Appendix A – Glossary and Definitions

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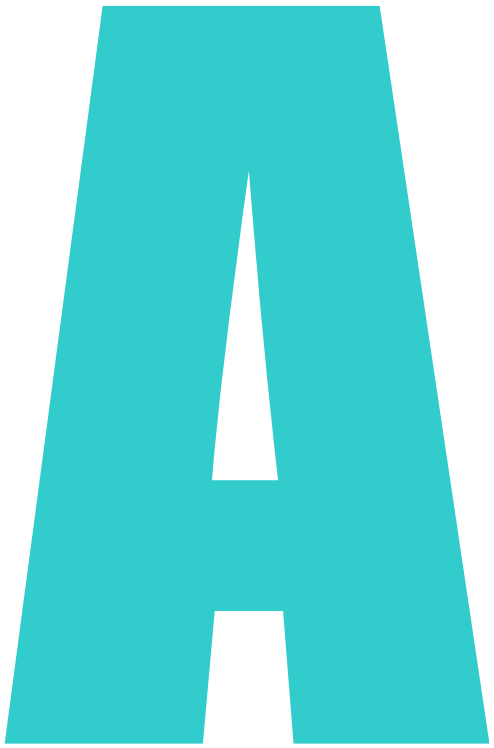

Glossary and Definitions

a.i. (Active Ingredient)
The chemical or substance in a pesticide product intended to kill, repel, attract, mitigate or control a pest or that acts as a plant growth regulator. The other ingredients in the formulation are referred to as inerts.

Absorbed Dose
The amount of a substance penetrating across the absorption barriers of an organism, via either physical or biological processes. Synonymous with internal dose.

Acute Exposure Estimate
Estimate of exposure from a pesticide or several pesticides with a common mechanism of toxicity during a one day (24 hour) time period.

Aggregate Exposure
The amount of a single substance available for interaction with metabolic processes or biologically significant receptors from multiple routes and pathways of exposure.

Aggregate Exposure Assessment
A process for developing an estimate of the extent of exposure of a defined population to a given chemical by all relevant routes and from all relevant sources (pathways).

Aggregate Risk
The risk associated with all pathways and routes of exposure to a single ch emical.

Algorithms
The computational equations used for the calculations of the risk assessments.

Benchmark Dose (BMD)
A statistical lower confidence limit on the dose producing a predetermined level of change in adverse response compared with background response. The BMD is derived by fitting a mathematical model to the dose-response data. A BMD10 is a benchmark dose with 10% change in adverse response compared with background response.

Biomonitoring
Measurement of a pesticide or its metabolites in body fluids of exposed persons, and conversion to an equivalent absorbed dose of the pesticide based on a knowledge of its human metabolism and pharmacokinetics.

Blended Commodities
Foods or food forms for which large-scale blending and mixing occurs at some time in the food chain to the consumer.

BW (Body Weight)
Usually expressed in kg.

Common Mechanism of Toxicity

Pertains to two or more pesticide chemicals or other substances that cause a common toxic effect by the same, or essentially the same, sequence of major biochemical events. Hence, the underlying basis of the toxicity is the same, or essentially the same, for each chemical.

CMG (Common Mechanism Group)

A group of pesticides determined to cause adverse effects by a common mechanism of toxicity. Not all members of a CMG will necessarily be incorporated in a cumulative risk assessment.

CWS (Community Water System)

A drinking water system specific to a designated community.

Concurrent Exposure (or Co-occurrence)

The potential human exposure by all relevant pathways routes that allows one chemical to add to the exposure of another chemical such that the total risk of a group of common mechanism chemicals is an estimate of the sum of exposures to the individual chemicals. The accumulation of the common toxic effect may or may not depend on simultaneous or overlapping exposures depending on duration and recovery time of the toxic.

Crop Groupings

EPA designated groupings of Raw Agricultural Commodities into groups according to similar morphologies (type, size, texture, etc.). Residue data generated on a few designated representative commodities can then be translated to the others in the crop group assuming use patterns are similar.

