is born.

Lifeline models the individuals starting with assignment of initial and fixed characteristics. This process begins with an individual from the Natality Database; data regarding this individual includes sex, mother's race/ethnicity, mother's education, mother's age, mother's census region, mother's urbanicity/setting and birth month. Mortality for simulated individuals is based on standard life tables (NCHS Vital Statistics of the U.S.); mortality is selected as a function of age, race, and sex.

Once "born" and initially housed, the simulated individual's growth is modeled using a biologically plausible model of patterns of change in physiology based on NHANES III data. Normal growth processes are monotonic (height and weight increase with age). Modeled parameters include height, weight, body surface area, and surface area of hands. Each year, the physiology of the individual is updated.

Each individual's mobility is modeled yearly and a binary decision made as to whether the individual moves or not. Based on Census and mobility data, LifeLine models the movement of individuals using information relating to region, tenure, income and urbanicity. If the simulated individual is selected to move, the nature of the new house is modeled based on mobility surveys and the American Housing Survey.[2] Characteristics of residences include the nature of the foundation, size of lot, area of finished space, number and types of room, number of floors, water supply of home, and income quartile. The survey information does not include individual room sizes, the footprint of the house on the lot, or the presence of a yard, so LifeLine assigns room dimensions and bases the presence/absence of yard, garden, and fruit trees from data in the National Home and Garden Pesticide Use Survey and the American Housing Survey.

Simulating Activities/Locations, Pesticide Use, and Daily Diets

Once the residence, ethnicity, age, sex and race are defined for the simulated individual, these data can be used to guide the selection of data on exposure related activities/locations, pesticide use, and daily diets. These predictive factors are usually determined by selecting records from (similar) individuals that match the modeled individual (binning).

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[2] Mobility is determined in a frequency table that provides the probability of moving or not moving to a specific type of home based on an individuals's current residence. The table is comprised of 33 cells, i.e., 4 census regions X 2 settings X 2 units X 2 tenures + Prob(Not moving).

Exposure related activities/locations in LifeLine are defined by NHAPS where record selection is determined by binning individuals based on age, sex, season, region, weekday/weekend, and residence type [3]. It should be noted that NHAPS does not track interactions with pets, playing golf, and gardening; assumptions concerning these activities and associated exposures are made independently by LifeLine (using EPA Residential Exposure SOPs) LifeLine data inputs related to activities/locations include general measure of activity level, surface area-normalized dermal transfer coefficient, clothing protection factor, fraction of hand that is placed in mouth, frequency of hand to mouth activity, refreshment rate for residues on hand, soil intake, and grass intake.

Exposure is estimated with modifications of the basic exposure equations from the EPA December, 1998 Draft Residential SOP's. Post-application exposures are modeled on whether a pesticide product is used that day. If not, residues are based on the previous applications with an adjustment for decline.

Residential Pesticide Use

The model treats residential pesticide use based on two categories. The first category includes residues that occur as a result of the homeowner using a pesticide product or hiring a commercial pesticide applicator. The second category is pesticide residues that the individual encounters that are applied by others (such as at golf courses or public heath uses).

The first category is estimated based on use/usage information supplied by the user and data on pest pressures taken from the National Home and Garden Pesticide Use Survey (NHGPUS). This would include information on the frequency of use of a pesticide in a residential setting and the pesticide residue concentrations that would result from its use. For example, a record from the NHGPUS might include information that, in a given residence, ants were treated in the kitchen three times per year with a crack and crevice spray. LifeLine uses this information to model both applicator and post-application exposures and accounts for declining residues for the latter set of exposures via user-entered data regarding pesticide degradation. Pesticide residues from the second category are estimated based on data supplied by the user.

Modeling Components for Dietary Exposure Assessment

Food Consumption: Food consumption information in LifeLine is derived from the USDA's Continuing Survey of Food Intakes by Individuals (CSFII). The most recent data available (surveys conducted in 1994 through 1996 with a supplemental children's survey in 1998) comprise a nationally-representative, statistically based survey of individuals residing in 50 states and DC. A total of 20,607 individuals were interviewed over the period of the survey. The interview design was for 2 non-consecutive days using in-person 24 hour recalls (ca. 3-10 days

[3] This results in a total of 108 bins – age and sex (9 bins); season and region (3 bins); weekday/weekend (2 bins); single vs. multi-family home (2 bins).

apart) covering all seasons of the year and all days of the week. Data collected in the surveys included information on sources, amounts, and time of consumption of foods, and sources and amounts of water consumed. LifeLine relates the foods, as reported in the CSFII, to raw agricultural commodities by way of recipe files. The most current food consumption survey (CSFII 1994-96,1998) is related to raw agricultural commodities by recipes supplied by USDA/EPA as a result of their collaborative production of the Food Commodity Intake Database (FCID), which serves as a companion data set in which intakes are presented in terms of food commodities rather than foods as consumed (for example, as wheat flour and whole egg rather than as noodles). The FCID has undergone revisions since its public release in 2000. Version 2.0 of LifeLine utilizes the original version of the FCID but will be revised in the near future to incorporate recent changes made by OPP in the FCID (the new OPP FCID is termed the "revised FCID").

Pesticide Residues: Pesticide residues on foods are modeled based on user input of either single, point-estimate values for raw agricultural commodities or a distribution of residues[4] These residue values may be modified by the user to account for any concentration or reduction of residues that may be expected from food processing, storage, cooking, etc.

Dietary Exposure: LifeLine models dietary exposure in two distinct phases.

In the first phase, a Food Residue File is used to create a unique distribution of residues for each food in the CSFII survey, as eaten. The residue values provided by the user (either deterministic single-valued point estimates or distributions) are applied with the user-supplied modifying factors to each food reported on each eating occasion in every CSFII record. The resulting distribution of food residues is tagged for identity and saved as a record. For example, Lifeline would model the distribution of residue concentrations on a cheese pizza by using residue values on each food component of that pizza (e.g., milk, wheat, tomatoes, etc.) along with a standard recipe for cheese pizza to produce a distribution of residue concentrations in pizza.

The second phase, the Exposure Assessment phase, employs the Food Residue Files and CSFII records for the amount of food reported eaten by each individual. Groups of records from the CSFII are selected that are consistent with the description of the population described by the system user (e.g., infants<1, children 3-5, etc.) These records define the dietary profiles of the individuals within that chosen population. The developers of LifeLine have extensively examined the CSFII records to reveal patterns of dietary habits that may be characteristically similar within groups of individuals and different between groups. CSFII records were analyzed in an effort to identify patterns of dietary behavior. Among the parameters that were examined were body mass index (BMI), caloric intake, frequency of eating within a day, characteristics of the eating occasions-number of foods per eating occasion, food selection overall-number of foods

[4] For a single point estimate, a tolerance of 1 ppm for chemical X on eggplant may be used to model the occurrence of residues in foods containing this raw agricultural commodity. For a distribution of residues, residues of chemical Y on wheat may be based on monitoring data available from the USDA Pesticide Data Program [PDP] which may be used to model residues in foods containing wheat products.

eaten per day and number of different foods eaten per day, and mass of food eaten per day per unit body weight. These parameters were examined together within a matrix of age, sex and season. There were few differences observed between males and females of the same age. These analyses were used to group food records into age-based bins as follows:

Bin 1: Nursing infants less than one year

Bin 2: Non-nursing infants less than one year

Bin 3: Age 1 year

Bin 4: Age 2 years

Bin 5: Age 3 years

Bin 6: Age 4 years

Bin 7: Age 5 years

Bin 8: Ages 6-7 years

Bin 9: Ages 8-11 years

Bin 10: Ages 12-14 years

Bin 11: Ages 15-25 years

Bin 12 Ages 26 and above

When an exposure analysis is run, a CSFII record is selected for each iteration from the appropriate bin of records to supply the mass of each food item consumed (note that this is not normalized to body weight). This value is multiplied by a concentration selected from the residue distribution for that food item as was built in the Food Residue Files. This product is saved and represents the mass of the pesticide ingested through that particular food item; the overall sum of such food item residues for a given individual within any specified time period (typically one day) represents the mass of pesticide residue to which the individual is exposed through the diet for this time period.

This process is repeated by drawing additional sets of residue values from the residue table to create a series of exposure values across a period (season) for that individual. The user has the option of either repeating that individual's same diet for the entire season or randomly drawing another diet from a similarly binned individual. Thus, the software allows estimation of these exposure values using the same CSFII individual record for a whole season or randomly drawing other CSFII records from the appropriate bin for each day of the season. It is important to note

that while LifeLine does track each individual's life history, this information in its entirety is not saved. There are three results saved for each season of each individuals life; the exposure from the maximum day within each season of an individual's life, the exposure from each season's average value within an individual's life, and a random exposure value from each season from an individual's life. If a person lives to be 70 years, for example, a total of 4 x 70 exposure records would be saved by the program (i.e., 4 seasons per year x 70 years). These would represent either the exposures from the maximum exposure day within each season, the average daily exposure for each season, or the exposure from a randomly selected day from each season.

The above process is repeated for the duration of this individual's life, saving a set of records -- containing the seasonal maximum, the seasonal average, or a random selection from the season – for each of the four seasons of each year. The completed individual exposure history represents one iteration of the assessment. The number of iterations employed can be selected by the system user.

Tapwater Exposure

Lifeline in able to evaluate exposures through tapwater. Each individual's consumption of tapwater is taken directly from CSFII and includes both direct water and indirect water (water from food).

On the residue side, the user can input either deterministic or distributional values of residue data for tapwater exposure. Residue concentrations in LifeLine are selected from 4 seasonal distributions in accordance with the season for which exposure is being assessed. Each of the four seasonal distributions can be optionally subdivided on the basis of region, setting (urban vs. rural), and type of water supply(e.g., public source, private well, etc.). These data are available for each simulated individual through the AHS. The same 4 residue values are repeated each year that the individual is in the home. In order to maintain reasonable consistency with prior concentrations to which an individual has been exposed, each household is randomly assigned a percentile and the corresponding seasonal values for that region, setting and water supply type is selected. In this way, upper percentile households will remain in the upper percentiles and lower percentile households will remain in the lower percentiles.

Dose Estimates

The model tracks a group of individuals through their lifetime, producing exposure histories. The histories consist of the route-specific doses for each day of an individual's life. These histories provide the basis for deriving a number of different estimates of dose. These include one day doses randomly chosen from within each season of an individual's lifetime. It is also possible to evaluate a group of consecutive days from an individual's exposure history over any given time period. Chronic and lifetime doses can be estimated by summing an individual's entire exposure history to produce a lifetime average daily dose. The distribution of these values

across individuals allows an evaluation of the distribution of the doses used for the assessment of chronic endpoints and carcinogenic risks. The model also tracks the mean and maximum daily dose (or group of daily doses) on a seasonal basis throughout an individual's lifetime. In this way, the model permits the user to explore exposure distributions from a wide range of perspectives.

B. The CARES Model

1) Past SAP Reviews

There has been one previous session with the SAP that was devoted to the CARES software (April 30 - May 1, 2002). This review focused on the operation and documentation of the software, the model design, and model results.

Copies of the presentation materials, Panel discussions, and final Panel report from this SAP meeting have been provided to this Panel as have the latest technical manual and users manual. In this section we will briefly summarize some of the features and operation of CARES. Complete details are provided in the source documents.

2) Model Background

In 2000, Crop Life America funded the Cumulative and Aggregate Risk Evaluation System, CARES, to address FQPA mandates for short-term, intermediate duration, and lifetime food, drinking water and residential aggregate and cumulative exposure and risk calculations. CARES development has proceeded through a cooperative team effort of Crop Life America staff and member company scientists and expert exposure and risk assessment consultants, Infoscientific, Inc., Novigen Sciences, Sielken & Associates Consulting, Inc. and Summit Research, with participation by EPA and USDA.

Recently the custody of CARES has been transferred to ILSI with the goal of making the model publically available while providing an administrative mechanism for distributing and maintaining the software. The primary technical responsibility for the development of the CARES software has and continues to be with InfoScientific, Inc. (Henderson, NV). Additional information is available from http://www.infoscientific.com/home.htm

Model Design

The CARES software consists of several modules, including a Population Generator; Dietary, Water, and Residential Modules; Aggregate and Cumulative Assessment Modules; and a Contribution and Sensitivity Analysis Module. The Population Generator is used outside of CARES to generate a reference population of 100,000 individuals selected from 5 million

individuals who completed the long form of the 1990 U.S. Census (the PUMS dataset containing 12,500 individuals) This PUMS dataset was sampled using a stratified random design to produce a 100,000 member CARES Reference Population (RP). Stratification was based on race/ethnicity and age/sex and designed so as to contain a certain minimum number of individuals to support analysis of upper percentiles of exposure for subgroups of interest. To account for this stratification, each member of the RP is appropriately re-weighted so that the RP as a whole is representative of the U.S. population as defined by the 1990 Census. Individual 365-day exposure profiles are created for each of these individuals by algorithms in the Dietary, Residential, or Drinking Water modules. The dose from exposure is aggregated and/or cumulated in the respective modules and a common risk metric is calculated. The Contribution and Sensitivity Analysis module permits the user to analyze the output from the Aggregate & Cumulative module to identify the contributing sources of exposure for individuals or subpopulations.

U.S. Census/PUMS data contains many descriptive variables of interest for each person in RP. However, the PUMS data is insufficient to completely model an individual's exposure. For example, the PUMS (and thus the RP generated from this) contains no data on the sampled individual's dietary consumption. The requirement to generate a comprehensive pesticide exposure profile for each individual in the RP makes it necessary to match individuals in the RP with individuals in other databases containing additional, more exposure-specific information. Since it is not possible to create an "exact" match, critical attributes in the reference population were matched to the same attributes in alternate surveys including the USDA's CSFII for data on consumption patterns and NHAPS for data on activity patterns. According to pre-established criteria, some attributes are matched exactly; for example, the sex and ethnicity of subjects reported in the Census are exactly matched to the same attribute reported for subjects in CSFII/FCID food intake databases. Other attributes were matched less precisely using a measure of dissimilarity (Gower's Similarity Index). For example age was given a high priority for closeness of matching in the age range from 1 to 12 years (exact by year up to age 12 and similar by month of birth), whereas youths were matched within a range of 12-19 years); after age 19, age was not given a priority for matching. In addition to age and sex, other criteria that were used to match individuals from the RP to other individuals (in the CSFII, NHAPS, or REJV [Residential Exposure Joint Venture]) include region, urban vs. rural status, household size, race/ethnicity, household income, poverty level/category, employment status, education level, and home ownership status.

Using this procedure, attributes not available for the reference population (e.g. daily food and water consumption) were assigned to individuals in the reference population based upon subjects in another survey, in this case CSFII/FCID. By combining the data available in the PUMS with matched data in the CSFII, the RP adds data on body weight, height, pregnancy status, as well as one-day food consumption data to the data available in the PUMS.

Dietary Consumption Profile

CARES next creates for each individual a 365 day consumption profile. CARES begins with the 1 or 2 days of records present for each individual in the CSFII and uses additional statistical matching to match similar individuals and develop consumption diaries as "fill-in" for remaining days of the year. This second round of matching used to "fill in" the remaining 363 days is similar to the first that was used to match the PUMS data and the CSFII data except that person-specific and day-specific characteristics were compared for the person in the RP to consumption days of other surrogates in the CSFII. Example parameters that were matched included the calendar date (ideally, to within +/- 7 days in order to preserve seasonal nature of consumption data), age, day of week, and characteristic diets (e.g., vegetarian, low fat, low salt, diabetic, etc.). Using this algorithm, the process finds the 3 to 5 person-days of consumption data which most closely fit the necessary requirements to be considered as an acceptable fill-in value and randomly selects one of these to be inserted into the consumption profile for the date of interest. This is done for each individual in the CARES RP until all 365 days of an individual's profile are filled.

Residential Exposures

Demographic information in the Census (e.g. region of the country, socio-economic status, housing type, pet status) is used in combination with user provided information on pesticide use (amount, frequency, and temporal pattern of use; dissipation; and transfer) and human behaviors that would bring the subject in contact with the chemical. Key elements for residential exposure modeling include the demographics of residents (e.g., region, family composition, sex, age, bodyweight); lifestyle patterns of residents (e.g., activity and product/product use patterns); and residential factors (e.g., housing type, air exchange rates, surface types, etc.) Based on this information, the CARES residential model uses an Event Allocation Module to create a temporal profile of residential-related product use occurrences, and includes a product co-occurrence matrix that can be derived from available survey instruments. The daily dose arising from residential exposure is calculated for up to 18 different scenarios selected based on EPA's Residential SOPs:

- Lawn Care
- Vegetable Garden Care
- Ornamental Plant Care
- Tree Care
- Pick Own Fruits/Vegetables
- Crack & Crevice Treatment
- Termite Control
- Rodent Control
- Pet Care
- Outdoor Fogger Use
- Indoor Fogger Use

- Indoor Treatment
- Paint/Wood Treatment
- Impregnated Materials
- Detergent/Handsoap Use
- Swimming Pool Use
- Golfer
- Public Use
- Custom (future)

Drinking Water Exposures

The daily dose from exposure via drinking water, is calculated by using regional and temporal specific pesticide concentrations provided by the user (based on monitoring and/or modeling), by water intake and body weight data in the CSFII/FCID, and demographic information in the Census.

C. The DEEM/Calendex Model

1) Past SAP Review

DEEM was the subject of an SAP review on February 29, 2000 and Calendex was considered in the Panel session of September 27, 2000. A key change in the DEEM/Calendex software that occurred with the release of DEEM-FCID/Calendex-FCID was the incorporation of the USDA/EPA Food Commodity Intake Database (FCID) as the means of translating CSFII foods as eaten to raw agricultural commodities for which EPA regulates pesticide uses. The FCID is a publicly available database and its incorporation into DEEM replaces the proprietary recipes that are part of the earlier versions of DEEM. Exponent has also decided to make this software available at a nominal annual licensing fee that covers production, shipping and handling costs. The details of the license agreements required can be found on the company web site (www.exponent.com).

Materials from previous SAP Panel consideration of DEEM/Calendex have been provided to the Panel as have the latest technical manuals and users manuals. In this section we will briefly summarize some of the features and operation of the software. Extensive additional detail is provided in these source documents.

2) Model Background

DEEM/Calendex - DEEM-FCID/Calendex-FCID Models

DEEM and Calendex are software systems developed by Durango Software and licensed and supported by Exponent (Formerly Novigen Sciences, Inc.). DEEM was developed as a model for conducting Monte Carlo dietary risk assessments; Calendex followed later as an additional module that allows calendar-based aggregate assessments of residential and water exposure. Both modules are required to conduct an aggregate assessment that includes a critical exposure commodity (CEC) report on food exposure. DEEM-FCID and Calendex-FCID are the most current versions of these modules and will be the subject of the remainder of this background segment.

DEEM-FCID

This module provides a probabilistic assessment of dietary exposure/risk for the US population or subsets of the population (several preset sub-populations are in the software but the user can define others). The population of interest is simulated from the CSFII using the FCID to relate foods as eaten to raw agricultural commodities. Estimation of residues on raw agricultural commodities are input by the user and can be any combination of residue distributions and single estimates. The user can set the number of desired iterations for the Monte Carlo assessment with an iteration involving the summing of exposure for one person in the CSFII on one day, derived from a random draw of residue concentrations for each food consumed for that day. The process is repeated for as many iterations as specified by the user with each iteration involving a random draw of residue concentration. Thus, the process works through all of the individuals in CSFII who responded for both days of the survey and who match the population parameters chosen by the user (age, sex, ethnicity, etc.). The resulting frequency distribution of the exposure estimates for all individuals on all days is used, after accounting for each survey respondent's sampling weight, to derive a frequency distribution of dietary exposure for the population chosen.