CAG (Cumulative Assessment Group)

A subset of the CMG. The CAG is that group of pesticides selected for inclusion in the cumulative risk assessment. The chemicals in the CAG are judged to have a hazard and exposure potential that could result in the expression of a cumulative risk.

Cumulative Exposure Assessment

A process for developing an estimate of the extent to which a defined population is exposed to two or more chemicals which share a common mechanism of toxicity by all relevant routes and from all relevant sources (pathways).

Cumulative Risk

The likelihood for the occurrence of an adverse health effect resulting from all pathways and routes of exposure to substances sharing a common mechanism of toxicity.

CSFII (Continuing Survey of Food Intake by Individuals)

USDA survey database which compiles food and water consumption data for a representative sample of the U.S. population.

CSU (Contribution, Sensitivity, Uncertainty)

In CARES, the module which allows the user to “look at” the output from the assessments and to determine contributions of various variables.

Decompositing

The process of statistically translating composite residue information into “individual item” residue information for monitoring data.

Deterministic

This approach uses point estimates, for example, single maximum values or average values, to represent input variables in an exposure model.

Dislodgeable Residues
The portion of a pesticide that is available for transfer from a pesticide treated surface.

Dose
The amount of a compound received by an individual, usually expressed as mg/kg BW and sometimes with an added dimension of time.

ECOFRAM (Ecological Committee On FIFRA Risk Assessment Methods)
Joint EPA, industry and academic work group on probabilistic risk assessment for pesticides.

ED_{10}
A statistical estimate of the dose which would cause an incremental effect of 10% in the exposed population, usually expressed as mg/kg BW/day. Also suggested for use as a "benchmark" dose in lieu of a NOEAL for calculating MOEs.

Environmental Degradate
Breakdown products of the parent pesticide in the environment; sometimes incorrectly called metabolites.

Event Allocation
The frequency of residential pesticide use is specified in this CARES module.

Exposure
Contact of a substance with the outer boundary of an organism. Exposure is quantified as the concentration of the agent in the medium in contact integrated over the time duration of that contact.

Exposure Assessment
The qualitative or quantitative determination or estimation of the magnitude, frequency, duration, and rate of exposure of an individual or population to a chemical.

Exposure Scenario
A combination of facts, assumptions, and inferences that define a discrete situation or activity where potential exposures may occur.

FCID (Food Commodity Intake Database)
EPA's database takes the individual eating event data from CSFII and summarizes it in 24-hour intervals for each person in the CSFII. Also, the CSFII includes missing values that were replaced by imputed values in the FCID.

Field Trials
Residue studies conducted on crops (usually by registrants) at maximum label rates and minimum PHI's to determine tolerance levels for registration.

FIRST (FQPA Index Reservoir Screening Tool)
A Tier 1 screening model from US EPA that estimates pesticide concentrations in surface water (using an index reservoir).

FDA Monitoring Data
Pesticide monitoring data collected by the FDA. Samples are collected at points of entry into the country for tolerance enforcement. Compliance samples are collected at distribution centers.

FQPA Safety Factor

Uncertainty Factor applied to pesticide reference doses, mandated by the Food Quality Protection Act of 1996, to provide extra protection for infants and children unless studies justify it can be removed.

FCT (Fraction Crop Treated)

An estimate of the acreage under cultivation that is actually treated with the pesticide at least once. It is expressed as a fraction of the total acreage in the US for that crop.

Index Chemical

The chemical selected as the basis for standardization of toxicity of components in a mixture. The index chemical should have a clearly defined dose-response relationship.

Index Reservoir

The reservoir, usually the most vulnerable, selected as the basis for the FIRST model.

Geographic Granularity

Drinking water assessment spatial resolution or smalle st geographic unit of analysis.

GW (Ground Water)

Water residing in a subsurface environment.