DEEM-FCID also has a Critical Exposure Commodity (CEC) module that allows the user to analyze exposure records that contribute to the higher end of the frequency distribution. The module can save records in the top few percentiles of the distribution containing information on the CSFII individual and consumption day used, the amounts of foods consumed, and the residue levels on these foods.

Calendex-FCID

Calendex-FCID provides for repeated daily DEEM-type analyses of dietary exposure along with residential and water components for up to a year. For the non-dietary part of the analysis the user supplies pesticide product use rates and frequency of application, etc., estimates of concentration changes on days before, during and after treatment. Exposure factors are provided by the model subject to modification by the user.

Data used in the model include:

1. The percent of households where the treatment will be applied during a typical year (for the entire US or by region)
2. The percent of these treated professionally and self treated by an occupant.
3. The exposure routes: inhalation, dermal, and oral
4. The maximum active exposure period for an application
5. Up to ten application scenarios and their probability of occurrence
6. The probability that a treatment occurs on any given day of the week and that the initial application is made on any given week of the year
7. Assignment of contact rates, residue amounts, and residue degradation parameters to each occupant age category included in the analysis, for all application scenarios or for any given set of application scenarios
8. Applicator exposure-related functions (including contact functions and residue functions) for inhalation, dermal and oral exposure

The population for non-dietary exposure is also modeled from the CSFII records.

The user can specify the dates of use of a pesticide product based on available information on seasonality of use.

Drinking Water Exposures

The daily dose from exposure via drinking water, is calculated by using regional and temporal specific pesticide concentrations provided by the user (based on monitoring and/or modeling), by water intake and body weight data in the CSFII/FCID, and demographic information in the Census.

III. Model Comparison/Contrast Summary

A. Introduction

Above, we have briefly described three aggregate models -- Lifeline, CARES, and DEEM/Calendex designed to estimate exposure to and risk from pesticides. These descriptions alluded to differences among the models that could be expected, at least in some cases, to result is differences in exposure estimates even when identical (or nearly identical) datasets are assessed. Such differences are of interest to OPP in a regulatory context, particularly if the differences are large, are systematic, or span regions of regulatory interest. This section of the document expands upon earlier discussions of the models with an emphasis on some of the fundamental differences in databases and approaches that each of the models take to estimate dietary exposure (food and water). Additional discussion in this section covers several base comparison analyses that OPP has performed. Finally, this section concludes with comparisons of simultaneous model runs performed with LifeLine and DEEM as part of our routine dietary

risk assessment procedure; these regulatory analyses compare the results of the two models in side-by-side runs.

B. Differences in LifeLine, CARES, and DEEM/Calendex

Important differences associated with the dietary modules of models include their design assumptions and data sources and databases which may lead to differences in estimated exposures. Some of the more potentially significant differences are in the:

- Reference population
- Binning Methodology by which each model groups individuals
- Reference population bodyweights
- Model (or sampling) weights

Table 1 below summarizes differences among the dietary modules of the three models, each of which are further described below.

Table 1

Factor	DEEM-Calendex	CARES	Lifeline
Reference Population	CSFII Survey	Census (PUMS)	Natality (NCHS)
Binning Methodology	Random (2 Day Diaries)	Gower Dissimilarity Index	Random (Age, Season)
RefPop Bodyweight	CSFII normalized	CSFII normalized	Lifeline (NHANES)
Model Weight	CSFII Survey	CARES (Stratified)	Equal Weights (Random)
Modeled Population	US Population	US Population	US Population (Natality, Mortality)

1) Reference Population

Each model begins with a somewhat different reference population as a basis of its exposure calculations. Briefly, LifeLine uses as a basis for its "starting population" natality data from the NCHS. It is through LifeLine's population generator that individuals are born, grow, move, age, and die. LifeLine tracks each day in each individual's life and develops an internally consistent exposure history based on cross-linked databases such as the U.S. Census Bureau's American Housing Survey, National Home and Garden Pesticide Use Survey, etc. CARES uses

as its reference population a data set of 100,000 individuals obtained from a 5% PUMS sample from the U.S. Census. This reference population has been designed to 1) contain a sufficient number of individuals in each of a number of regulatory subpopulations of concern such that high-end exposure percentiles can be adequately predicted; and 2) be representative, after weighting, of the U.S. population as a whole. DEEM uses the USDA's CSFII as the foundation of its calculations using each reported individual (or, more precisely, each of the ca. 40,000 person-days) directly in its exposure estimates.

2) Binning Methodology

The three models also differ in the methods and characteristics which are used to group individuals into common bins. Such binning is necessary in order to permit the use of multiple databases to estimates longitudinal exposure. For dietary exposure estimates, LifeLine groups individuals by age and season (age groups are: non-nursing infants, nursing infants, 1 y.o. 2 y.o., 3 y.o. 4 y.o. 5 y.o. 6-7 y.o., 8-11 y.o., 12-14 y.o., 15-25 y.o. and 26+ y.o.). That is, to generate a series of diets for an individual over that individual's lifetime, LifeLine matches (and draws from) only those individuals which have similar ages and only from those consumption diaries that arose from the specific season of interest. For example, in creating a series of consumption diaries for the spring season for a 6 year old child, only consumption diaries for children aged 6 or 7 that were obtained by CSFII during the spring are used. When in the LifeLine model the season advances to summer or the child becomes 8, the matches are taken from only those bins. Other factors such as ethnicity, sex, and region do not play a role. It is in this way that a longitudinal series of diets for each LifeLine individual over that individual's lifetime is constructed. CARES uses similar binning methodology, except the CARES bins are constructed using additional criteria presented earlier in this document. Matches are constructed based on the Gower dissimilarity index. With DEEM, the CSFII diaries are used directly; consumption diaries are only used for those individuals reporting 2 days of consumption.

3) Reference Population Bodyweights

The three models also differ with respect to how bodyweight is used. Both DEEM and CARES estimate exposure as the product of consumption (on a g food/kg bodyweight basis as derived from CSFII) and pesticide residue concentration (ug pesticide/g food). For Lifeline, the amount consumed (in grams) is obtained from the CSFII and the body weight is assigned to each individual (for each individual's year) by means of a survey-based mathematical algorithm which considers how weight is related to height and how height changes with age.

4) Model Weights

Model weights used by each of the exposure softwares are different. Lifeline is self-weighting in the sense that individuals are "born" on the basis of (and in direct proportion to) natality data from the NCHS. [5] The CARES reference population is weighted so as to produce a

[5] Each individual born in Lifeline has an implicit model weight of 1. This is because the births are in direct proportion to actual births in the U.S. – as reflected in the 1990 Natality data. Lifeline offers a second

population similar to that of the U.S. population as determined by the 1990 Census. DEEM uses CSFII sampling weights directly which, in turn, reflect the U.S. population.

C. LifeLine vs. DEEM Comparisons

OPP has been using the DEEM exposure software since approximately 1998 and has an extensive history of performing and evaluating dietary risk assessments with this model. Beginning in November 2003, OPP risk assessments have been performed with both DEEM (or DEEM/Calendex) and LifeLine. This has been done in order to compare in a systematic fashion the estimated exposures obtained from DEEM with those obtained from LifeLine using data from regulatory reviews. Overall, OPP has found close agreement between the DEEM and LifeLine estimated exposures. Typically, differences have been less than 3% at the 95th percentile, less than 10% at the 99th percentile and less than 20% at the 99.9th percentile for assessments using acute endpoints. For comparisons using chronic endpoints, percent differences have generally been less than 5%. A more complete comparison of these results is presented Appendix B. As can be seen, for most of the concurrent runs, there is little substantive difference between exposures as predicted by DEEM and those as predicted by LifeLine[6].

D. 1000 ppm Tomato Consumption Analyses

OPP has also performed additional QA/QC checks on each of the three models by estimating the exposure that would result from residues of 1000 ppm in a single commodity. This was done in LifeLine, DEEM, and CARES for fresh tomatoes[7]. The resulting predicted exposures (in mg/kg) exactly correspond to the consumption values which were used by the model if consumption is expressed in g food/kg bodyweight (see Appendix A for a derivation of this result). The following table presents these results at various percentiles:

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option by which individuals can use weights which reflect CSFII weights.

[6] However, differences do exist and can potentially be more pronounced for certain assessments. It can be difficult to quantitatively pinpoint the exact reasons for these differences since each software model is distinct and can use different base assumptions and different databases. Determining the reasons for these differences can be important in those cases where the results span thresholds which hold regulatory significance. One of the topics of this SAP is to present OPP's attempt to produce a standardized procedure by which the reasons for these differences can be more fully explained.

[7] This corresponds to Food Commodity Code 8003750 and Food Form 110 in DEEM and CARES; in Lifeline, this corresponds to Crop Group 8, Food 3750, and Food Form 110.

Table 2 Comparison of Lifeline, CARES, and DEEM-FCID Model Predictions for 1000 ppm Tomato Input using 100%CT				
Age Group	Percentile	Model-Predicted Consumption g food/kg bw		
		Lifeline	CARES	DEEM-FCID
Children 3-5 yrs old	99.9	10.45	10.82	9.10
	99	4.02	3.57	3.58
	95	1.11	1.13	1.17
Adults 20-49 yrs old	99.9	6.26	6.69	5.35
	99	2.90	2.47	2.30
	95	1.32	1.33	1.13

As can be seen, the predicted values are reasonably similar to each other which reflect overall similarity in model databases for consumption of this commodity.

IV. Approximating Consumption Distributions for Models via SAS Simulations

A. Introduction

Detailed technical documentation is provided for each of the probabilistic risk assessment models (technical & user manuals, previous SAP materials, etc.) regarding its reference population, binning design, and modeling weight. A model's reference population and its binning design together determine the expected (or actual) frequencies that the CSFII consumption diaries are used in a simulation. The model weights project those simulated exposure days up to the modeled population. Since the selection of food diaries and food residues are statistically independent, the food consumption patterns and the anticipated residue distributions may be analyzed separately. In particular, the distribution of food consumption for a population subgroup (e.g., grams of apple juice consumed/day by 3 to 5 year olds) can be estimated using the information regarding the model's design, and analyses for single RAC scenarios can be compared and contrasted based on each model's design and may be performed without performing a monte carlo simulation via CARES, LifeLine, or DEEM/Calendex (discussion of limitations below).

Figure 1 Consumption Distribution for Apple Juice, 3to5 Year Olds

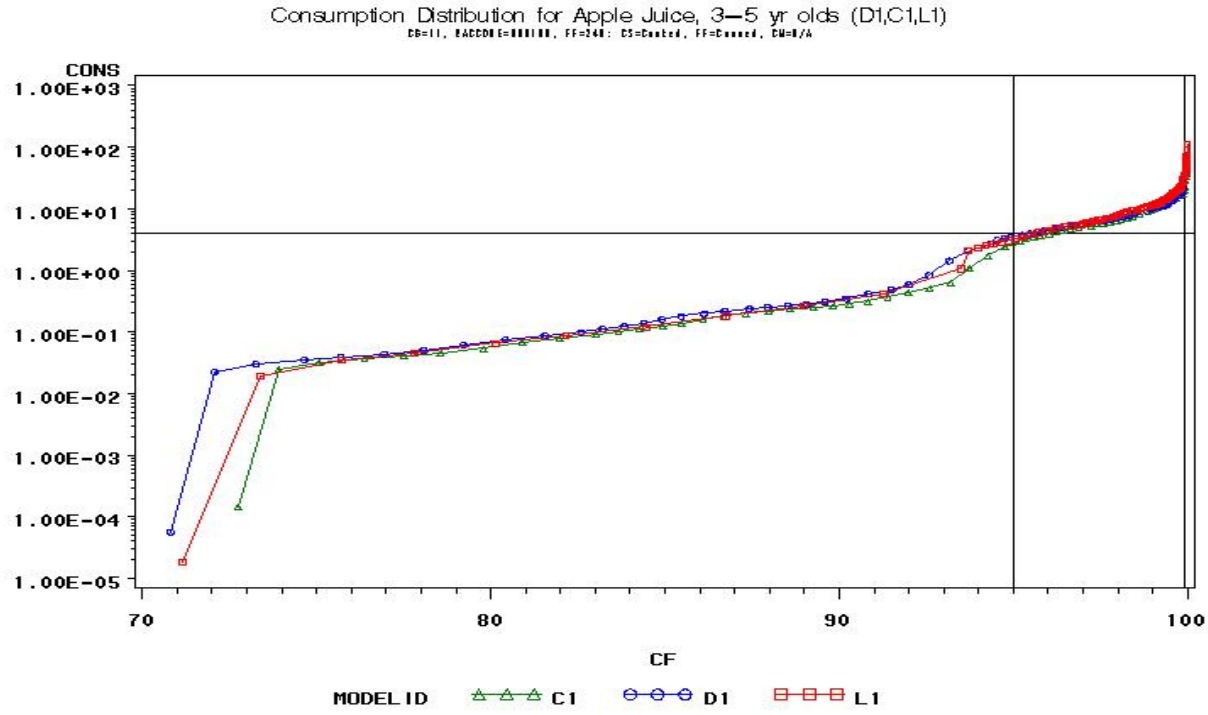


Figure 1 (above) was produced in a SAS simulation of dietary consumption of apple juice for each model (CARES=C1, DEEM=D1, and Lifeline=L1) and illustrates that approximately 5% of the time (days), toddlers (3 to 5 year olds) drink almost 4 grams/kg bwt of apple juice in a day (weighted). These consumption distributions differ for the three models since each model will differ in their expected frequencies for using the CSFII diaries, and weights applied for each use. All three model approximations provide reasonably similar predictions of apple juice consumption above the 95th percentile (weighted) via the SAS simulation. This graphical comparison suggests that residues at 10 ppm (e.g., tolerance) will provide exposure of at least 0.04 grams ai/kg bwt/day for 5% of the projected exposure days. At lower percentiles - and for different RACs, the three models may produce different predicted consumption amounts due to varying designs (@95%: 3.76-DEEM-Calendex, 2.85-CARES, 3.23-Lifeline).

We compared the predictions from these approximated models to the predictions from the actual models for a series of simple scenarios to evaluate the accuracy of these model approximations. In particular, we assumed a single residue of 1,000 ppm on a single RAC. Based on the dietary exposure algorithm explained in Appendix A, the predicted exposures from this scenario is equivalent to the model's distribution of amount consumed (grams food/kg bwt).

The consumption approximations (SAS simulations) to each of the respective models enable us to predict which RACs will produce larger differences across these models. The ability to

approximate the respective probabilistic risk assessment models also provides a cost effective means to evaluate the effects of the various models' design features. These model approximations may be used to help determine why the different models produce different (or similar) predictions - e.g., one can observe that CARES uses a particular diary much more (or less) frequently than DEEM or LifeLine in generating the exposure distribution for that subgroup.

By modifying the respective approximated SAS-simulation models, we can also obtain a better understanding of the effects of various modeling design features. For example, one can quantitatively assess the following types of issues: What is the consequence of DEEM utilizing only 2 day diaries? How might the DEEM-Calendex model predictions change if the Reference Population was somehow extended such that the 1 day diaries were also included in the assessment? What is the consequence of the CARES binning algorithm (Gower Dissimilarity Index)? Does CARES provide higher (lower) exposure since some diaries with high (low) consumption values are used with relatively high (low) frequency? For LifeLine what is the consequence of random drawing from the age-season bin? What is the effect of using the CSFII survey weights to sample food diaries? Can we expect to find larger effects for certain RACs? What is the effect of the LifeLine model using its physiometric models for bodyweights to determine consumption (=Amount consumed/Lifeline Bodyweight)? These SAS model approximations can also be used to obtain a quick estimate of both the model's exposure at the upper percentile (99.9th), as well as the major commodities contributing to exposure at that upper percentile. These single RAC approximations also enable us to determine relatively quickly if a particular set of residues will provide for levels of exposure that exceed some magnitude of concern.

A limitation to these model approximations is that one is not able to estimate an individual's co-occurrent exposure from multiple foods (RAC-food forms) in separate consumption distributions. And so while we know that 5% of the person-days may have apple juice consumption exceeding 2 grams/kg bwt, we do not know what other items these high apple juice consumers are having that day. One needs to run the full probabilistic risk assessment model to account for co-occurrent exposure from multiple foods (RACs). However, CEC analyses performed on actual food exposure assessments have shown most individuals at the high exposure tail (i.e., 99.9th percentile) obtain most of their daily exposure from a single RAC. Therefore we believe it is appropriate to use these model approximations to obtain a rough estimate of the models' exposure at the 99.9th percentile, as well as identify the RACs that contribute to exposure (i.e., Critical Exposure Commodities or 'CEC assessment') at this upper percentile.

Next, we will provide some background information on the USDA CSFII survey and describe how the consumption distributions were approximated for the DEEM-Calendex, CARES and the LifeLine models respectively using SAS. For DEEM-Calendex, an alternative 'DEEM-Calendex' approximation was developed using all of the food diaries. For Lifeline, two alternative 'Lifeline' model approximations were developed using SAS. The first alternative model uses the CSFII respondents reported (or imputed) bodyweights rather than the Lifeline's bodyweight models to calculate consumption. The second alternative model approximates if the

CSFII survey weight option is selected. The last section highlights the approach for aggregating exposure via the full probabilistic model from multiple RACs, and computing a CEC report for these individuals using the SAS approximation model in the upper percentiles.

B. The 1994-96, 1998 Continuing Survey of Food Intake by Individuals (CSFII)

The 1994-96 CSFII Survey was designed primarily to obtain updated information on food consumption patterns in the US. The 1998 supplement was designed to collect additional data for children up through age 9. These data have been used by nutritionists and by program analysts evaluating the impacts of various food programs administered by the USDA (i.e., food stamps, WIC). The survey design produced several sets of survey weights. Two survey weights that are of interest here are: (i) the 1 day weights for those participating in the 1994-96, 98 Survey (WT4_DAY1), and (ii) the 2 day weights for those participants in the 1994-96, 98 survey that provided two days of food diaries (WT4_2DAY).

Table 3 provides some summary statistics regarding the 1994-98 CSFII survey. There were 12,364 households that participated in the survey. At least one member of the household provided at least one day of food diary. Overall, 21,662 individuals provided at least one day of food diaries. Of this total population, 20,607 individuals provided two days of food diaries. This relatively high two day participation rate of 95.1% (=20,607/21,662) did not vary significantly across age groups. [The 1989-91 CSFII survey collected as many as three days of food diaries from individual participants.] The survey sample sizes indicate an oversampling of children: the survey collected food diaries for 1,551 infants, 2,191 1-2 year olds, 4,579 3-5 year olds, and 2,188 6-12 year olds. The survey also collected data from 2,938 females between 13 and 49 years old - the EPA category for females of child bearing age.

Table 3 CSFII Descriptive Statistics

AGE	Total Persons	Total Persons w/2 Day Diets		Total Persons			Total Daily Diets	
		Male	Female	w/ 2 Day Diets	w/ 1 Day Diets	Total Daily Diets	2 Day	1 Day
US General Population	21,662	10,439	10,168	20,607	1,055	42,269	41,214	1,055
Infants (0 year old)	1,551	723	763	1,486	65	3,037	2,972	65
1 to 2 years old	2,191	1,048	1,048	2,096	95	4,287	4,192	95
3 to 5 years old	4,579	2,230	2,161	4,391	188	8,970	8,782	188
6 to 12 years old	2,188	1,084	1,005	2,089	99	4,277	4,178	99
13 to 19 years old	1,281	603	619	1,222	59	2,503	2,444	59
20 to 49 years old	4,970	2,358	2,319	4,677	293	9,647	9,354	293
50+ years old	4,902	2,393	2,253	4,646	256	9,548	9,292	256
Females 13 to 49	3,079	0	3,079	2,938	141	6,017	5,876	141

Data on the individual's bodyweight was not collected for approximately 3.7% (=808/21,662) of the individuals in the survey. The USDA provided a means for imputing bodyweights based on the respondents age and sex. These values and decision rules are presented in Table 4.