Hazard

The adverse effects or toxicity.

HI (Hazard Index)

The sum of each exposure divided by it's RfD.

HUC (Hydrologic Unit Codes)

Hierarchical classification of hydrologic drainage basins in the US.

LOAEL (Lowest Observed Adverse Effect Level)

The lowest dose at which an adverse an adverse effect is seen.

LOD (Limit of Detection)

Statistical method for handling non-detectable pesticide residues in food. The level at or below which residues cannot be detected for that method.

LOQ (Limit of Quantification)

Statistical method for handling non-quantifiable residues in food. The level below which residues cannot be reliably quantified for that method.

Market Basket Data

Pesticide residue data based on sampling food at the consumer purchasing level. Samples are collected at the grocery store or supermarket level and treated as the average consumer prepares before analyzing (i.e. peeling, washing but not cooking).

Metabolite

Break down product of the parent pesticide in plants or animals.

MOE (Margin of Exposure)

The point of departure divided by a human environmental exposure of interest, actual or hypothetical.

Monte Carlo Analysis

One of several mathematical techniques for performing probabilistic assessments. The method relies on the computational powers of modern computers to simulate the range and frequency of all possible outcomes of a process based on repeatedly sampling from the inputs provided by the user. These inputs are combined according to the model that is specified by the user.

NOAEL (No Observed Adverse Effect Level)

The dose at which no adverse toxic effect is seen.

ND (Nondetectable Residues)

Pesticide residue analysis that indicates the pesticide cannot be detected at or above the LOD of the method.

Occupational Exposure

How much pesticide a person may receive directly from use at or for the workplace.

Pathway of Exposure

The physical course a pesticide takes from the source to the organism exposed (e.g. through food or drinking water consumption or residential pesticide use).

%CT (Percent Crop Treated)

An estimate of the acreage under cultivation that is actually treated with the pesticide at least once. It is expressed as a percentage of the total acreage in the US for that crop.

PPE (Personal Protective Equipment)

Equipment used to reduce exposure to pesticides when applying to crops or harvesting. (i.e. safety glasses, gloves, long pants, etc.).

Pesticide

A compound used to control a pest. A pest can be an insect, plant or any organism, such as a mold or bacteria.

Pesticide Residue

The amount of the original chemical (known as parent) or breakdown products (known as metabolites) that remain on the medium of concern (i.e. food, drinking water, skin, etc.).

PHED (Pesticide Handlers Exposure Database)

A large database of actual pesticide exposure studies that EPA uses to estimate exposure when data are not available for a specific chemical exposure scenario.

PDP Monitoring Data (Pesticide Data Program)

USDA's Agricultural Marketing Service program, started in 1971, in which selected commodities are analyzed for pesticide residues. Samples are collected at US distribution centers and treated as an average consumer would prepare before analyzing.

POC (Point of Comparison)

Dose at which a uniform response occurs.

POD (Point of Departure)

Point on the dose-response curve where each chemical's response is close to or within the background level of response, in other words, the dose at which effects from a pesticide are first distinguishable. Depending on the data available and the purpose of the analysis, there are differing procedures for estimating points of departure.

PAD (Population Adjusted Dose)

The reference dose of a pesticide adjusted for the FQPA safety factor.

Potential Dose

The amount of a chemical contained in material ingested, air breathed, or bulk material applied to the skin.

Post-Application Exposure

Exposures from any residues that remain in and around the home after a pesticide is used.

PHI (Pre-Harvest Interval)

The interval between the last application of pesticide and harvest of the crop.

Probabilistic Assessment

The use of a statistical technique (e.g. Monte Carlo) to quantify both the range of exposures to pesticide residues and the probability or chance of exposure to any particular level.

Processing Factors

Factors that account for increase or decrease in residues in foods or in water due to preparation (i.e. washing, cooking, peeling) or treatment (i.e. filtration, chlorination).

PUMS (Public Use Micro Data Sample)

PUMS is a statistically reliable dataset provided by the Bureau of the Census, Economics and Statistics Administration that contains sufficient data and statistical weightings for sampled individuals to be representative of the 1990 U.S. population. This dataset is approximately a 30% sample from the portion of the U.S. population that received the long form so that the total number of individuals in PUMS is equivalent to 5% of the U.S. Population.

PRZM/EXAMS

Przm-3 and EXAMS-II are both US EPA environmental fate models that simulate field-scale pesticide transport for Tier 2 screening assessments. The Pesticide Root Zone Model (PRZM-3) simulates leaching and run-off from a field; the output from PRZM is linked to the Exposure Analysis Modeling System (EXAM-II) to simulate pesticide concentrations in surface water.

RAC (Raw Agricultural Commodity)

Foods broken down into their simplest components are composed of the RACs. This is the crop/commodity that EPA registers and assigns tolerances (i.e., wheat, corn, apples, tomatoes, etc.) from field trial data.

Residential Exposure

EPA uses this term to refer to any exposure to any person who lives in a home beyond the diet and outside the occupational setting. Exposures that occur as a result of pesticide applications in schools, parks, and day care centers are included under this term.

RfD (Reference Dose)

The NOAEL divided by the UF.

Risk

The likelihood of adverse effects, usually expressed as an MOE, fraction of RfD, the HI, or a probability.

Risk Mitigation

If some uses of a registered pesticide are found to pose unreasonable human health or ecological risks, EPA explores ways to mitigate or manage the risks by modifying or ending the problematic use.

Route of Exposure

The way a chemical enters an organism after contact (e.g. inhalation, oral, dermal). Note that all three routes of exposure can occur within an exposure pathway. A pathway is not route specific.

SCI-GROW

This Tier 1 screening model, Screening Concentration in Ground Water, identifies pesticides that are not expected to reach ground water, due to the nature of their properties. This empirical model from the US EPA is based on actual monitoring data collected for a number of pesticides that serve as benchmarks.

Sensitivity Analysis

Effect of changing the value of single variables in the risk assessment to see the magnitude of the change to the outcome.

Source Code

The actual programming code that is the basis for the algorithms and the model.

SW (Surface Water)

Water located above ground.

SOP (Standard Operating Procedures)

Methods developed by the agency to address over 40 different exposure scenarios for residential exposure assessment.

Surrogate Data

Substitute data or measurements on one substance (or population) used to estimate analogous or corresponding values for another substance (or population).

Tier Process

Current regulatory policy provides for various levels (“tiers”) of exposure assessment in which various simplifying assumptions are successively relaxed. AS the tier increases the amount of refined or more realistic data used in the assessment increases.

Tolerance

The maximum, legal limit of a pesticide that is allowed to remain in or on a treated commodity as it enters interstate commerce. Usually expressed in parts per million (ppm).

Toxic Effect

An effect known (or reasonably expected) to occur in humans that results from exposure to a chemical substance and that will or can reasonably be expected to endanger or adversely affect quality of life.

TEF (Toxic Equivalency Factor)

When products have a common mechanism of toxicity, it may be possible to normalize the dosage of each product to that of a reference product. For example if 10 mg/kg BS/day of Chemical A produces the same effects as 1 mg/kg BW/day of the reference chemical. The TEF applied to chemical A would be 0.1-fold.

Toxicity Endpoint

A dose where no adverse effects are measured.

Transfer Coefficient

Residue transfer rate to humans during the completion of specific activities, calculated using concurrently collected environmental residue data.

Uncertainty

Lack of knowledge about specific factors, parameters, or models.

UF (Uncertainty Factor)

Uncertainty factors applied to account for inter- and intra-species differences in relation to toxic effects, and uncertainties associated with the data.