A total of 41,214 (=20,607x2) diaries were collected from the 20,607 'two-day' participants, the one-day diaries contributed another 1,055 diaries which provide for a total of 42,269 daily food diaries in the 1994-98 CSFII database. The DEEM and DEEM-Calendex models utilized only the 41,214 two day diaries in its exposure model. As noted below, CARES provides the theoretical possibility of using all diaries; however, the particular Food Match table in the CARES model (Version 2.0) does not include about 1,000 food diaries.

Table 4 Imputing CSFII Bodyweights				
	Male		Female	
Age	Bwt - kg	No. of Missing	Bwt - kg	No. of Missing
0-6 months	6	59	6	71
7-12 months	9.4		9.4	
1 yr old	11.8	31	10.8	48
2 yr old	13.6	64	13	65
3 yr old	15.7	110	14.9	113
4 yr old	17.8	88	17	137
5 yr old	19.8	76	19.6	48
6 yr old	23	49	22.1	46
7 yr old	25.1	21	24.7	24
8 yr old	28.2	20	27.9	27
9 yr old	31.1	20	31.9	12
10 yrs old	36.4	16	36.1	10
11 yrs old	40.3	12	41.8	8
12 yrs old	44.2	8	46.4	4
13 yrs old	49.9	0	50.9	6
14 yrs old	57.1	6	54.8	8
15 yrs old	61	4	55.1	4
16 yrs old	67.1	1	58.1	6
17 yrs old	66.7	0	59.6	0
18+ yrs old	70	62	60	281
TOTAL		647		918

C. Food Recipes

The food recipes provide a breakout for each of the 9,746 food items reported in the CSFII survey (e.g., hamburger), into Raw Agricultural Commodities, or RACs. Each RAC belongs to a EPA crop group (CG). All RACs are also assigned a 3 digit code indicating the cooked status (CS), food form (FF), and cooking method (CM) pertaining to that RAC in that food item. Following conventional practice, these three characteristics are in total referred to as the 'Food Form', and the acronym FF is interpreted as the concentration of these three classifications CS-FF-CM.

These recipes are important for pesticide risk assessments since food residue data are usually available for individual RAC-FF's. The three models use slightly different versions of recipes. Also, the EPA regulates pesticides on specific food crops (RACs), and so risk managers often mitigate dietary exposure to pesticides using restrictions on use of a pesticide on particular RACs.

The three models are currently using different recipes. The Lifeline recipe is most different from the FCID recipes used in DEEM-Calendex and CARES. There are 548 RACs in the Lifeline recipes, 467 RACs in the FCID recipes. The Lifeline recipe contains 73 distinct food forms (FF), while FCID contains 32 distinct food forms. There are a total of 4,724 distinct RAC-FFs in the Lifeline recipe, and 2,410 distinct RAC-FFs in the FCID recipes. Table 5 presents the various types of foodforms (FF) available in the FCID and Lifeline recipes. The Lifeline recipes contain some FFs that are not present in the DEEM-Calendex nor CARES recipes. The three recipes also differ in some of the quantitiative estimates of levels of RAC-FFs in a particular food as eaten. For example, the Lifeline recipe estimates that 'Orange juice, babyfood' (CG=10,RAC=002411,FF=240) accounts for 5% of the total mass of 'Mixed fruit juice with lowfat yogurt, babyfood' (672501500), while DEEM-FCID estimates that 'Orange juice, babyfood' accounts for 15% of the total mass. Both types of differences, the latter in particular, may have a non-trivial effect upon the model predictions.

The FCID recipe file contains 2,410 unique RAC-Food Forms, while the Lifeline recipe contains 4,724 unique RAC-Food Forms. One difficulty in comparing model dietary estimates is assigning residue values to the corresponding RAC-FF in each of the models.

Table 5 Food Forms

Cooking Status		Food Form		Cooking Method	
CS	Description	FF	Description	CM	Description
1	uncooked	1	fresh	1	baked
2	cooked	2	frozen	2	boiled
6	frozen meal	3	dried	3	fried
7	salad	4	canned	4	fried or baked
8	sandwich	5	cured, pickled, smoked, salted	5	boiled or baked
9	not specified	8	other	8	not specified
7	salad	9	not specified	9	not specified as to further cooking
8	sandwich			0	N/A
9	not specified				

Lifeline Food Forms: 110,112,120,130,150,180,190,210,211,212,213,214,215,218,219,220,221,222, 223,224,228,229,230,231,232,233,234,238,239,240,241,242,245,248,249,250,251,252,253,255,258,259,280, 281,282,283,284,288,289,290,291,292,293,294,295,298,299,621,710,718,788,790,792,798,890,893,898,920, 930,980,990,998,xxx. **FCID Food Forms**: 110,112,120,130,150,210,211,212,213,214,215,220,221,222, 223,224,230,231,232,233,234,240,241,242,245,250,251,252,253,255,900.

The approximations for each of the models used the Lifeline recipe to convert food items to RAC-FFs. We wanted to control for differences caused by the use of different recipes so that we could identify the effects of other modeling design features (Reference Population, binning method, model weights) to explain differences the model predictions. Since Lifeline is planning to adopt the revised FCID recipe in the near future, our SAS model approximations for all three models will also be modified to use the revised FCID recipes.

Figure 2 Models' Use of Food Recipes

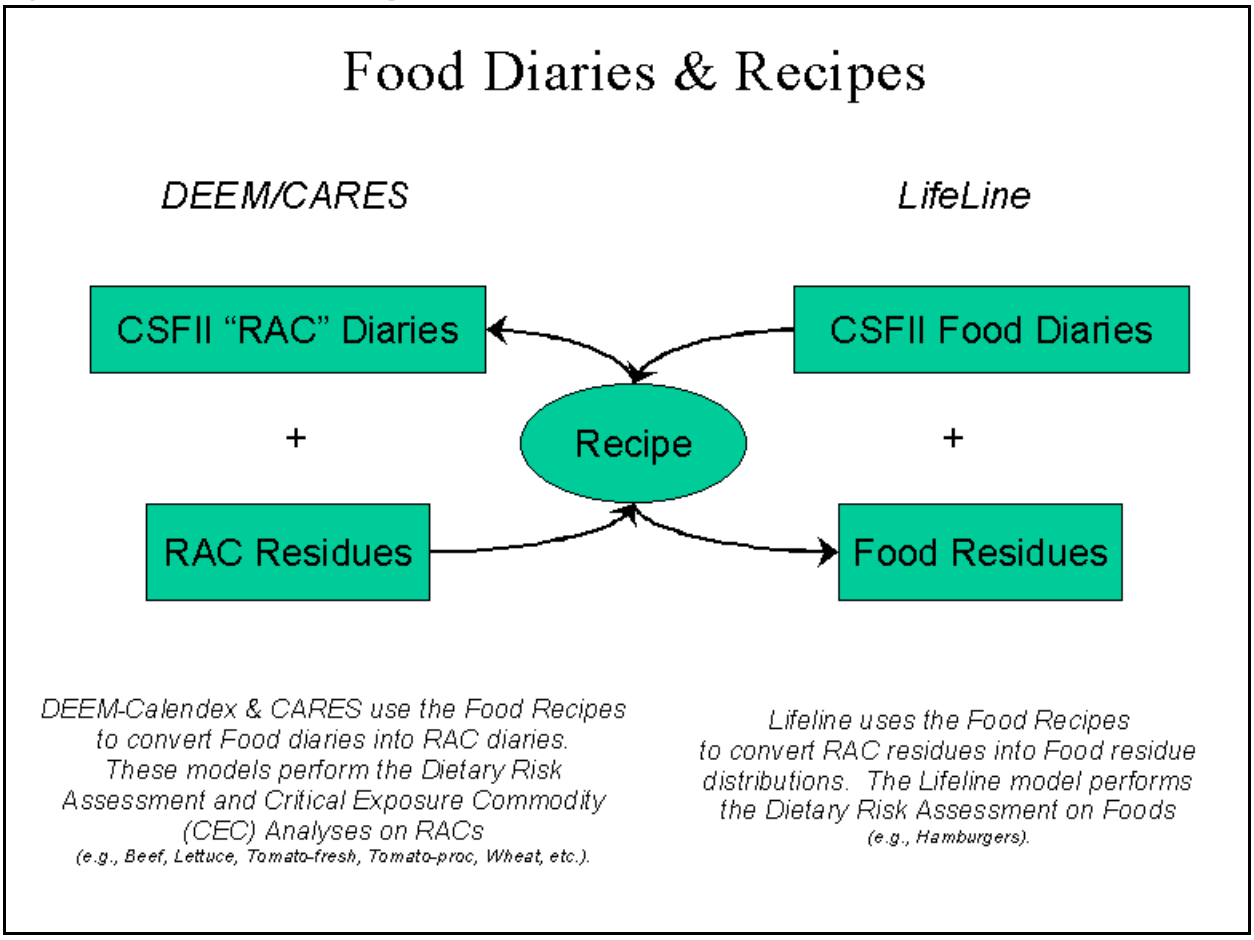


Figure 2 illustrates how the three models use the food recipes. The DEEM-Calendex and CARES models use their respective FCID recipes to convert food items reported in the CSFII food diaries into EPA RAC-FFs. These 'RAC-FF' diaries are used by these models in the probabilistic simulations. The models take the residue values (or distributions) entered by the user for each RAC-FF, and conducts a Monte Carlo analysis randomly drawing a residue for each corresponding RAC-FF to estimate exposure during that simulated day. In contrast, the Lifeline model takes the RAC-FF residues that have been input by the user, and uses the food recipes to convert these RAC-FF residue values (and/or distributions) into residue distributions for the food items. For example, residues on beef, fresh tomatoes (FF=110) and processed tomatoes (i.e., ketchup, FF=240), lettuce, wheat, and sesame seeds are converted to a residue distribution for 'hamburger' that reflect the sum of the corresponding residues of the percent of mass that each RAC-FF contributes to the overall mass of the hamburger. The Lifeline model then takes these food residue distributions, and performs a Monte Carlo risk assessment, randomly drawing a food residue for each food item reported in the daily diary. The advantage of this approach is that a user can (in principle) conduct the risk assessment using monitoring residues from actual food samples (e.g., total diet study may analyze hamburger platters), if such data are available. The disadvantage of this approach is that it complicates CEC analyses at the RAC-FF level. The initial objective of these SAS model approximations was to provide a method for ascertaining the

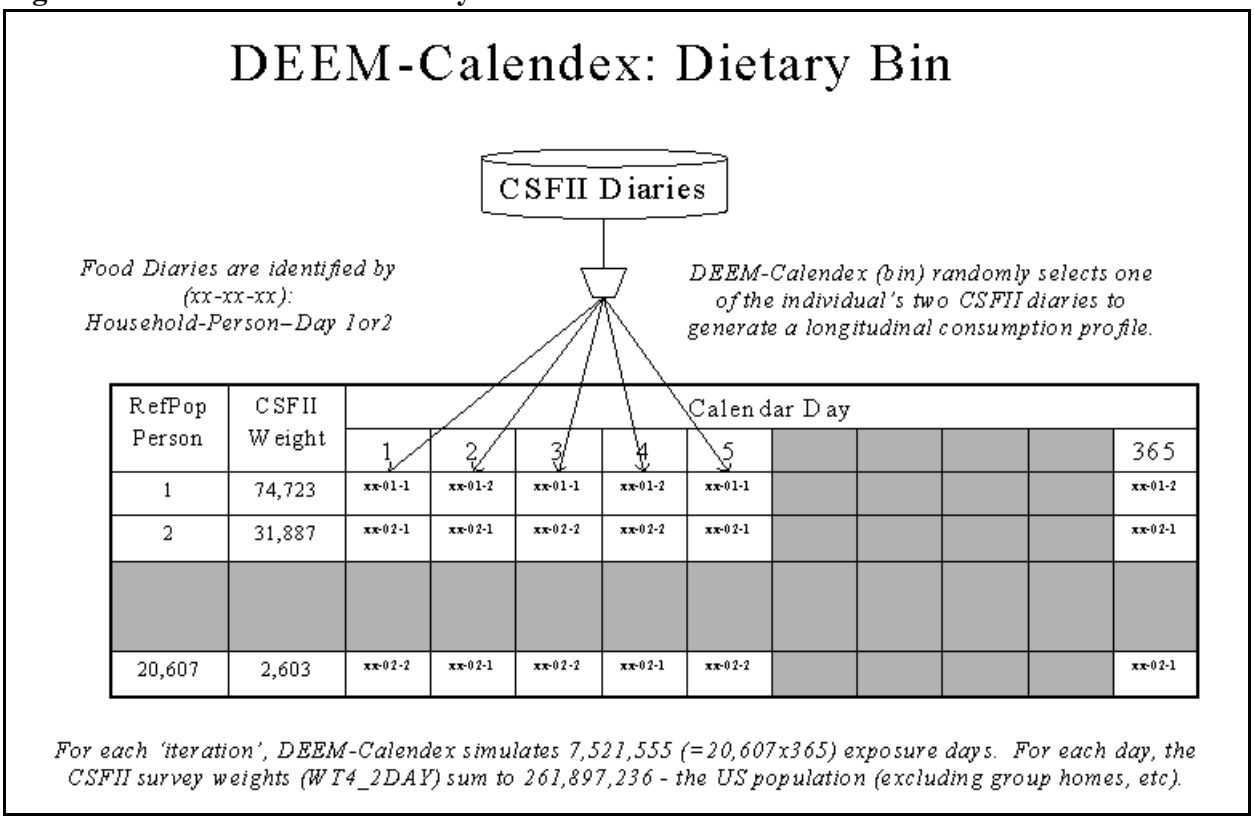
critical commodities using the Lifeline model. The pre-run analyses of the residues should provide us with an *a priori* expectation of the overall risk, as well as knowing if a particular RAC will by itself provide exposure that exceed some level of concern. In other words, if the benchmark (aPAD) in the example (above) were 0.001 grams ai/kg bwt/day, then for consumers at the upper percentile (99.9th), the residues at the 10 ppm (tolerance) level would provide higher dietary exposure (0.04 g ai/kg bw) than this benchmark.

D. DEEM-Calendex SAS Model Approximation

As noted, the model's reference population and its binning design together determine the expected (or actual) frequencies that the CSFII consumption diaries are used in a simulation.

For DEEM-Calendex, all of the diaries have the same expected frequency of being used in a simulation. As Figure 3 illustrates, each of the 20,607 individuals in the Reference Population have exactly two food diaries, and the binning design is comprised of randomly selecting one of these two diaries to generate the 365 day consumption profile. Therefore, each diary is used an expected 182.5 times (=365x0.5) per 'iteration'. While the actual frequency of use of each diary during any particular simulation cannot be determined from the DEEM-Calendex output, the actual frequencies should fluctuate very close to this expected value (i.e., by the law of large numbers, as the number of iterations increases, the percent of the time each of the two diaries are selected will approach 50%).

Figure 3 DEEM-Calendex Dietary Bin



For any particular day (1 - 365), the model (CSFII) weights sum to 261,897,236 - the estimated US population in 1990 excluding individuals living in group homes (military, hospitals, etc.). The CSFII survey has a set of survey weights for these 20,607 individuals that provided two days of food diaries, as well as another set of survey weights for all 21,662 individuals that provided at least one food diary [These survey weights include 15 individuals that did not consume any food during the day.] Since the DEEM-Calendex reference population is based on the CSFII survey design using only two day diaries, the two day CSFII survey weights (WT4_2DAY) are applied to each use of that diary. Also, since all food diaries have the same expected frequency of use for simulated exposure days (182.5 x # iterations), that expected frequency (a constant) may be dropped from calculating the relative weights for each CSFII diary. Therefore, the CSFII survey weights (WT4_2DAY) are sufficient for approximating the consumption distributions for DEEM-Calendex, DEEM, and the CSFII survey.

In approximating the consumption distributions, we constructed groups of diaries based on the amount consumed, to limit the total number of data points to 100 to approximate each of the RAC distributions. Therefore, each data point (after the top 20) represents consumption from more than one diary. For this grouping scheme, all consumption distributions have a uniform format (at most 100 data points), which in turn facilitates writing programming code that uses these approximated models to assess pesticide exposure as described later. The groupings were developed as follows: for each RAC, the top (highest) 20 consumption diets were entered as distinct values (CNT_IND) to obtain high resolution at the upper consumption levels. The next 100 high consumption diets (21 to 120) were designated in groups of ten (the last group may be composed of fewer than 10 individuals). For each of these groups, the average consumption of the RAC was calculated, and the total weights were summed to obtain a representative consumption and model weight for that group; the average consumption and summed weights were entered as distinct values. The next 400 high consumption diets (121 to 520) were designated into twenty groups of twenty, and average amounts consumed and total weights were developed for each of these 20 groups (the last group may have fewer than 20 individuals). Similar progression was made with the maximum size of the subsequent groups set at 50, 100, 1000, 5000, and if needed, the 100th group included everyone else. The maximum number of consumers for any single RAC-FF is 42,269 - the total number of food diaries in the entire CSFII survey. Since the grouping scheme needs to account for the possibility of a high number of consumers for some RAC-FF (e.g, indirect drinking water), the last groups (C96-C99) represent a potentially large number of people shown in Table 6. [A future modification may be used to tailor the groupings for RAC-FF based on the number of consumers in the respective age groups.]

Table 6 Grouping Consumption Diaries

CSFII Top Consumers (Descending)	Maximum Number of Consumers	Indicator for Consumption Groups	Weight
1 to 20	1	C1 to C20	Single Value
21 to 120	10	C21 to C30	Sum of 10
121 to 520	20	C31 to C50	Sum of 20

521 to 1,520	50	C51 to C70	Sum of 50
1,521 to 3,020	100	C71 to C85	Sum of 100
3,021 to 13,020	1,000	C86 to C95	Sum of 1,000
13,021 to 33,020	5,000	C96 to C99	Sum of 5,000
33,021+	5,000+	C100	Sum of Rest

For each RAC-FF, the total weights were summed to obtain the total number of 'consumers' within that subgroup. This total was subtracted from the total population in that subgroup (261 million for the US population - and smaller figures for subgroups), to obtain a 'zero' consumption individual. For these consumption approximations, these 'zero' consumption records were merged back into the data base before the indicators were developed, and so the 'last' group may represent either just the non-consumers, or some of the diaries with low consumption plus the remaining non-consumers. [Future modifications are to account for these non-consumers as a distinct group.]