Validation

All software testing, verification, and associated life-cycle documentation are classified as system validation. Validation determines how well the model is able to characterize hazard, exposure and risk compared to that occurring in the real world. For the CARES project, eight categories are defined in Appendix F.

Variability

Differences attributed to true heterogeneity or diversity in a population or exposure parameter.

Verification

Verification of the underlying exposure assessment models is conducted through the five categories of software testing listed in Appendix F.

VIC (Vector of Individual Characteristics)

The Census based or other database characteristics for each member in the Reference Population that are used by any component of CARES. The characteristics or traits used for matching between databases.

Vulnerability

The susceptibility of a water source for contamination with pesticide residues because of location, cropping practices, type of source, etc

Appendix B – Population Generator White Paper

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B

CARES

Population Generator

CARES White Paper

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CARES Population Generator

Reference Population, Individual Characteristics, and Matching

This paper describes the current state of the Population Generator methodology for creating a Reference Population, determining the Vector of Individual Characteristics for each member of the Reference Population, and the associated matching of information from multiple databases. The methodology is in the process of being fine-tuned to optimize its performance characteristics, and the details of the methodology may change slightly as necessary.

Executive Summary

The Population Generator supports the Cumulative and Aggregate Risk Evaluation System (CARES) characterizations of exposure and aggregate and cumulative doses and risks in the U.S. population or a user-specified subpopulation of the U.S. Population.

The Population Generator creates a Reference Population containing 100,000 representative individuals from the U.S. population. These individuals are real people randomly selected from the 1990 U.S. Census (see Section 2.4 and Appendix A for a detailed description of the stratified sample design).

The distributions of the percent of the total weight over the strata for age/gender, race/ethnicity, and Census division in the U.S. Census (5% PUMS) and the Reference Population are qualitatively very similar.

With a sample size of 100,000 for the Reference Population, subpopulations of freque nt interest (e.g., specified by age/gender, race/ethnicity, etc.) contained at least 5,000 people. A sample size of 5,000 ensures that estimates of the 95-th, 99-th, and 99.9-th quantiles have a high probability of being close to their true subpopulation values (Section 2.3).

CARES uses the people in the Reference Population as the starting point for all characterizations of exposure, dose, and risk. The Reference Population is a fixed set of people that does not vary from analysis to analysis. The estimated exposures, doses, and risks for the individuals in the Reference Population do vary from analysis to analysis. The Reference Population's distributions of exposures, doses, and risks parallel those in the U.S. population or subpopulation in that they are based on a representative sample of real people from the U.S. population or subpopulation.

An individual's exposure, dose, and risk depend on numerous characteristics of the individual (e.g., age, gender, race/ethnicity, body weight, geographic location, income, type of residence, and activity patterns). The dietary (food and water) and non-dietary calculations in CARES reflect this dependence and incorporate the individual's characteristics. The Population Generator provides these characteristics to the dietary and non-dietary modules for each individual whose exposure, dose, and risk is being evaluated.

The Population Generator determines individual characteristics by starting with a Reference Population of people from the 1990 U.S. Census (the 5% Public Use Microdata Sample, or PUMS, provided by the Bureau of the Census). This guarantees that the combination

of the Census characteristics (age, gender, etc.) for a person being analyzed in CARES is a realistic combination in the sense that it is a combination corresponding to a real person in the U.S. population.

The individual's characteristics that are not in the Census are appended to the Census characteristics as needed from other databases. For example, food consumption is appended based on USDA's Continuing Survey of Food Intakes by Individuals (CSFII) database and the companion EPA's Food Commodity Intake Database (FCID).

The portions of an individual's vector of individual characteristics (VIC) that are in the Census are set equal to those Census values. The portions of the VIC that are not in the Census are filled in with the values for a person in another database who is matched to the Census individual.

It is impossible to match an individual in the Census with the exact same individual in another database. The identities of sampled persons in most surveys are unknown. But more importantly, the same individuals are unlikely to be present or represent the same age groups in samples taken at different times. (An infant in 1997, for example, could never exist in the full1990 Census let alone the PUMS.) Thus, a Census individual is matched to a similar (but not necessarily identical) person in another database.

Because certain activities of importance in at least some FQPA assessments, such as pregnancy, are unique to females, matched individuals are not allowed to cross gender lines. That is, Census females are always matched with females in other databases, and Census males are always matched to males in other databases.

The general strategy with respect to characteristics other than gender is to match individuals that have similar (if not identical) characteristics. More specifically, the strategy is to determine for each sampled Census individual a measure of how similar each person in the other database is to the Census individual, and then match the Census individual to a person in the other database on the basis of this similarity measure.

The similarity measure is calculated using relevant characteristics that are in common between the two databases. The similarity measure is a single number obtained by pooling the relative similarity evaluated for each characteristic.

The similarity measure reflects the objective of the matching. For example, if a Census individual is being matched to a person in CSFII primarily for the purpose of obtaining food consumption information, then the similarity measure reflects the importance of matching characteristics with respect to food consumption. Because food consumption is not in the Census, a Census individual is not matched to a CSFII person on the basis of food consumption itself. Rather, the Census person is matched using the common characteristics (e.g., age/gender, race/ethnicity, and region) to the extent that they are associated with food consumption differences (see Section 4.3 for further details).

Each sampled Census individual is matched to a person in CSFII. The matched CSFII person fills in some parts of the VIC for the Census individual. Specifically, the matched CSFII person fills in a body weight, nursing or pregnancy status, and one or two days of food consumption. The remaining days in the 365-day calendar profile of food consumption for the Census individual are filled in by calendar-specific days of food consumption from other persons in CSFII who are similar to the CSFII person matched to the sampled Census individual (see Section 5 for further details).

1. Supporting the Objectives of CARES

The Population Generator supports the objectives of CARES.

CARES characterizes the exposures and the aggregate and cumulative doses and risks in the U.S. population or a user-specified subpopulation of the U.S. population. Individuals in the target population are expected to have different exposures, doses, and risks. CARES des cribes the distribution of exposures, doses, and risks among the individuals.

A "Population Generator" is the process used to create a representative set of individuals from the U.S. population. This representative set of individuals from the U.S. population is the "Reference Population." The Reference Population is composed of a large number of real people randomly selected from the 1990 U.S. Census. CARES uses the real people in the Reference Population as the starting point for all characterizations of exposures, doses, and risks.

Distributions of exposures, doses, and risks are derived from the estimated exposures, doses, and risks for the individuals in the Reference Population. The Reference Population is a fixed set of real people that does not vary from analysis to analysis. The estimated exposures, doses, and risks for the individuals in the Reference Population do vary from analysis to analysis.

The user may specify that a particular CARES analysis only include a subpopulation of the Reference Population. For example, the user can specify that the distributions of exposures, doses, and risks be derived only from the children in the Reference Population.

The distributions of exposures, doses, and risks parallel those in the U.S. population or specified subpopulation in that they are based on a representative sample of real people from the U.S. population or a user-specified subpopulation.

An individual's exposure, dose, and risk depend on numerous characteristics of the individual (e.g., age, gender, body weight, geographic location, income, type of residence, and activity patterns). The dietary (food and water) and non-dietary equations and models in CARES reflect this dependence and incorporate the individual's characteristics. The Population Generator provides these characteristics to the dietary and non-dietary modules for each individual whose exposure, dose, and risk is being evaluated.

The Population Generator determines individual characteristics by starting with a Reference Population of real people from the U.S. Census. This guarantees that the combination of the Census characteristics (age, gender, etc.) for a person being analyzed in CARES is a realistic combination in the sense that it is a combination corresponding to a real pers on in the U.S. population. Furthermore, the joint distribution of these characteristics in CARES is the same as the joint distribution in the U.S. population. For example, the frequency of individuals that are male, age 40, live in South, etc. is the same as in the 1990 U.S. Census. This faithfulness to the U.S. population is guaranteed in CARES but is not guaranteed by procedures that start with artificially created individuals.