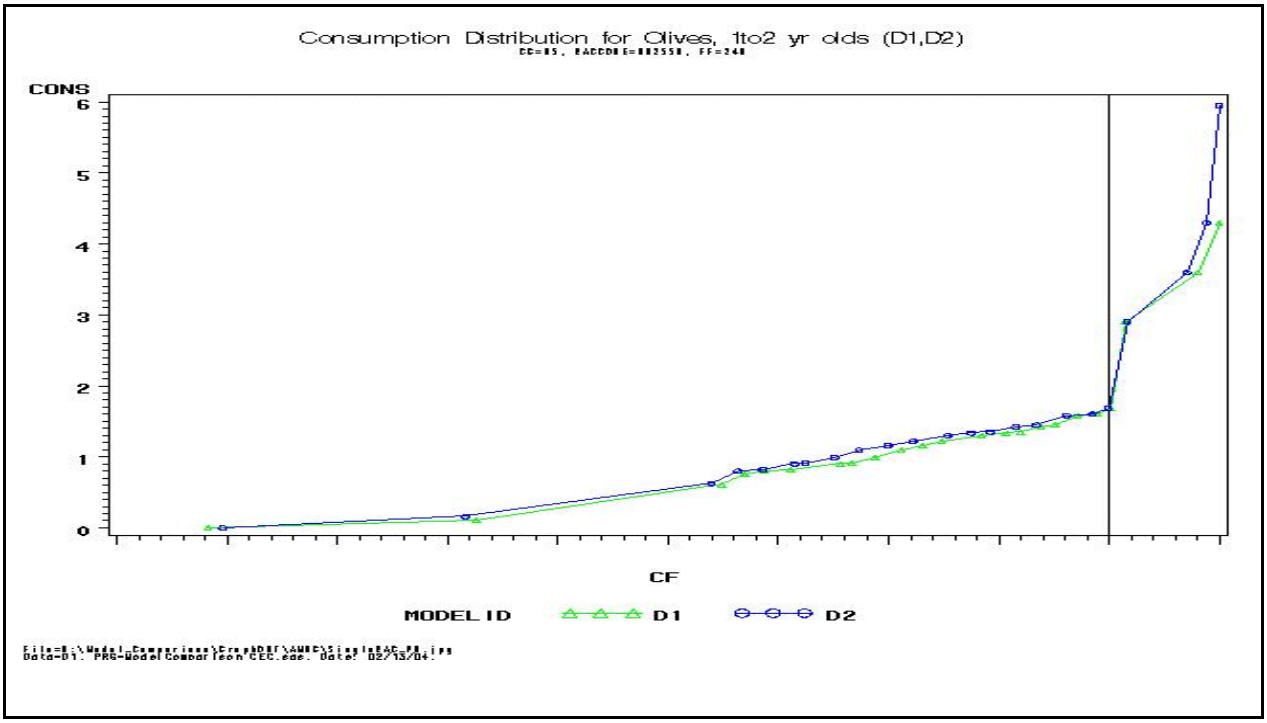


Figure 4

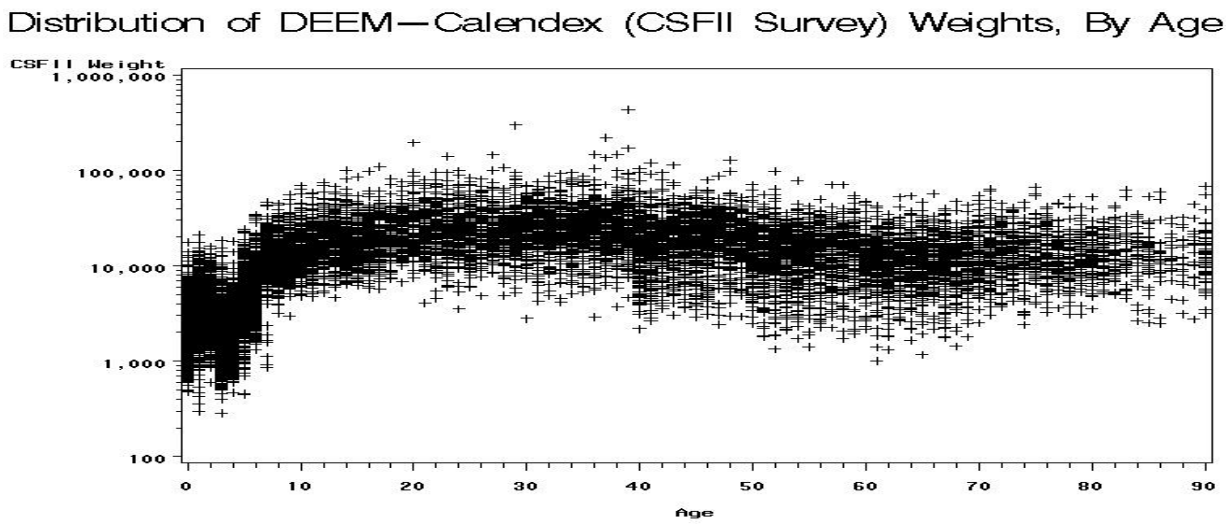
We also developed an alternative model (D2), all uses of the food diaries, including the 'one day' diaries, were used to construct the consumption distributions for each subgroup. Since we are increasing the number of individuals in each subgroup, we need to use the CSFII survey's 'Day 1' weights (WT4_DAY1 vs. WT4_2DAY) to construct these distributions. For example, there are an 95 additional 1 to 2 year olds (2,096 to 2,191 toddlers), increasing the total number of daily diaries from 4,192 to 4,287 (See Table 3). As Figure 4 indicates, the exclusion of these 95 food

diaries affects the consumption distribution for olives among 1 to 2 year olds (CG=95, RAC=002350, FF=240) at the 100th percentile. The toddler (ID=12312-01-1; refers to CSFII HouseholdID-PersonID-DayCode) that consumed the maximum amount of olives per kg bwt (5.95 grams/kg bwt) in this age group is found among the 95 '1 day' diaries that are not included in the DEEM-Calendex model. The next highest olive consumer (4.29 grams/kg bwt) is among the two day respondents (24808-01-2). This latter toddler actually consumed a bit (0.5 grams) more olives than the highest consumer: 68 grams of 'olives, green, stuffed' (foodcode = 755100300, 86%) versus 67.5 grams of 'olives, black' (foodcode = 755100200, 100%), but he was also heavier (13.61 kg bwt versus 11.34 kg bwt), thereby reducing his consumption (68x0.86/13.61 = 4.29 < 5.95 = 67.5/11.34).

As noted earlier, DEEM-Calendex uses the CSFII survey weights as its model weights. The model weights are used to project the simulated exposure days to the modeled population. The overall contribution of a CSFII diary is determined by the frequency of use (canceled out in DEEM-Calendex), and the model weights. In Figure 1, these weights (CSFII survey weights) are reflected in the horizontal distances between the data points. As the consumption distribution indicates, there is variability in the weights among the highest 20 consumption data points. The following 10 data points (~between the 95th percentile and 90th percentile) have larger weights since these points represent groups of 10 individuals - and hence the CSFII survey weights for these ten individuals were summed accordingly. Similarly, the subsequent data points (~between the 76th percentile and the 90th percentile are even larger since each point represents groups of 20 individuals.

Figure 5 depicts variability in the CSFII survey weights. As noted earlier, the 1998 supplemental survey targeted infants and children, and so the CSFII survey contains a disproportionately larger number of infants 7% (~1,551/21,662) than the US population. Therefore, the survey weights for infants (and toddlers) are low so that the projected population proportionately reflects the children in this age group.

Figure 5 Distribution of DEEM-Calendex model (CSFII) weights



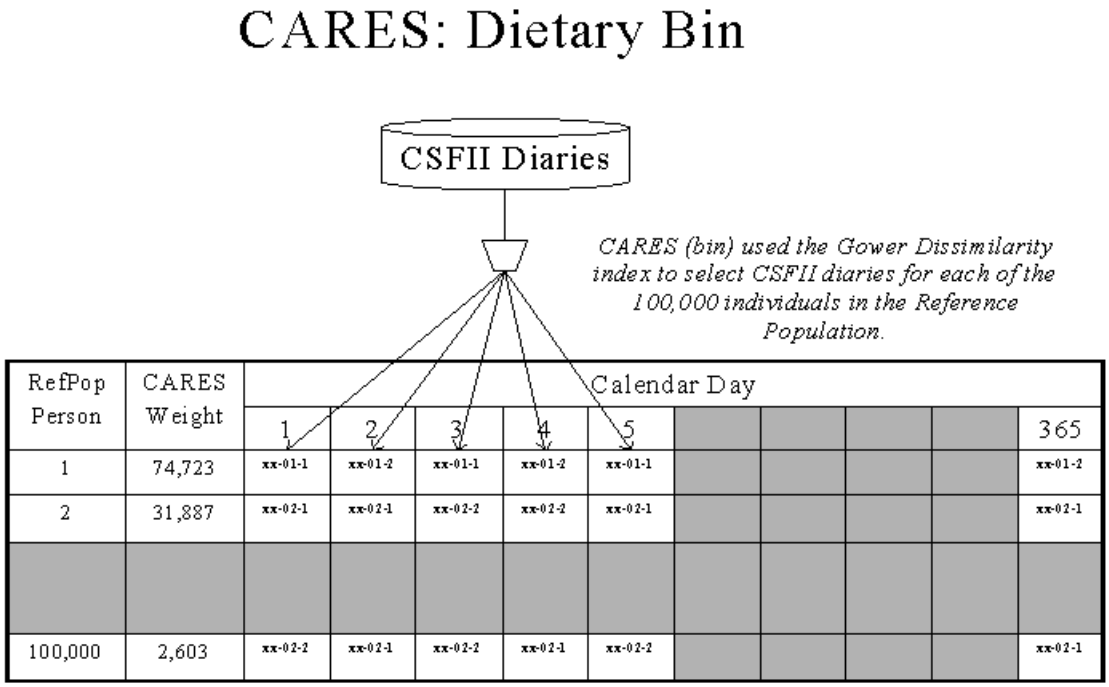
[The population subgroups (EPA subgroups) of concern are the Infants, 1 to 2 year olds, 3 to 5 year olds, 6 to 12 year olds, 13 to 19 year olds, 20 to 49 year olds, 50 plus, Females 13 to 49 year old (childbearing age), and the total US population.]

These probabilistic models, including DEEM-Calendex, do not attempt to model each individual in the US, but rather, the reference populations attempt to approximate consumption patterns across the modeled (US) population. DEEM-Calendex uses the CSFII survey weights to project each simulated exposure day up so as to represent the population represented by that survey respondent. A large survey weight indicates that the respondent represents a large number of individuals with similar demographics, having similar daily food intakes. DEEM-Calendex allows users to specify the number of iterations that each diary will be simulated - i.e., for each iteration, a new set of residues are drawn for each of the food commodities (RACs) to obtain the daily dietary exposure. These iterations can be thought of as the model's attempt to capture some of the variability that might be accrued to such a food diary.

E. CARES SAS Model Approximation

As noted earlier, the CARES model uses Gower Dissimilarity Indices and an algorithm to determine the probability that a particular CSFII diary would be selected in populating the consumption profiles for each of the 100,000 individuals in the CARES Reference Population. The Gower Dissimilarity Indices set constraints on which diaries qualified to be in particular bin, and a particular diary was selected randomly from this bin. If the number of diaries fell below a minimum figure (3 diaries), then the time window was expanded to increase the possible diaries in the resulting bin, and a diary would then be randomly chosen from this lot. The resulting Food Match table is a particular outcome of 36,500,000 multinomial trials. Conceptually, one could use this information on the CARES model design to compute and tabulate the probabilities and overall expected frequency of using each CSFII diary. However, we adopted the simpler approach of tabulating the actual frequencies that each diary was used, and summing the corresponding model weights in each instance. This process is depicted in Figure 6.

Figure 6 CARES Dietary Bin



For each day, the CARES model weights sum to 241,343,436. For the entire 100,000 person reference population, CARES simulates 36,500,000 exposure days (100,000 x 365) for the modeled year.

The fact that CARES provides a defined, fixed Food Match table allows us to evaluate the binning mechanism (as done here) independent of any model simulations. Since the CSFII diaries for the entire 365 day period are determined beforehand and permanently fixed in the Food Match Tables (12 tables - one for each month), the RAC-FF consumption distributions remain the same during all CARES simulation (regardless of pesticide/residue scenario). In contrast, the consumption distributions will vary slightly from simulation to simulation for both the DEEM-Calendex and LifeLine models since the CSFII diaries are selected on the fly (unless the same random seed is specified in DEEM-Calendex). To approximate the consumption distributions for these two models, the expected (rather than actual) contribution from each of the CSFII diaries is calculated using the information regarding the respective reference populations, binning methods, and model weights, to estimate the consumption distributions. To approximate the consumption distributions for the CARES model, we used the actual frequencies and corresponding model weights to tabulate the contributions from each of the CSFII diaries.

Table 7 CARES Model Weights & Frequency of Using Diaries

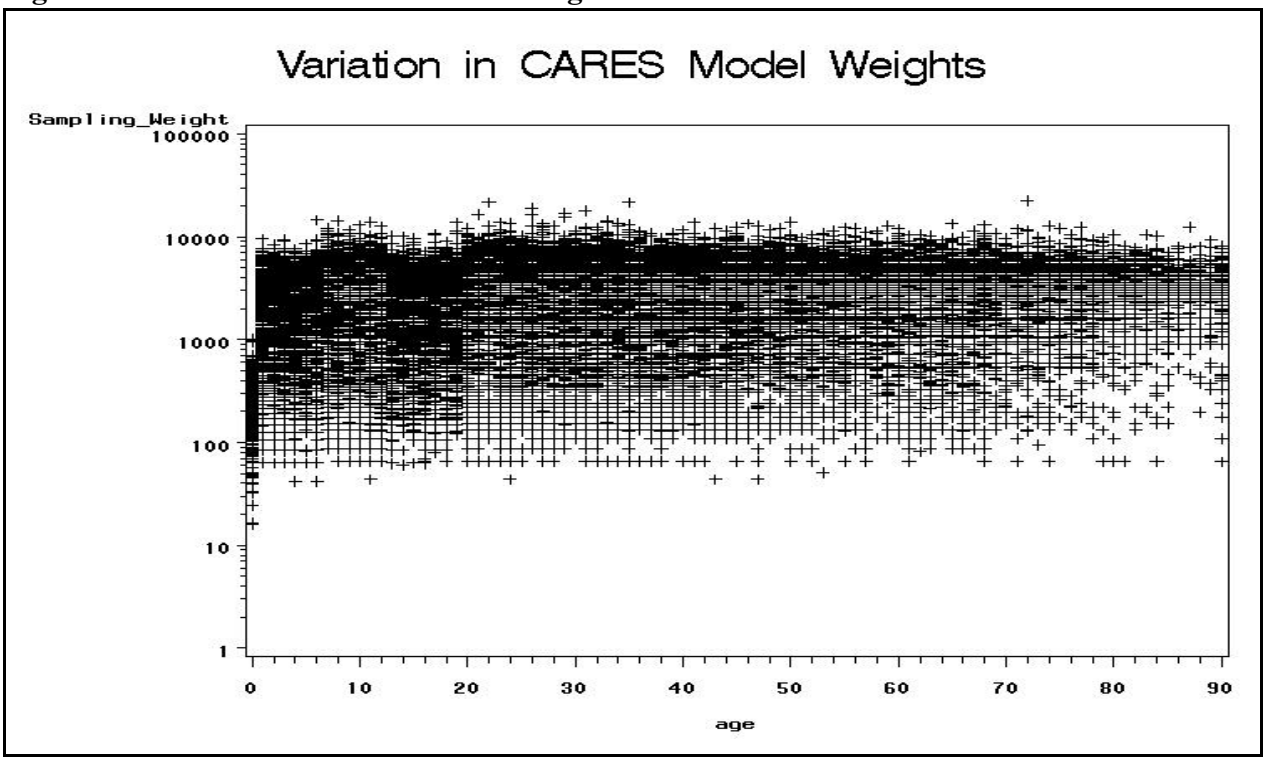
CARES Reference Population	RefPop Count	Projected Population - Each Day	Total Simulated Exposure Days	Age Range of CSFII Diets	Total # CSFII Diets in Bin	CARES Diaries Used	CSFII Diaries not Used
Total	100,000	241,343,436	36,500,000		42,269		
Infants	20,003	3,164,483	7,301,095	Infants (1)	3,037	3,033	4

1 to 2	3,367	7,558,715	1,228,955	1 to 2	4,287	4,263	24
3 to 5	4,985	11,015,723	1,819,525	3 to 5	8,970	8,576	394
6 to12	8,653	24,758,100	3,158,345	6 to12	4,277	4,277	0
13 to19	10,019	22,749,174	3,656,935	13 to19	2,503	2,503	0
20 to 49	33,538	110,317,123	12,241,370	20 to 90	9,647	13,230	591
50 Plus	19,435	61,780,118	7,093,775	20 to 90	9,548	12,886	1,227
Females13to49	22,205	67,350,407	8,104,825	F13 to 49		7928	

The actual frequencies of use of CSFII diaries CARES range from zero to 23,649. Table 7 provides a breakout of these frequencies. Many of the food diaries that are not used in CARES belong to individuals that provided two days of diaries (used by DEEM-Calendex). Presumably, these CSFII individuals did not match closely with the CARES Reference Population as far as the Gower Dissimilarity Indices are concerned. Demographic analyses of these non-match population needs to be done.

The CARES model weights were based on the stratified random sampling design of the US Census-PUMS data base used to generate the 100,000 individuals in the CARES Reference Population. These model weights sum to 241,343,436, the projected US population. [Slight

Figure 7 Variation in CARES Model Weights



difference with the CSFII projected population - may be due to differential use of annual Census estimates.] The CARES development team designed a large populaton of infants (<1 yr old) so that inference testing could be performed. Therefore, the number of infants in the CARES Reference Population is 20,003, a disproportionately large number of individuals as compared to the US population (~1.3%). Like the CSFII survey weights (model weights used in DEEM-

Calendex), the CARES model weights also vary considerably across the Reference Population. This is illustrated in Figure 7. The model weights for infants are much lower than the weights for older persons (>1 yr old) due to over representation of infants in the CARES Reference Population. However, there is considerable variability in the magnitude of these weights for all ages. These model weights range from 0 to 22,351.

Figure 8 Consumption Approximation for CARES Apple Juice

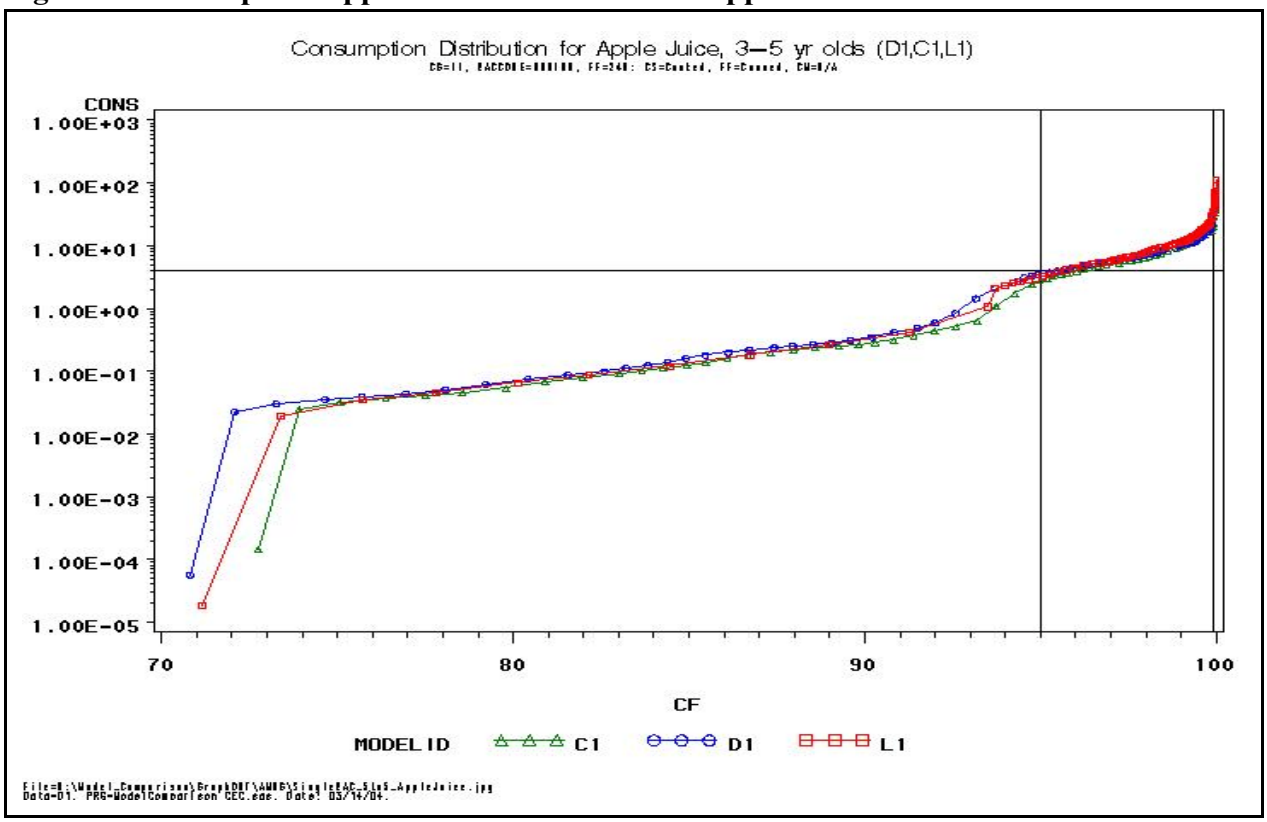


Figure 8 depicts the CARES approximation for apple juice consumption for 3to5 year olds. The distributions overlap very closely throughout this population. Figure 9 depicts the CARES approximation for olives (FF=240). For this RAC-FF, both CARES (C1) and the alternative DEEM-Calendex model (D2) that includes the one day diaries have a maximum consumption of approximately 6 grams/kg bwt for the 3 to 5 year old age group. The approximation to the baseline DEEM-Calendex model (D1) that includes only the two day diaries reaches its maximum consumption at 4 grams/kg bwt. The discrepancy is due to the fact that the 1 to 2 year old with the highest olive consumption was among the individuals that provided only one day of food diaries (CSFII ID=). The model approximations for DEEM-Calendex (D1) and CARES (C1) cross due to the fact that CARES does not use one of the food diaries (frequency=0) that reported relatively high consumption of olives, whereas the DEEM-Calendex model uses this diary (among the two day diaries) in simulating exposure for this subgroup. Therefore, the model predictions would switch with DEEM-Calendex (D1) producing higher exposure estimates in this range than the CARES model (C1). At the 99.9th percentile, all three models provide the same expected consumption (~1.8 grams/kg bwt/day).

Figure 9 Consumption Approximation for 3 Models for Olives (FF=240)

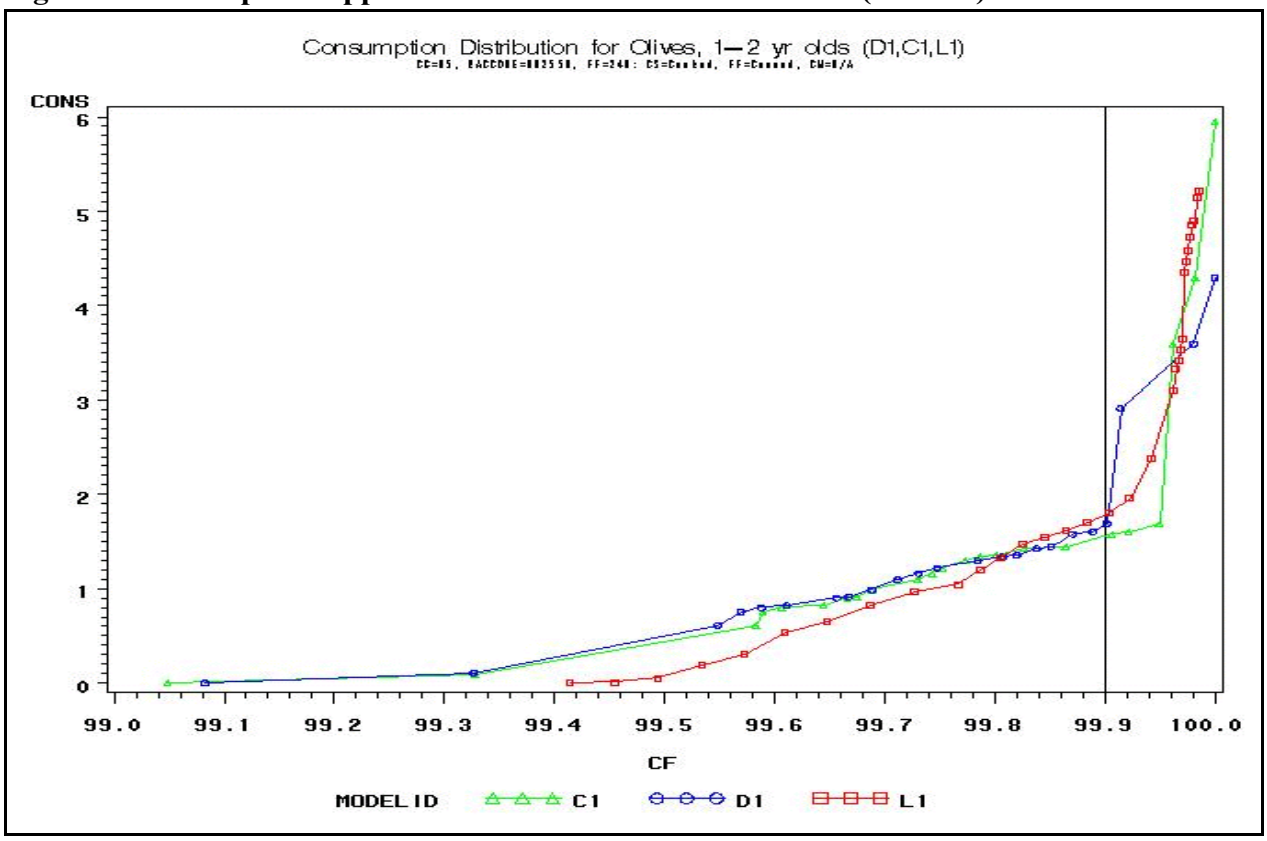


Figure 10 Consumption Distribution for Fresh Papayas (3-5 yrs old)

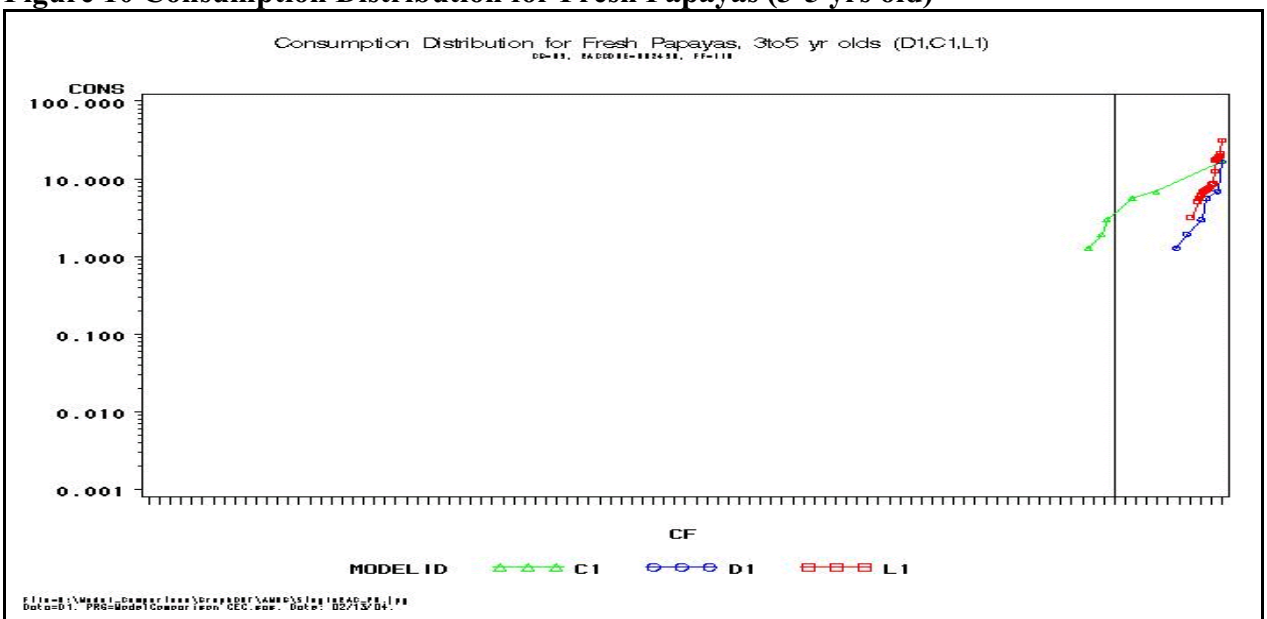


FIGURE 10 SingleRAC Comparisons for Fresh Papaya (3to5 year olds)

For fresh papaya consumption among 3to5 year olds (see Figure 10), the CARES' model generates exposure (>0) at the 99.9th percentile while Calendex and Lifeline models do not have any exposure at this upper percentile. The following explains the reason for this difference: CARES uses the diaries of 3to5 year olds with high papaya consumption relatively more than the other two models, and weights these simulated exposure days more than DEEM-Calendex or Lifeline. There are seven 3to5 year old CSFII food surveys that reported fresh papaya consumption:

(1) ID=40008-05-1, Amt=16.75 gm/kg, N=1128, Total Weight=2,456,395;
(2) ID=52017-01-2, Amt=6.89 gm/kg, N=418, Total Weight=887,559;
(3) ID=33328-01-1, Amt=5.58 gm/kg, N=220, Total Weight=497,387;
(4) ID=33328-01-2, Amt=5.58 gm/kg, N=211, Total Weight=467,672;
(5) ID=32306-01-1, Amt=2.97 gm/kg, N=95, Total Weight=191,917.
(6) ID=12322-01-1, Amt=1.93 gm/kg, N=225, Total Weight=497,128;
(7) ID=51326-01-1, Amt=1.28 gm/kg, N=368, Total Weight=792,879;
Toddler (ID=33328-01-1) consumed papayas on both days.

As noted earlier, each CSFII diary is weighted to account for both the frequency of use and the model weights applied as expected in the corresponding model. This overall weight is reflected in the chart as the horizontal distance between the consumption values.

As Table 7 indicated, the CARES Reference Population consist of 4,985 3to5 year olds, which provides for a total of 1,819,525 (=4,985x365) simulated exposure days. With a potential total of 8,970 3to5 year old food diaries, the average number of times that each food diary would be used to populate those 1.8 million exposure days is 203 (=1819525/8970) times per diary. Since CARES' model weights project these 4,985 3to5 year olds up to 11,015,723 toddlers, the average model weight for each simulated day is 2,209 (=11015723/4985). Therefore, each diary would have an average 'Total Weight' of 448,243 (=203 days x 2,209 avg wgt/day). Similarly, multiplying the average total weight by the total number of diaries obtains the total number of projected person-days in this population (8970 diaries x 448243 avg wgt/diary = 11015723 toddlers x 365 days/toddler).

The CARES' Food Match used the diaries for the top two papaya consumers a total of 1,128 amd 418 times, respectively; much higher than the average 203 times. This higher than average frequency contributed to average total weights: 2,456,395 and 887,559 respectively; much higher than the average diary weight of 448,243. When running the actual models for a simple scenario (1000 ppm), CARES provided a figure higher than the SAS approximated model (C1) at the 99.9th percentile (16.72 vs. 5.59). [note: Total Weight for this high consumption diary of 2,456,395 is 0.06% (of 11,015,723x365)- not quite 0.1% of the Total 365 day projected person days. The total weights for top three diaries sum to approximately 0.1% of this total projected person days.] Both Calendex (D1) and Lifeline (L1) projected zero consumption at the 99.9th percentile and below, just as the approximated models. The next section provides an overview of how the Lifeline model was approximated.

F. Lifeline SAS Model Approximation

Lifeline models an individual from birth to death (Lifeline provides an option for either setting the number of years all individuals live, or applies mortality statistics based on race, sex and ethnicity to set the probability that an individual dies (maximum age=85)). To assess dietary exposure, Lifeline randomly selects CSFII diaries from bins based on the individuals' age and season. As noted, there are 12 age-related groups in which diets are binned - Infants have two bins based on breastfeeding status. Lifeline assigns each infant to be either a breastfeeding infant, or a non-breastfeeding infant throughout the first year of life.

Table 8 reproduces these age-season bins displaying the number of CSFII diaries in each of these bins. Lifeline assigns each individual-infant as being breast fed or not. The individual's sex has a slight influence on this assignment (~27% of females and 25% of males are breastfeeding infants). If the individual is a breastfeeding child, then each of the 187 diaries in this bin has a 1 in 187 chance of of being drawn on any given day during the winter season (Infants are assumed to be breastfeeding the entire year - no distinction made by age in months). Lifeline provides an option of using the CSFII survey weights as a 'weight' to select from these diaries. Under this option, the probability that Lifeline will select a particular diet among the 187 diaries available in the Infant-Breastfeeding-Winter bin is proportionally related to the relative size of that diaries' CSFII survey weight.

For any particular individual simulated, some diaries may be selected more than once. Since a food diary can only be selected based on the corresponding season, the maximum frequency that a diary can be selected to a particular individual is 90 days. Lifeline also allows the option of fixing the diet for the entire season. This option may be useful for bounding the variability in exposures for subchronic exposure assessments (i.e., average daily exposure over a 7 day, 14 day or 30 day period). For the entire population, we anticipate that each of the diaries in each of the dietary bins are selected with some expected frequency (depending upon the Reference Population). We have used this information to estimate the contribution that each CSFII diary has in the respective probabilistic risk assessment models.

As Table 8 indicates, the smallest dietary bin is the 176 diaries in the Fall-Infants-Breastfeeding. One of the concerns with all modelers is the size of these bins. One reason cited for not including other factors in this binning design (e.g., sex, race, ethnicity, geography) is that each additional factor reduces the size of the average bin proportional to the number of categories. Therefore, adding sex as a criterion for a bin would reduce the smallest bin size from 187 (Infants-Breastfeeding-Winter) to at most 93 (=187/2), adding race (3 categories) in addition to sex would reduce that bin by an additional 3 factor to 31 (=93/3), and so on.

Table 8 Size of Lifeline Dietary Bins					
Lifeline Dietary Bin (Age)	Total Sample	Winter	Spring	Summer	Fall
Infants Breastfeeding	846	187	227	256	176
Infants Non-Breastfeeding	2,191	503	562	703	423
1	2,124	561	528	555	480
2	2,163	480	568	625	490
3	3,595	793	838	1,102	862
4	3,641	795	941	1,159	746
5	1,734	420	454	487	373
6 to 7	1,764	451	491	449	373
8 to 11	2,149	511	589	548	501
12 to 14	1,175	260	237	373	305
15 to 25	3,444	741	929	903	871
26+	17,443	3,800	4,455	4,876	4,312
All Ages	42,269	9,502	10,819	12,036	9,912

Table 9 Lifeline Model: Distribution of Bodyweights (kgs), By Age & Age_Bins

		Percentiles												
AGE	mean	0	5	15	25	35	45	50	55	65	75	85	95	100
0	8.3	5.5	7.2	7.6	7.8	8.0	8.2	8.3	8.3	8.5	8.7	9.0	9.4	15.2
1	11	7	9	10	10	11	11	11	11	11	12	12	13	22
2	13	8	11	12	12	13	13	13	13	14	14	15	16	29
3	15	9	13	13	14	14	15	15	15	16	16	17	18	34
4	17	10	14	15	16	16	17	17	18	18	19	20	21	39
5	20	11	16	17	18	19	19	20	20	21	22	23	25	44
6	23	12	18	19	20	21	22	22	23	24	25	26	29	53
7	26	13	20	22	23	24	25	26	26	27	28	30	33	67
8	30	14	22	25	26	27	29	29	30	31	33	35	39	83
9	34	16	25	28	30	31	33	33	34	36	38	40	45	105
10	39	17	28	31	33	35	37	38	39	41	43	46	53	131
11	44	19	31	35	38	40	42	43	44	47	50	54	61	164
12	51	21	35	40	43	45	48	49	51	54	57	62	71	206
13	57	22	38	44	48	51	54	56	57	61	65	70	81	222
14	62	22	41	47	51	55	58	60	62	66	71	78	91	222
15	66	22	41	48	53	57	61	63	66	71	76	84	99	222
16	66	22	41	48	53	57	62	64	66	71	76	84	100	222
17	66	22	41	48	53	58	62	64	66	71	76	84	100	222
18	66	22	41	48	53	58	62	64	66	71	76	84	100	222
Lifeline_Bwt Bins U														
6-7 year old	24	12	18	20	21	22	23	24	24	25	27	28	32	67
8-11 year old	37	14	24	28	30	32	34	35	36	39	42	46	54	164
12 year old	51	21	35	40	43	45	48	49	51	54	57	62	71	206
13-14 year old	60	22	39	45	49	53	56	58	60	63	68	74	86	222
15-19 year old	66	22	41	48	53	57	62	64	66	71	76	84	100	222

20 year old	66	22	41	48	53	58	62	64	66	71	76	84	100	222

As noted earlier, Lifeline divides the amount consumed, as reported in the CSFII survey, by the Lifeline modeled body weights to calculate consumption (=grams of food consumed/kg bwt). The Lifeline model generates body sizes (height, body weight, body surface area) for each of the individuals based on sex, race and ethnicity. Lifeline has 12 physiometric models - one for each of the demographic groups: 2 Sexes (Male, Female), 3 Races (White, Black, Other) and 2 Ethnicity groups (Hispanic, Non-Hispanic). These models were developed based on a regression analyses of the NHANES data. We could have generated body weight distributions using these 12 physiometric models and weighting each of the groups according to their respective percent of the Reference Population (based on the Natality data). Rather than proceed with that approach, we simply estimated the body weight distributions from actual Lifeline runs.

Table 9 presents body weight distributions for various ages that were generated from 5 runs of 7,500 people run through age 85. For infants, Lifeline generated body weights ranging from 5.5 kgs to 15.2 kgs. Lifeline uses the modeled body weights at the midpoint of the person's years (month 6 for infants). For adults (17 year olds - people in all demographic subgroups stop growing in both height and body weight after reaching this age), body weights range from 22 kg to 222 kgs. Since Lifeline also selects food diaries from the food (age) bins, the food diary of an 11 year old may be used to model dietary exposure for an 8 year old, and vice versa. Therefore, additional grouping of these body weight distributions can be generated to minimize the permutations of body weight and food diaries synthesized to approximate the Lifeline model. In particular, the bodyweight distributions were grouped for 6 to 7 year olds, 8 to11 year olds, 13 to14 year olds, 15 to19 year olds, and 20+ year olds, based on the intersection of the dietary (age) bins.

While the body weights distributions vary across the 12 demographic subgroups, it is not necessary to generate different distributions since Lifeline does not use those factors (sex, race, ethnicity) in its dietary bin (i.e., Lifeline may assign the food diary of a female-white-hispanic to a male-black-Non-Hispanic).

The following steps outline the procedure for approximating the Lifeline model:

(1a) For each age_group, select all the CSFII records in the Diet Bin (Table 10);

(1b) For Females 13-49, the CSFII records in the 15-25 diet bin need to be duplicated to account for permutations with the two body weight bins (15-19 year old & 20+ year old);

(2) Match each CSFII record with a different body weights in the corresponding body weight bin (0%, 25%, 50%, 75%, 100%), calculate the consumption (amount consumed/Lifeline body weight) and output each of these synthesized diets;

(3) Compute the Lifeline weight as the number of years that the individual is expected to draw from that age bin (e.g., draw from 1 year old bin for only 1 year, but from the 26+ year bin for 36 years);

(4) For each RAC-FF, calculate the total number of consumers (Sum weights for all

consumers);

(5) For each RAC-FF, calculate the total number of non-consumers = total weight - total consumers.

The Lifeline model weights reflect the total expected number of times that the CSFII diary will be used when running Lifeline. These weights are presented in the last column of Table 10 for the corresponding age diet bins. For the first year of life, each individual will draw from either the breastfeeding bin (~26% chance), or the non-breastfeeding bin (~74% chance). Therefore, the CSFII survey weights for infants-breastfeeding are set at 0.26, and the weights for non-breastfeeding infants are set at 0.74. [Sex was averaged.] For the first year of life, each individual will draw for one period (90 days) from each of the 4 seasonal-1 year old bins. The weights are set to 2 for CSFII diaries in the 6 to 7 year old range, since all individuals will draw from that age-seasonal bins for two periods (once each while 6 years old and again at 7 years old). Similarly, CSFII diaries in the 8 to11 years old range have weights of 4 since the individual lives during ages 8 to11.

Since race and sex are not used in binning diets, the total frequency and the probability of drawing a particular diary are equivalent. Otherwise, the total frequencies are conditional upon the relative proportions of each demographic subgroup (i.e., if those factors are used in binning, then Female-White-NonHispanic diaries are weighted much more (0.3025) than Female-Other-NonHispanic diaries (0.0245) - adjustments are proportional to the expected shares of the respective subpopulations.

Table 10 LifeLine Diet (Age) Bin, Bodyweight Bin, and Model Weights

EPA Age Group	LifeLine (L1) Dietbin	LifeLine (L1) Body weight bin	BreastFeeding Pct	Weight #years
All Infants <1 year old	Infants-BF	All Infants <1	0.26	1
All Infants <1 year old	Infants-NBF	All Infants <1	0.74	1
Children 1-2 years old	1 year old	1 year old	1	1
Children 1-2 years old	2 year old	2 year old	1	1
Children 3-5 years old	3 year old	3 year old	1	1
Children 3-5 years old	4 year old	4 year old	1	1
Children 3-5 years old	5 year old	5 year old	1	1
Children 6-12 years old	6-7 year old	6-7 year old	1	2
Children 6-12 years old	8-11 year old	8-11 year old	1	4
Children 6-12 years old	12-14 year old	12 year old	1	1
Youth 13-19 years old	12-14 year old	13-14 year old	1	2
Youth 13-19 years old	15-25 year old	15-19 year old	1	5
Adults 20-49 years old	15-25 year old	20 year old	1	6
Adults 20-49 years old	26+ years old	20 year old	1	24
Adults 50+ years old	26+ years old	20 year old	1	36
Females 13-49 years old	12-14 year old	13-14 year old	1	2
Females 13-49 years old	15-25 year old	15-19 year old	1	5
Females 13-49 years old	26+ years old	20 year old	1	24
Females 13-49 years old	15-25 year old	20 year old	1	6

Figure 11 depicts the individual's life in the LifeLine model. During the first year of life, the individual will either be assigned food diaries (for each of the 4 seasons) from the breastfeeding bins (p=0.26, average of male and females), or the non-breastfeeding bins (p=0.74). During ages 1 through 5, the individual will be assigned food diaries for one year from each of the corresponding diet bins. Since the individual's age and the CSFII diet bin age match exactly, the model approximation synthesized LifeLine diets matching the body weight of a one year old with the CSFII diet of one year olds. During ages 6 through 7, the individual may select from this enlarged dietary age bin. Therefore, CSFII diaries in this age bin are weighted twice the amount that diets in the 1 through 5 age range, and the approximated model synthesizes LifeLine diets matching these CSFII diets with possible body weights of 6 to 7 year olds. Similarly, during ages 8 through 11, the approximated model synthesizes LifeLine diets matching the diets in this bin with LifeLine body weights in this age range. During age 12, the LifeLine model may assign to that individual diets from the 12 to 14 years old diet bin. Therefore, the approximated model synthesizes diets by matching diets in this bin with the body weights of 12 year olds. For the 6 through 12 year subgroup (EPA group), the approximated model uses CSFII diaries for ages 6 through 14 (three dietary bins). Similarly, for the EPA subgroup 13 through 19, the approximated model uses CSFII diaries for ages 12 through 25 (two dietary bins). For the EPA subgroup 20 through 49, the approximated model uses CSFII diaries for ages 15 through high (two dietary bins: 15 to 25, and 26+). For the EPA subgroup 50+, the approximated model uses CSFII diaries for ages 26+. And for the Females age 13 through 49 subgroup, the approximated model uses CSFII diaries for ages 12 through 91.

	Mortality Rate=0%	-	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
	Lifeline Age	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	19	20	25	26	49	50	85	Lifetime
CSFII Age	EPA Age Group LL DietBin	Infants	1to2		3to5			6to12							13to19				20to49				50Plus		
0-BF	0 - BF	0.25																							0.25
0-NBF	0 - NBF	0.75																							0.75
1	1 yr old		1																						1
2	2 yr old			1																					1
3	3 yr old				1																				1
4	4 yr old					1																			1
5	5 yr old						1																		1
6	6to7 yr olds							1	1																2
7																									
8	8to11 yr olds																								4
9										1	1	1	1												
10																									
11																									
12	12to14 yr olds																								3
13														1	1	1									
14																									
15	15to25 yr olds																1	1	1	1					11
25																									
26	Ages 26+																				1	1	1	1	60
49																									
50																									
91																									
	E{#Yrs|LL Age}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	86
	E{#Yrs|LL DietBin}	1	1	1	1	1	1	2		4				1	2		5		6		24		36		86
	E{#Yrs|EPA AgeGroup}	1	2		3			7							7				30				36		86

Figure 11

The model approximations generated for LifeLine assume that the mortality rate option is not used (i.e., all individuals in the simulation live up through age 85 or whatever year is specified). If the mortality rate option is used, then the model weights are adjusted to reflect the expected probability that the individual will live and draw upon the corresponding age bins. As an extreme case, suppose the mortality statistics were such that all individuals lived through age 26, then died (p=1). Then the approximated model for the 20 to 49 year subgroup would draw upon the 15 to 25 year bin for 6 years (age 20-25), and 1 year from diet bin 26+. For the CSFII diaries in the 26+ dietary bin, the weights would be 1, rather than 24 (LifeLine years 26-49).

In addition to the approximating the LifeLine (L1), we developed two alternative models based on alternatives assumptions regarding the LifeLine design. The first alternative model (L2) assumes the same dietary bins, but applies the CSFII body weights that were reported (or imputed) for the respective diaries, rather than synthesizing CSFII diaries for the LifeLine physiometric model. This alternative model attempts to capture the effect of the LifeLine binning design (frequency of use and model weights applied) upon the LifeLine's estimated exposures.

The second alternative model (L3) differs from the baseline model (L1), by using the CSFII weights as a factor in drawing diaries from the corresponding age bins. This model approximation attempts to approximate LifeLine if the CSFII weight option is selected. The purpose of this model is to also identify the effects of using this option. The CSFII diaries with relatively high survey weights will be weighted accordingly.

Lifeline differs from DEEM-Calendex (and CARES) in its use of the Lifeline-modeled body weights as well as differing frequencies of using CSFII diaries and corresponding model weights. Therefore, one can use the two alternative Lifeline models to identify the effects of these two factors. The effect of using the CSFII body weights (L2) is to control for the variability created by the Lifeline model (Lifeline body weights), so as to identify the effects of Lifeline's binning design (frequency of using diaries and model weights) upon differences in model predictions. Intuitively, if the individuals with high consumption (grams food/kg bwt) also have relatively large CSFII survey weights, then the Lifeline model would provide lower consumption at the upper end since these diaries would be weighted equally (equal chance of being selected) as the other CSFII diaries - whereas DEEM-Calendex would weight these simulated exposure days much more than the simulated exposure days performed on the other diaries - with relatively smaller CSFII survey (and model) weights.

The next alternative model approximation (L3) assumes that the CSFII survey weights option is used to run Lifeline model. Lifeline allows users to select this option, which uses the CSFII survey weights to affect the relative probability of selecting a diary within a particular bin. Therefore, the expected frequencies that a diary is used is proportional to its CSFII survey weight (e.g., a diary with a CSFII survey weight equal to 10,000 is expected to be used 10 times more often than a diary with a CSFII survey weight equal to 1,000). In this model approximation, the Lifeline-modeled body weight distributions are retained. Since the diaries are used in proportion to their respective CSFII survey weights, running Lifeline using this option will provide similar estimates to DEEM-Calendex in so far as the frequency of use of diaries is concerned. Future work will demonstrate how these three model approximations (L1, L2, L3) may be used to

identify the effect of the two major factors affecting the differences between Calendex and Lifeline - Lifeline's anthropomorphic (body weight) models, and its binning design.

G. Approximating Aggregate Dietary Exposures for Multiple RACs

While the SAS model approximations do not reproduce the actual aggregate model results (diaries beyond the top twenty are aggregated (and LifeLine recipes are used for D1 and C1), they do provide similar exposures for Single RAC analyses. For assessing pesticides with multiple uses, we need to sum exposures across these RAC-FFs. Simply summing exposures for RAC-FF at various percentiles (e.g., 99.9th) would grossly overestimate exposure at that percentile since no individual is at the high consumption percentile for all RACs. While individuals do consume multiple RAC-FFs during a day, consumers having high consumption for one RAC-FF, will have moderate or lower consumption for other RAC-FFs. Analyses of DEEM CEC (Commodity Exposure Contribution) data indicate that simulated exposure days at the upper percentiles receive most of that total daily exposure from one RAC-FF.

Figure 12 depicts the percent aPAD contributed from the highest RAC-FF, the percent aPAD contributed from all other RAC-FFs, and the total percent aPAD for individuals at the top 0.2%.

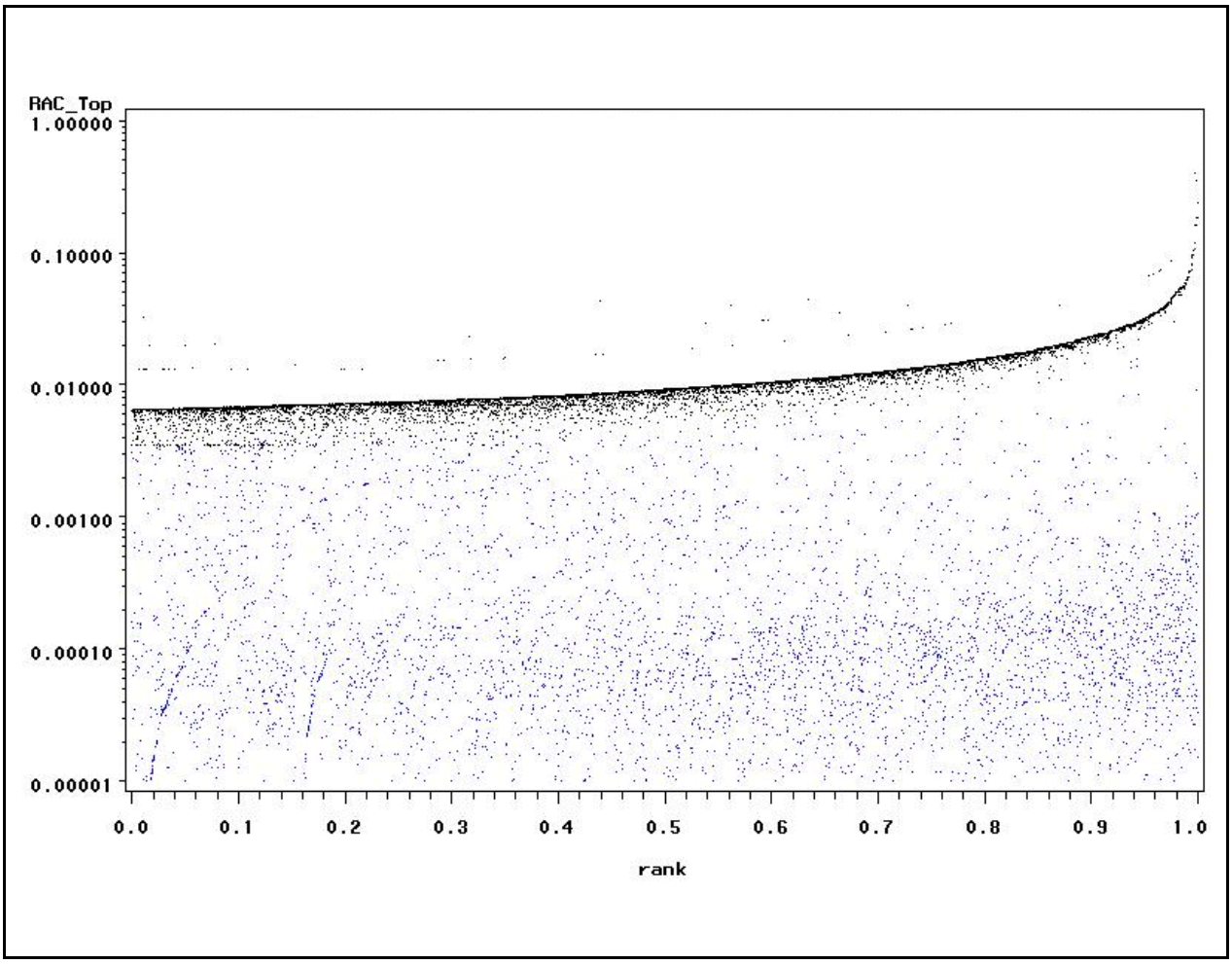


Figure 12

Most of the simulated exposure days in this upper percentile received the majority of their exposure from a single RAC-FF. We use this information to base our assumption that individuals at the upper percentiles receive all of their daily exposure from one RAC-FF, we approximate the aggregate exposure for the population by adding probability mass from the simulations for each RAC-FF residue distribution. Specifically, we can output exposures at the upper percentiles from the 99.9th to the 100th percentile in increments of 0.01, sort these exposures from lowest to highest, and select the top 10 increments to obtain the exposure at the 99.9th level, and the commodities contributing to exposure at this level.

Based on the importance of the top contributing RAC-FF, we approximate the aggregate exposure for the population by adding probability mass from the simulations for each RAC-FF residue distribution. Specifically, we can output exposures at the upper percentiles from the 99.9th to the 100th percentile in increments of 0.01, sort these exposures, and select the top 10 increments to obtain the exposure at the 99.9th level, and the commodities contributing to exposure at this level. Table 11a presents this for the MultiRAC example (3 to 5 year old). This model approximation

projects that 0.01% of the population that consumes strawberries has exposure of at least 0.02261 gm/kg/day. The increment with the next highest exposure occurs to the 99.99th percentile of prune juice consumers at 0.02006 gm/kg/day. The next increment of strawberry consumers have exposures of at least 0.01349 gm/kg/day. The tenth increment of exposure occurs among the 99.97th percentile of plum consumers at 0.006984 gm/kg/day. This value provides an estimate for exposure at the 99.9th percentile, of 69.84% of the aPAD (=0.006984/0.01).

Table 11a Exposure at the Upper Percentiles for Selected RAC-FFs (D1)

RAC	FoodForm	Mean	99.94	99.95	99.96	99.97	99.98	99.99	100
Apple, fruit with peel	uncooked; fresh; N/A	1.05E-05	2.671E-03	2.916E-03	3.150E-03	3.402E-03	3.951E-03	**4.702E-03**	9.829E-03
Peach	uncooked; fresh; N/A	3.154E-06	1.115E-03	1.327E-03	1.785E-03	2.652E-03	3.854E-03	**6.246E-03**	5.374E-02
Plum	uncooked; fresh; N/A	1.124E-05	**4.705E-03**	**5.335E-03**	**5.922E-03**	**6.984E-03**	**8.420E-03**	**1.227E-02**	1.139E-01
Plum- babyfood	cooked; canned; N/S	2.407E-06	9.042E-04	1.034E-03	1.617E-03	2.307E-03	3.463E-03	**5.301E-03**	6.490E-02
Plum, prune, juice	N/S; N/S; N/A	6.45E-06	1.064E-04	2.127E-04	1.213E-03	2.716E-03	**7.696E-03**	**2.006E-02**	4.103E-01
Olive	cooked; canned; N/A	4.688E-06	2.309E-03	2.743E-03	3.473E-03	4.682E-03	**6.466E-03**	**1.003E-02**	4.224E-02
Strawberry	uncooked; fresh; N/A	1.05E-05	3.372E-03	4.373E-03	**5.732E-03**	**8.393E-03**	**1.349E-02**	**2.261E-02**	1.767E-01
Strawberry, juice	cooked; canned; N/A	7.81E-06	3.275E-03	3.843E-03	4.531E-03	**5.384E-03**	**6.529E-03**	**8.263E-03**	3.411E-02

Table 11b presents the contributions of each of these commodities to the total exposure for the top 0.2%. The 'contribution to total exposure' is calculated by summing up the top twenty increments by RAC. Strawberries account for 28.8% of the total exposure to this group. Plums account for 25.0% of total exposure, prune juice accounts for 15.9% of the total exposure, and so on. Although apple, fruit with peel has the highest average exposure to this subgroup (1 to 2 year olds) of this set of RACs at 1.05E-05 gm/kg/day (Table 11b), it accounts for only 2.7% of the total exposure. This is due to the fact that a relatively high percent of 1 to 2 year olds consume apples, and receive some exposure from this RAC, but at relatively lower levels based on the anticipated residues.

Table 11b Summing Probability Mass

RAC	Food Form	Contribution to Total Exposure *	% Cont
Apple, fruit with peel	uncooked; fresh; N/A	4.702E-03	2.7%
Peach	uncooked; fresh; N/A	6.246E-03	3.6%
Plum	uncooked; fresh; N/A	4.364E-02	25.0%
Plum- babyfood	cooked; canned; N/S	5.301E-03	3.0%
Plum, prune, juice	N/S; N/S; N/A	2.775E-02	15.9%
Olive	cooked; canned; N/A	1.649E-02	9.4%
Strawberry	uncooked; fresh; N/A	5.022E-02	28.8%
Strawberry, juice	cooked; canned; N/A	2.018E-02	11.6%
Total		1.745E-01	100.0%

* Sum of exposure at percentiles: e.g., Olive 1.649E-02 = 1.003E-02+6.466E-03.

This approach to estimating exposure at the 99.9th percentile will tend to underestimate exposure to the degree that some individuals in this upper percentile receive their total daily exposure from

multiple RAC-FFs - thereby pushing down the distribution for individuals receiving their exposure from a single RAC-FF.

H. Other Applications of the Model Approximation

While the primary use of model approximations is to discern the reasons for different model predictions, other applications of these models include:

* Ability to provide relatively quick (~1 minute) a priori expectations on what exposure levels are at the upper percentiles,
* Ability to generate approximate CEC reports, including detecting infrequent, high exposure events (low PCT, high residue/consumption),
* Enhance transparency with regards to exposure by pulling anecdotal consumption and residue values for 'back-of-the-envelope' calculations,
* Ability to QC the residue data inputs (finding problems with Olives in CARES, Plums/Prunes in Lifeline, Pears in CARES),
* Ability to conduct quick uncertainty analyses with respect to various parameters, in particular, the percent of crop treated, and processing factors.
* Ability to evaluate variations of existing models. For example, if CARES develops a new Food Match table. Or the new version of Calendex provide the ability to specify binning factors (gender, race, ethnicity, etc.) for developing longitudinal consumption profiles.

V. Introduction to Hypothetical Case Study and Analysis of Results

In order to compare estimated exposures from the three models (LifeLine, CARES, and DEEM), OPP developed a case study for a hypothetical chemical (Chemical A). While not reflective in its entirety of any specific pesticide, the scenario is realistic to a variety of registered agrochemicals. Thus, Chemical A can be considered a composite chemical of sorts whose application scenarios are based on real-world use and application parameters. The following paragraph provides a short synopsis of the scenarios which were modeled in the case study.

> *Chemical A is one of the more widely used broad-spectrum insecticides in agriculture and residential lawn care markets. Thus, exposures are expected to occur through food, drinking water, and residential lawncare pathways. Registered end-use formulations include flowable concentrates (FlC), granulars (G), pelleted/tableted (P/T), ready-to-use (RTU), and wettable powders (WP). Depending on the crop, these formulations may be applied under a variety of application scenarios (e.g., dormant, prebloom, foliar and soil (broadcast). The insecticide is registered for use on over 300 sites in agriculture. Agricultural uses include fruit and nut tree, fruit and vegetable, and grain crops. More than 100 tolerances are established for this chemical with greatest amount (in lbs) used on apples, pecans, and grapes. Chemical A is also used by homeowners in residential settings for lawn care. No other residential uses exist.*

OPP normally assesses exposure in its routine assessments for the following age groups:

infants <1, children 1-2 y.o.; children 3-5 y.o.; children 6-12 y.o.; youth 13-19 y.o.; adults 20-49 y.o; adults 50+ y.o., and females 13-49 y.o. For this case study, only the analyses for children 3-5 y.o. and adults 20-49 y.o. will be presented. OPP believes that these two groups are most appropriate for the comparisons that will be performed. For the dietary aspect of exposure, these two groups are considered to have divergent eating patterns and cover a broad spectrum of potential exposure sources from foods. While the residential exposure aspect of the equation is not being assessed in this document, we expect that such comparisons will be made in the future and these two age groups are most appropriate for this comparison: adults 20-49 are considered under both the applicator and post-applicator scenarios and children 3-5 y.o. is the youngest age group which might reasonably have post application exposures from playing for extended periods on lawns.

Given the above general description of exposure scenarios, OPP developed input files for each of the three models. As is routine for OPP risk assessments, input files were generated for food commodities based primarily on PDP data (using fied trial and for water based exposures based on PRZM-EXAMS simulation.

These input files were used to generate dietary exposure estimates from all three models[8]. Given the different assumptions and databases used, exposure estimates from each of the three models would not be expected to be identical, but should rather be reasonably similar to each other. As can be seen in Table 12, for food only, water only, and food + water, estimated exposures are reasonably similar

Table 12 Estimated %aPAD's through Food, Water, and Food + Water pathways for LifeLine, DEEM, and CARES For Chemical A.

Exposure Medium	Age Group	95th percentile			99th percentile			99.9 percentile		
		LL	DEEM	CARES	LL	DEEM	CARES	LL	DEEM	CARES
FOOD	Children 3-5 y.o.	4	12	5	18	24	21	77	81	89
	Adults 20-40 y.o.	1	3	2	7	8	7	32	29	34
WATER	Children 3-5 y.o.	3	3	3	15	15	15	78	80	89
	Adults 20-40 y.o.	1	2	2	7	10	11	37	52	60

[8] LifeLine generates estimates of exposure distributions by season (e.g, distributions of exposures to1 year olds in the springtime); these are not directly comparable to the exposure estimates provided by DEEM/Calendex or CARES which estimate overall distributions of exposure across all seasons. Thus, OPP used the LifeLine season-specific exposures and generated comparable figures to which comparisons with DEEM and CARES could be made.

FOOD + WATER	Children 3-5 y.o.	7	14	9	28	34	32	115	116	129
	Adults 20-40 y.o.	3	5	4	12	15	16	52	62	68

For this hypothetical example, the aPAD = 0.01 mg/kg; the percentages in this table represent the percent of this aPAD which is occupied for Children 3-5 y.o. and Adults 20-49 y.o. at the 95th, 99th, and 99.9th percentiles. Each model's estimated exposure can be calculated by multiplying the percent of the aPAD occupied (expressed as a decimal) by the aPAD.

It is of interest to OPP to identify those commodities which contribute to some substantial degree to exposures. Both CARES and DEEM have this capability which was used to determine the significant contributors for Chemical A. While Lifeline currently does not have this capability, this report option is currently being developed and is expected to be present in future releases. These are listed below for both the 3-5 y.o. age group (Table 13) and the 20-49 y.o. adult group (Table 14) along with their relative rankings.

Table 13 DEEM-FCID and CARES CEC for Ages 3-5

	DEEM-FCID 3-5 yrs old		**CARES 3-5 yrs old**	
RACs	**Share of Total Exposure**	**# High Exposure Events**	**Share of Total Exposure**	**# High Exposure Events**
Strawberry- uncooked	20.86 (1)	1,190 (1)	25.87 (1)	406 (1)
Pear- uncooked[b]	0.62 (15)	0	16.60 (2)	209 (3)
Olive- cooked	13.31 (2)	973 (2)	13.29 (3)	216 (2)
Strawberry juice- cooked	13.01 (3)	900 (3)	8.64 (4)	107 (5)
Almond- cooked	2.48 (7)	440 (4)	7.59 (5)	119 (4)
Blueberry- uncooked	3.33 (5)	427 (5)	5.01 (6)	58 (6)
Peach- uncooked	3.93 (4)	263 (6)	3.84 (7)	56 (7)
Nectarine- uncooked	3.08 (6)	229 (7)	3.32 (8)	50 (8)

Apple, fruit with peel- uncooked	2.23 (8)	38 (12)	2.04 (9)	14 (14)
Raspberry- uncooked	1.35 (12)	0	1.74 (10)	21 (10)
Grape- uncooked	1.56 (11)	82 (8)	1.65 (11)	16 (13)
Apple sauce- cooked	1.63 (10)	51 (9)	1.28 (12)	9 (15)
Apple juice- uncooked	1.71 (9)	39 (11)	1.27 (13)	13 (1)
Apricot dried- uncooked	0.45 (17)	45 (10)	1.17 (14)	19 (11)
Raspberry juice- uncooked	1.13 (13)	0	1.06 (15)	24 (9)
Beef liver- cooked	0.90 (16)	9 (14)	1.01 (16)	17 (12)
Blackberry juice- uncooked	0.08 (19)	16 (13)	0.95 (17)	3 (17)
Snap beans- cooked	0.76 (14)	0	0.77 (18)	7 (6)
Beets garden tops- uncooked	<0.01 (20)	0	0.74 (19)	0
Okra- cooked	0.36 (18)	0	--	0

Briefly, rankings are performed by the DEEM and CARES programs by totaling exposure over all commodities for all individuals and apportioning that total exposure by commodity. For example, if a Chemical X is registered on only two commodities (A and B) and the sum of all exposures to Chemical X over all individuals is 30 g, this exposure would be apportioned between Commodities A and B. If the total of all exposures to all individuals through Commodity A is 20 grams and that through B is 10 grams, then exposure through Commodity A would be 20 g/30 g or 67% and that through Commodity B would be 10 g/30 g or 33%. It is in this way that the percentages above were derived. This information is used by the risk assessor to suggest which commodities are signicant risk contributors and is confirmed by the risk assessor by re-running the analyses with the commodities of interest removed.

[b] OPP has noted the signficant differences in rankings for pears and beet tops between DEEM-FCID and CARES. We contacted the CARES developer regarding this discrepancy. They identified a slight programming error for the case of pears with respect to use and generation of percent crop treated values. They are now investigating reasons for the slight discrepancies for garden beet tops. We expect that additional updated information will be provided at the SAP meeting.

Table 14 DEEM-FCID and CARES CEC for Ages 20-49				
	DEEM-FCID 20-49yrs old		**CARES 20-49 yrs old**	
RACs	**Share of Total Exposure**	**# High Exposure Events**	**Share of Total Exposure**	**# High Exposure Events**
Strawberry- uncooked	16.08 (2)	253 (1)	20.64 (1)	52 (2)
Pear- uncooked[b]	0.32 (16)	0	12.42 (4)	37 (3)
Olive- cooked	21.06 (1)	136 (3)	16.62 (2)	9 (7)
Strawberry juice- cooked	4.32 (4)	27 (6)	1.59 (11)	1 (11)
Almond- cooked	4.94 (3)	237 (2)	15.11 (3)	55 (1)
Blueberry- uncooked	3.57 (7)	93 (4)	5.99 (6)	20 (5)
Peach- uncooked	3.65 (6)	17 (7)	6.07 (5)	10 (6)
Nectarine- uncooked	3.72 (5)	9 (8)	3.19 (9)	5 (8)
Apple, fruit with peel- uncooked	0.83 (12)	0	1.14 (12)	0
Raspberry- uncooked	1.54 (9)	0	2.23 (10)	5 (8)
Grape- uncooked	0.60 (14)	2 (10)	0.26 (16)	0
Apple sauce- cooked	0.15 (18)	0	0.03 (19)	0
Apple juice- uncooked	0.10 (19)	1 (12)	0.06 (18)	0
Apricot dried- uncooked	0.46 (15)	5 (9)	0.39 (15)	2 (10)
Raspberry juice- uncooked	0.22 (17)	0	0.18 (17)	0
Beef liver- cooked	2.35 (8)	39 (5)	1.07 (14)	0
Blackberry juice- uncooked	0.07	0	--	0

Snap beans- cooked	1.28 (10)	2 (10)	1.14 (13)	0
Beets garden tops- uncooked[b]	0.72 (13)	1 (12)	5.58 (7)	31 (4)
Okra- cooked	0.05 (21)	0	3.96 (8)	0

Briefly, rankings are performed by the DEEM and CARES programs by totaling exposure over all commodities for all individuals and apportioning that total exposure by commodity. For example, if a Chemical X is registered on only two commodities (A and B) and the sum of all exposures to Chemical X over all individuals is 30 g, this exposure would be apportioned between Commodities A and B. If the total of all exposures to all individuals through Commodity A is 20 grams and that through B is 10 grams, then exposure through Commodity A would be 20 g/30 g or 67% and that through Commodity B would be 10 g/30 g or 33%. It is in this way that the percentages above were derived. This information is used by the risk assessor to suggest which commodities are signicant risk contributors and is confirmed by the risk assessor by re-running the analyses with the commodities of interest removed.

[b] OPP has noted the signficant differences in rankings for pears and beet tops between DEEM-FCID and CARES. We contacted the CARES developer regarding this discrepancy. They identified a slight programming error for the case of pears with respect to use and generation of percent crop treated values. They are now investigating reasons for the slight discrepancies for garden beet tops. We expect that additional updated information will be provided at the SAP meeting.

Table 15 Model Approximation CEC for 3 to 5 year olds									
				DEEM-Calendex		CARES		Lifeline	
Pct aPAD at 99.9th				47.6%		%48.5%		51.4%	
RAC	FF	RAC	Food Form	Pct Contribution	#Occurrences > aPAD	Pct Contribution	#Occurrences > aPAD	Pct Contribution	#Occurrences > aPAD
003600	240	Strawberry, juice	status: cooked;form: canned;method: N/A	29.4% (1)	116 (3)	24.3% (2)	116 (3)	28.8% (2)	364 (3)
003590	110	Strawberry	status: uncooked;form: fresh;method: N/A	23.8% (2)	245 (1)	25.1% (1)	248 (1)	29.0% (1)	675 (1)
002350	240	Olive	status: cooked;form: canned;method: N/A	21.1% (3)	84 (6)	21.9% (3)	87 (4)	16.6% (3)	277 (5)
000070	110	Apple, fruit with peel	status: uncooked;form: fresh;method: N/A	7.3% (4)	16 (10)	7.2% (4)	16 (9)	7.8% (4)	123 (9)
002600	110	Peach	status: uncooked;form: fresh;method: N/A	4.1% (5)	67 (8)	4.2% (5)	65 (7)	4.1% (5)	236 (6)
003590	240	Strawberry	status: cooked;form: canned;method: N/A	4.0% (6)	73 (7)	3.9% (6)	75 (6)	4.0% (6)	209 (7)
001620	298	Fish- shellfish, mollusc	status: cooked;form: not specified;method: not specified	3.7% (7)	0 (10)	3.5% (8)	0 (10)	0% (9)	0 (10)
000110	212	Apple, sauce	status: cooked;form: fresh;method: boiled	3.4% (8)	20 (9)	3.1% (9)	18 (8)	3.5% (7)	157 (8)
002300	110	Nectarine	status: uncooked;form: fresh;method: N/A	3.2% (9)	85 (5)	3.6% (7)	79 (5)	3.1% (8)	356 (4)
001750	110	Grape	status: uncooked;form: fresh;method: N/A	0% (10)	117 (4)	3.1% (9)	117 (2)	3.1% (8)	413 (2)
000030	230	Almonds	status: cooked;form: dried;method: N/A	0% (10)	247 (1*)	0% (10)	245 (2)	0% (10)	548 (2*)

For both age groups, the SAS model approximations provided lower estimates on the %aPAD at the 99.9th for this MultiRAC case example. For 3 to 5 year olds, the model approximations underestimated DEEM-Calendex (47.6% vs 81% of aPAD), CARES (48.5% vs 89%), and Lifeline (51.4% vs 77%) shown in Table 15. Similarly, for the 20 to 49 year old age group, the model approximations underestimated DEEM-Calendex (16% vs 29% of aPAD), CARES (16% vs 34%), and Lifeline (24% vs 32%). As noted, using the model approximation to estimate aggregate exposure will tend to underestimate exposure at the 99.9th percentile due to several reasons: (1) exposure from other commodities are not included, and (2) adding increments of 0.01% of the population may overlook some individuals consuming a commodity that have infrequent (<0.01%), but high exposure.

The potential for commodities having infrequent but high exposure is illustrated with the contribution from almonds. While the models predict almonds to have a moderate share of contribution to total exposure, the models (and model approximations) also indicate that almonds can produce many simulated exposure days with high exposure. Reviewing the data inputs, we have: (i) relatively high residues (14 - 45 ppm), (ii) assumed only one

percent of the almond crop treated, and (iii) relatively low percent of diaries with almond consumption. The high residue data reflects OPP's typical use of field trial data for nuts (PDP generally monitors fruits and vegetables). The approximated consumption distributions (D1, C1, L1) indicates that less than four percent of the food diaries have any consumption of almonds. Therefore, almonds' share of total exposure among the top 0.2% is low since there is a relatively low probability of matching a high consumption with a treated (high residue) commodity. On the other hand, almonds could produce relatively high exposure - if residues were at tolerance (or field trial) levels (e.g., 0.25 grams/kg bwt x 40 ppm = 0.01 mg ai/kg bwt = 100% aPAD). In contrast, strawberries contribute a relatively high share of total exposure even though those residues are smaller (0.005 to 5.3 ppm), since the percent of crop treated is higher (PCT=27%), and strawberry consumption is greater than almonds in both prevalence (fresh strawberries are consumed almost 7% of the days) and amount (up to 28 grams/kg bwt; in 1% of all simulated exposure days, strawberry consumption exceeds 3.5 gms/kg bwt/day).

Like the actual models, the model approximations also ranked fresh strawberries, strawberry juice and olives among the top contributors in terms of the share that these commodities contribute to the total exposure among 3 to 5 year olds at the top 0.2% of the population. Strawberries also rank high in terms of the number of occurrences that the commodity in and of itself provided exposure that exceeded the aPAD. While fresh grapes also rank high in this measure, it ranks low in terms of its overall share. Grapes do not have high residues (maximum value is 0.94 ppm), but there is one diary that reported high consumption (63 grams/kg bwt). Similarly, almonds did not provide any contribution in the model approximation CECs for this age group, but it ranks high as far as the number of occurrences that it provides.

Table 16 Model Approximation CEC for 20 to 49 year olds									
				DEEM-Calendex		CARES		Lifeline	
Pct aPAD at 99.9th				16.2%		16.6%		22.4%	
RAC	FF	RAC	Food Form	Pct Contribution		Pct Contribution		Pct Contribution	
002350	240	Olive	status: cooked;form: canned;method: N/A	48.6% (1)	11 (4)	44.3% (1)	17 (4)	36.3% (1)	90 (5)
003590	110	Strawberry	status: uncooked;form: fresh;method: N/A	22.4% (2)	70 (1)	21.8% (2)	82 (1)	20.1% (2)	219 (2)
002600	110	Peach	status: uncooked;form: fresh;method: N/A	4.6% (3)	5 (6)	13.0% (3)	19 (3)	4.9% (6)	127 (3)
003600	240	Strawberry, juice	status: cooked;form: canned;method: N/A	4.4% (4)	3 (7)	3.3% (7)	4 (7)	8.4% (4)	78 (7)
002300	110	Nectarine	status: uncooked;form: fresh;method: N/A	3.7% (5)	8 (5)	3.7% (5)	13 (6)	0% (10)	82 (6)
003590	240	Strawberry	status: cooked;form: canned;method: N/A	3.6% (6)	14 (3)	3.9% (4)	15 (5)	4.1% (7)	94 (4)
000030	230	Almond	status: cooked;form: dried;method: N/A	3.4% (7)	49 (2)	3.6% (6)	78 (2)	0% (10)	351 (1)
002350	291	Olive	status: cooked;form: not specified;method: baked	3.2% (8)	0 (8)	0% (10)	0 (8)	3.6% (9)	0 (9)
001620	298	Fish- shellfish, mollusc	status: cooked;form: not specified;method: not specified	3.2% (9)	0 (8)	0% (10)	0 (8)	3.8% (8)	0 (9)
001620	213	Fish- shellfish, mollusc	status: cooked;form: fresh;method: fried	3.0% (10)	0 (8)	0% (10)	0 (8)	0% (10)	0 (9)
000070	110	Apple, fruit with peel	status: uncooked;form: fresh;method: N/A	0% (11)	0 (8)	3.3% (7)	0 (8)	7.3% (5)	2 (8)
001620	292	Fish- shellfish, mollusc	status: cooked;form: not specified;method: boiled	0% (12)	0 (8)	3.1% (9)	0 (8)	11.5% (3)	0 (9)

In Table 16 (adults 20 to 49 years old), the approximated models also ranked olives and strawberries as the major commodities in terms of their shares of total exposure among 20 to 49 year olds at the upper percentile. Strawberries and almonds rank atop the commodities in terms of frequency of contributing to high exposure in and of itself. While strawberries is ranked high in part due to the number of diaries containing high strawberry consumption, there are relatively fewer diaries with high almond consumption and, therefore, almonds have only a small share of total exposure. Due to the relatively high residue values used in this MultiRAC scenario, a modest amount of almond consumption is required to obtain high exposure. For example, an individual needs to consume only 0.2 grams/kg bwt of almonds to obtain exposure exceeding the aPAD with residues of 45.8 ppm. Fish-shellfish, mollusc again appear in the Lifeline and DEEM model approximations' CEC report, but contributed relatively little in the actual CEC reports (<0.5% for the 20to49 population in DEEM). The relatively high contribution in the Lifeline approximated model due to its relatively low weight in DEEM-Calendex (CSFII survey weight=) and CARES.

VI. Summary and Future Activities

OPP has previously sponsored several presentations to the FIFRA Scientific Advisory Panel on the LifeLine, CARES, and DEEM/Calendex pesticide exposure models. The models all permit a time-based integration of both residential and dietary (food and water) exposures to pesticides. This is performed probabilistically, such that aggregation (or combining) of residues across multiple routes is accounted for in an appropriate and realistic manner.

The objective of the analysis described in this document is a comparison of dietary exposures (food + water) as estimated by each of the three models. Specifically, EPA has used each of the three models and a common data set based on a hypothetical chemical to further explore how the models differ both in the exposure estimates they produce and in the assumptions, methods, algorithms, and techniques which they use: each of the three models differ in their base "reference" populations, in their binning methodologies, in their assumptions regarding bodyweight, and in the model weights used by the program to project the reference population to the U.S. population as a whole. To the extent that these– and other– differences may produce different estimates of exposure at various percentiles of interest, such differences are of interest to OPP in a regulatory context. This is particularly true if the differences are large, are systematic, or span regions of regulatory interest. The food (alone), water (alone), and food + water exposure estimates at the 95th, 99th, and 99.9th percentiles produced by each of the three models for the common hypothetical data set are generally quantitatively similar . The relatively small differences observed in this exercize are in general keeping with what OPP has found in its systematic comparisons of estimated exposures from DEEM and Lifeline from concurrent analyses performed for regulatory reviews. In these comparisons, OPP has found close agreement between the exposure estimates producted by DEEM and those produced by LifeLine.

In an effort to explore in greater detail specific reasons for (the generally minor) differences in estimated exposures among the three models, OPP developed SAS approximations to these three models. These SAS approximation models specifically permit the isolation of factors related to the Reference Population, Binning Procedures, Sampling Weights, and individual Body Weights which cannot be isolated by running the individual models. Section IV of this document describes the development of these SAS approximation models and some analyses performed by the Agency using these SAS approximation models to compare and contrast model design features of DEEM-Calendex, CARES, and LifeLine. Based on these analyses the Agency concludes that the SAS approximation models tracks actual model results very closely for single Raw Agricultural Commodity (RAC) analyses, and reasonably well for the multi-RAC analyses. Thus, OPP concludes that differences in exposure estimates between the three models can be, by use of the SAS-model approximations, attributed to specific, identifiable differences between models with respect to assumptions, data sources, algorithms, and methods.

OPP is planning a number of additional future exploratory and other activities to futher investigate and evaluate these and other exposure software models. Some of these future

activities include the following:

- The exposure estimates provided here were based on three models – Lifeline, CARES, and DEEM or DEEM-Calendex – and were based on exposures through only the dietary (food and water) pathways. Similar analyses and comparisons are planned in which an additional model (SHEDS) is included and in which the residential pathways are considered.

- Currently, the models use slightly different modications/versions of the CSFII or FCID databases for food consumption. OPP has recently slightly revised this database to be consistent with OPP's current policies with respect to foods and food forms, and has provided this revised FCID database to the model developers. We anticipate that this common, revised food consumption database will be incorporated into each model by the model developers.

- OPP recognizes that it is important to be able to correlate or validate model-predicted exposures with measured exposures in the "real world", where possible. There is increasing interest in biomonitoring and an increasing number of studies being performed by EPA's Office of Research and Development (ORD) which make such model validation exercises possible (or at least allow "order-of-magnitude" comparisions to be made).

- The focus of this current comparison was on estimates of 1-day dietary (food + water) exposure . Future comparison efforts will be directed at longer-term (>1 day) exposures which incorporate all three exposure pathways (food, water, and residential). The EPA ORD's STAR grant program is currently involved in collecting integrated longitidual information regarding exposures across multiple pathways. We anticipate working closely with ORD in this process in developing this critical model input information.

Appendix A: Derivation of Equivalence of "Exposure" and "Consumption" Following Single-RAC Analysis Using 1 ppm

Mathematically,

Exposure = Consumption X Residue

$$\frac{\text{mg chemical}}{\text{kg bw/day}} = \frac{\text{kg food}}{\text{kg bw/day}} \times \frac{\text{mg chemical}}{\text{kg food}}$$

$$\text{Consumption} = \frac{\text{Exposure}}{\text{Residue}} = \frac{\frac{\text{mg chemical}}{\text{kg bw/day}}}{\frac{\text{mg chemical}}{\text{kg food}}}$$

$$= \frac{\frac{1}{\text{kg bw/day}}}{\frac{1}{\text{kg food}}}$$

$$= \frac{\text{kg food}}{\text{kg bw/day}}$$

Ergo, if residue is set at **1 ppm** and concentration factors turned off using DEEM™ software,
then *exposure = "consumption* $\frac{\text{kg food}}{\text{kg bw}}$*"*

Expressed another way:

If an individual consumes a food containing 1 ppm (i.e., 1 mg/kg produce) and is "exposed" to 1 mg pesticide /kg bodyweight, then that individual MUST have consumed a total of 1 kg of produce to obtain that exposure since Concentration X Consumption = Exposure and 1 mg chemical/kg produce x 1kg produce/kg bw = 1 mg chemical / kg b.w. Eating 1 kg of produce containing 1 ppm (=mg chemical/kg produce) is the ONLY way an individual can receive an exposure of 1 mg chemical/kg b.w (assuming consumption of a single RAC). Eating 2 kg produce is the only way an individual can be exposed to 2 mg/kg bw.

Similarly for 3, 4, and 5 kg of produce. Thus, to obtain the amount eaten from the output of Lifeline, CARES, or DEEM, one would need to take the "exposure" output following insertion of 1 ppm as a concentration expressed as "mg pesticide /kg b.w." and consider it as kg produce. Ergo, putting in 1 ppm into Lifeline, CARES, or DEEM will result in an "exposure" output which really reflects kg produce consumed. [and by similar logic, putting in 1000 ppm concentration into CARES will result in g produce consumed/kg b.w.]

Appendix B :Comparison of DEEM and Lifeline Dietary (Food Alone) Assessment Results for 14 OPP Assessments

This Appendix provides summary information for numerous concurrent analyses done for DEEM-FCID and Lifeline using equivalent data sets. These analysis represent actual regulatory assessments and were done for the purpose of comparing expsoure estimates produced by DEEM-FCID and Lifeline. Although the current document focuses on acute (one day) exposures, included here for completeness are comparisons of expsure estimates for the two models of both acute and chronic exposure estimates.

Summary of Chronic Dietary Exposure and Risk for Chemical 1				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.001128	4.2	0.001063	3.9
All Infants (< 1 year old)	0.003715	14	0.003657	14
Children 1-2 years old	0.006284	23	0.006303	23
Children 3-5 years old	0.004064	15	0.004341	16
Children 6-12 years old	0.001743	6.5	0.001702	6.3
Youth 13-19 years old	0.000873	3.2	0.000814	3.0
Adults 20-49 years old	0.000577	2.1	0.000686	2.5
Adults 50+ years old	0.000620	2.3	0.000664	2.5
Females 13-49 years old	0.000654	2.4	0.000790	2.9

Summary of Chronic Dietary Exposure and Risk for Chemical 2				
Population Subgroup	DEEM-FCID™		LifeLine™	
	Exposure (mg/kg/day)	%cPAD	Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.000053	<1	0.000049	<1
All Infants (< 1 year old)	0.000023	<1	0.000021	<1
Children 1-2 years old	0.000125	<1	0.000109	<1

Summary of Chronic Dietary Exposure and Risk for Chemical 2				
Population Subgroup	DEEM-FCID™		LifeLine™	
	Exposure (mg/kg/day)	%cPAD	Exposure (mg/kg/day)	% cPAD
Children 3-5 years old	0.000128	<1	0.000113	<1
Children 6-12 years old	0.000089	<1	0.000078	<1
Youth 13-19 years old	0.000053	<1	0.000047	<1
Adults 20-49 years old	0.000042	<1	0.000042	<1
Adults 50+ years old	0.000035	<1	0.000041	<1
Females 13-49 years old	0.000040	<1	0.000048	<1

Summary of Chronic Dietary Exposure and Risk for Chemical 3				
Population Subgroup	DEEM™-FCID		LifeLine™	
	Exposure (mg/kg/day)	%cPAD	Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.001343	<1.0	0.001125	<1.0
All Infants (< 1 year old)	0.005829	3.4	0.004902	2.9
Children 1-2 years old	0.007105	4.2	0.006381	3.8
Children 3-5 years old	0.004832	2.8	0.004442	2.6
Children 6-12 years old	0.002200	1.3	0.001869	1.1
Youth 13-19 years old	0.000763	<1.0	0.000654	<1.0
Adults 20-49 years old	0.000639	<1.0	0.000710	<1.0
Adults 50+ years old	0.000849	<1.0	0.000745	<1.0
Females 13-49 years old	0.000703	<1.0	0.000790	<1.0

Summary of Chronic Dietary Exposure and Risk for Chemical 4				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.000259	26	0.000235	24
All Infants (< 1 year old)	0.000408	41	0.000371	37
Children 1-2 years old	0.000408	120	0.001170	117
Children 3-5 years old	0.001204	78	0.000775	78
Children 6-12 years old	0.000779	46	0.000424	42
Youth 13-19 years old	0.000213	21	0.000187	19
Adults 20-49 years old	0.000151	15	0.000166	17
Adults 50+ years old	0.000164	16	0.000164	16
Females 13-49 years old	0.000158	16	0.000188	19

Summary of Chronic Dietary Exposure and Risk for Chemical 5				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.001719	8.6	0.00175	8.8
All Infants (< 1 year old)	0.000886	4.4	0.00087	4.3
Children 1-2 years old	0.001548	7.7	0.00140	7.0
Children 3-5 years old	0.001727	8.6	0.00163	8.1
Children 6-12 years old	0.001593	8.0	0.00142	7.1
Youth 13-19 years old	0.001429	7.1	0.001429	6.9
Adults 20-49 years old	0.001824	9.1	0.00181	9.1
Adults 50+ years old	0.001760	8.8	0.00189	9.4
Females 13-49 years old	0.001872	9.4	0.00194	9.7

Summary of Chronic Dietary Exposure and Risk for Chemical 6				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.000012	<1	0.000012	<1
All Infants (< 1 year old)	0.000036	<1	0.000031	<1
Children 1-2 years old	0.000028	<1	0.000027	<1
Children 3-5 years old	0.000028	<1	0.000027	<1
Children 6-12 years old	0.000019	<1	0.000017	<1
Youth 13-19 years old	0.000011	<1	0.000011	<1
Adults 20-49 years old	0.000009	<1	0.000010	<1
Adults 50+ years old	0.000008	<1	0.000010	<1
Females 13-49 years old	0.000009	<1	0.000011	<1

Summary of Chronic Dietary Exposure and Risk for Chemical 7				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.000168	3.4	0.000159	3.2
All Infants (< 1 year old)	0.000139	2.8	0.000124	2.5
Children 1-2 years old	0.000346	6.9	0.000316	6.7
Children 3-5 years old	0.000295	5.9	0.000276	5.5
Children 6-12 years old	0.000214	4.3	0.000190	3.8
Youth 13-19 years old	0.000151	3.0	0.000136	2.7
Adults 20-49 years old	0.000160	3.2	0.000148	2.9
Adults 50+ years old	0.000127	2.5	0.000149	3.0
Females 13-49 years old	0.000137	2.7	0.000159	3.2

Summary of Chronic Dietary Exposure and Risk for Chemical 8				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.001977	18	0.001903	17
All Infants (< 1 year old)	0.003438	31	0.003565	32
Children 1-2 years old	0.007519	68	0.007396	67
Children 3-5 years old	0.005737	52	0.005627	51
Children 6-12 years old	0.003918	31	0.003195	29
Youth 13-19 years old	0.001772	16	0.001668	15
Adults 20-49 years old	0.001368	12	0.001454	13
Adults 50+ years old	0.001165	11	0.001409	12
Females 13-49 years old	0.001276	12	0.001671	15

Summary of Chronic Dietary Exposure and Risk for Chemical 9				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.000015	<1	0.000014	<1
All Infants (< 1 year old)	0.000017	<1	0.000014	<1
Children 1-2 years old	0.000032	<1	0.000027	<1
Children 3-5 years old	0.000036	<1	0.000034	<1
Children 6-12 years old	0.000027	<1	0.000024	<1
Youth 13-19 years old	0.000019	<1	0.000017	<1
Adults 20-49 years old	0.000012	<1	0.000012	<1
Adults 50+ years old	0.000008	<1	0.000011	<1
Females 13-49 years old	0.000012	<1	0.000014	<1

Summary of Chronic Dietary Exposure and Risk for Chemical 10				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.000030	0.1	0.000019	0.1
All Infants (< 1 year old)	0.000062	0.3	0.000033	0.1
Children 1-2 years old	0.000073	0.3	0.000051	0.2
Children 3-5 years old	0.000062	0.3	0.000039	0.2
Children 6-12 years old	0.000041	0.2	0.000024	0.1
Youth 13-19 years old	0.000025	0.1	0.000016	0.1
Adults 20-49 years old	0.000025	0.1	0.000017	0.1
Adults 50+ years old	0.000025	0.1	0.000017	0.1
Females 13-49 years old	0.000024	0.1	0.000017	0.1

Summary of Chronic Dietary Exposure and Risk for Chemical 11				
Population Subgroup	DEEM-FCID™ Chronic Dietary		Lifeline™ Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD	Dietary Exposure (mg/kg/day)	% cPAD
General U.S. Population	0.000242	0.8	0.000232	0.8
All Infants (< 1 year old)	0.000661	2.2	0.000554	1.9
Children 1-2 years old	0.000548	1.8	0.000539	1.8
Children 3-5 years old	0.000535	1.8	0.000505	1.7
Children 6-12 years old	0.000373	1.2	0.000346	1.2
Youth 13-19 years old	0.000238	0.8	0.000224	0.8
Adults 20-49 years old	0.000197	0.7	0.000198	0.7
Adults 50+ years old	0.000153	0.5	0.000191	0.6
Females 13-49 years old	0.000185	0.6	0.000228	0.8

Results of Acute Dietary Exposure Analysis using DEEM-FCID™ for Chemical 12						
Population Subgroup	95th Percentile		99th Percentile		99.9th Percentile	
	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD
General U.S. Population	0.101406	10	0.213266	21	0.448222	45
All Infants (< 1 year old)	0.151252	15	0.293004	29	1.450145	145
Children 1-2 years old	0.312671	31	0.517028	52	0.834925	83
Children 3-5 years old	0.225240	23	0.395847	40	0.699340	70
Children 6-12 years old	0.135445	14	0.231391	23	0.351494	35
Youth 13-19 years old	0.090982	9.0	0.197597	20	0.311376	31
Adults 20-49 years old	0.067129	7.0	0.125381	13	0.281385	28
Adults 50+ years old	0.059752	6.0	0.101368	10	0.188474	19
Females 13-49 years old	0.073419	16	0.134416	30	0.265744	59

Results of Acute Dietary Exposure Analysis using Liefline for Chemical 12						
Population Subgroup	95th Percentile		99th Percentile		99.9th Percentile	
	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD
General U.S. Population	0.097052	10	0.207462	21	0.437302	44
All Infants (< 1 year old)	0.154129	15	0.312935	31	0.610843	61
Children 1-2 years old	0.311978	31	0.523393	52	0.886922	89
Children 3-5 years old	0.241526	24	0.402838	40	0.778797	78
Children 6-12 years old	0.132602	13	0.241125	24	0.430791	43
Youth 13-19 years old	0.084961	8	0.165164	17	0.351044	35
Adults 20-49 years old	0.073839	7	0.142175	14	0.304764	30
Adults 50+ years old	0.070479	7	0.133929	13	0.288166	29
Females 13-49 years old	0.085414	19	0.164400	37	0.352814	78

Results of Acute Dietary Exposure Analysis using DEEMFCID™ for Chemical 13						
Population Subgroup	95th Percentile		99th Percentile		99.9th Percentile	
	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD
General U.S. Population	0.008452	0.7	0.016173	1.3	0.031253	2.5
All Infants (< 1 year old)	0.002563	0.2	0.029559	2.4	0.093307	7.5
Children 1-2 years old	0.007620	0.6	0.021525	1.7	0.066148	5.3
Children 3-5 years old	0.009497	0.8	0.021198	1.7	0.051612	4.1
Children 6-12 years old	0.08621	0.7	0.015757	1.3	0.035078	2.8
Youth 13-19 years old	0.007489	0.6	0.014684	1.2	0.020221	1.6
Adults 20-49 years old	0.008826	0.7	0.016380	1.3	0.029998	2.4
Adults 50+ years old	0.008090	0.7	0.015325	1.2	0.026120	2.1
Females 13-49 years old	0.009456	0.8	0.016869	1.4	0.030134	2.4

Results of Acute Dietary Exposure Analysis using Lifeline™ for Chemical 13						
Population Subgroup	95th Percentile		99th Percentile		99.9th Percentile	
	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD
General U.S. Population	0.00894	0.7	0.01777	1.4	0.03462	2.8
All Infants (< 1 year old)	0.00250	0.2	0.03374	2.7	0.09576	7.7
Children 1-2 years old	0.00766	0.6	0.02469	2.0	0.05985	4.8
Children 3-5 years old	0.00919	0.7	0.02137	1.7	0.04860	3.9
Children 6-12 years old	0.00808	0.6	0.01623	1.3	0.03416	2.7
Youth 13-19 years old	0.00721	0.6	0.01509	1.2	0.03205	2.6
Adults 20-49 years old	0.00903	0.7	0.01783	1.4	0.03174	2.5
Adults 50+ years old	0.00931	0.7	0.01795	1.4	0.03300	2.6
Females 13-49 years old	0.00983	0.8	0.01955	1.6	0.03418	2.7

Results of Acute Dietary Exposure Analysis using DEEMFCID™ for Chemical 14						
Population Subgroup	95th Percentile		99th Percentile		99.9th Percentile	
	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD
General U.S. Population	0.000035	0.01	0.000070	0.02	0.0000190	0.06
All Infants (< 1 year old)	0.000142	0.05	0.000218	0.07	0.000394	0.13
Children 1-2 years old	0.000070	0.02	0.000157	0.05	0.000831	0.28
Children 3-5 years old	0.000066	0.02	0.000121	0.04	0.000680	0.23
Children 6-12 years old	0.000046	0.02	0.000077	0.03	0.000166	0.06
Youth 13-19 years old	0.000028	0.01	0.000043	0.01	0.000096	0.03
Adults 20-49 years old	0.000024	0.01	0.000051	0.02	0.000130	0.04
Adults 50+ years old	0.000022	0.01	0.000046	0.02	0.000091	0.03
Females 13-49 years old	0.000023	0.01	0.000046	0.02	0.000117	0.04

Results of Acute Dietary Exposure Analysis using Lifeline™ for Chemical 14						
Population Subgroup	95th Percentile		99th Percentile		99.9th Percentile	
	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD	Exposure (mg/kg/day)	% aPAD
General U.S. Population	0.000035	0.01	0.000069	0.02	0.0000187	0.06
All Infants (< 1 year old)	0.000013	0.04	0.000220	0.07	0.000398	0.13
Children 1-2 years old	0.000073	0.02	0.000175	0.06	0.000546	0.18
Children 3-5 years old	0.000067	0.02	0.000115	0.04	0.000505	0.17
Children 6-12 years old	0.000044	0.01	0.0000788	0.03	0.000216	0.07
Youth 13-19 years old	0.000029	0.01	0.000053	0.02	0.000114	0.04
Adults 20-49 years old	0.000028	0.01	0.000054	0.02	0.000119	0.04
Adults 50+ years old	0.000028	0.01	0.000056	0.02	0.000119	0.04
Females 13-49 years old	0.000031	0.01	0.000058	0.02	0.000136	0.05

Summary of Cancer Dietary Exposure and Risk for Chemical 15				
Population Subgroup	Exposure (mg/kg/day)		MOE	
	DEEM-FCID™	Lifeline™	DEEM-FCID	Lifeline
General U.S. Population	0.000499	0.001308	3.4e+04	1.3e+04

Summary of Cancer Dietary Exposure and Risk for Chemical 16				
Population Subgroup	Exposure (mg/kg/day)		MOE	
	DEEM-FCID™	Lifeline™	DEEM-FCID	Lifeline
General U.S. Population	0.000028	0.000019	1.64 x 10-7	1.13 x 10-7

Summary of Cancer Dietary Exposure and Risk for Chemical 17				
Population Subgroup	Exposure (mg/kg/day)		MOE	
	DEEM-FCID™	Lifeline™	DEEM-FCID	Lifeline
General U.S. Population	0.000015	0.000014	1.1e+06	5.92 x 10-7