The individual's characteristics that are not in the Census are appended to the Census characteristics as needed from other databases. For example, food consumption is appended based on USDA's Continuing Survey of Food Intakes by Individuals (CSFII) database and EPA's Food Commodity Intake Database (FCID).

One of the primary functions of the Population Generator is to ensure that the individual characteristics used in the dietary and non-dietary calculations are consistent. For example, the individual's gender in one calculation is the same as that individual's gender in every other calculation. All of the individual's characteristics that are used by more than one module for calculating exposures and risks for that individual are determined and stored in a common location by the Population Generator. This enhances the consisten cy between dietary and non-

dietary calculations. (In some cases, other CARES modules will add additional individual characteristics by simulation. When these characteristics need to be shared by other modules, they are also stored in the common area.)

Another function of the Population Generator is to ensure that the individual's characteristics are determined in a reasonable manner. Rather than artificially simulating an individual's entire lifetime starting from birth, the individual's characteristics are the characteristics of real individuals in databases. For example, forty-year-old males are characterized by database information on forty-year-old males as opposed to projecting these characteristics over forty years starting at birth.

An individual's characteristics are determined by databases related to the U.S. population or subpopulations. No single database has all of the individual's characteristics needed to evaluate that individual's exposure, dose, and risk. Thus, the information in several databases has to be pooled. The Population Generator does this pooling starting with data from the U.S. Census—a 5% Public Use Microdata Sample (PUMS).

The Population Generator pools information from different databases in a reasonable and statistically appropriate manner. The objective of the Population Generator is for its Reference Population of individuals to have the same joint distribution of dietary and non-dietary exposure (and risk) as occurs in the U.S. population or the user-specified subpopulation.

The Population Generator and its resultant Reference Population of representative individuals from the U.S. population support the objectives of CARES.

2. Reference Population

2.1 Goals

A goal of the Population Generator is to have the distribution of individual exposures, doses, and risks in the Reference Population agree with that of individuals in the U.S. population or a user-specified subpopulation. Furthermore, the marginal exposure distributions are to agree by age group, gender, race, and geographic location.

The Population Generator deals with real people at the time the databases are assembled. For example, seventy-year-old people are described today as opposed to seventy years in the future.

The Reference Population is a very large fixed sample of individuals from the U.S. population. By having a fixed sample of individuals as opposed to a sample that varies from analysis to analysis, differences in CARES' analyses are due to differences in chemicals and exposure scenarios being analyzed as opposed to random differences in the individuals being analyzed.

CARES results using a common Reference Population can also be more readily compared to other analyses based on different exposure algorithms or input data without having the comparison confounded by two different methods of selecting the individuals representing the U.S. population.

2.2 Composition

The Reference Population is composed of a sample of real people from the 1990 U.S. Census.

The sample is drawn from the 5% Public Use Microdata Sample (PUMS) purchased from Bureau of the Census, Economics and Statistics Administration, U.S. Department of Commerce (Census, 1992):

> "The file contains individual weights for each person and housing unit which, when applied to the individual records, expand the sample to the total population." (page AB-1)
>
> "Each PUMS file provides records for States and many of their geographic levels. The heirarchy is shown below: The 5% sample identifies every State and various subdivisions of the State called 'Public Use Microdata Areas', each with at least 100,000 persons. These PUMAs were primarily based on counties, groups of counties, and places. When these entities have more than 200,000 persons, PUMAs can represent parts of counties, places, etc. None of these PUMAs on the 5% sample crosses state lines." (page AB-2)

2.3 Size

The number of persons in the Reference Population was chosen so that typical statistical inferences would perform well.

In CARES exposures, doses, and risks are calculated for each person in a sample from the U.S. population or a user-specified subpopulation. The corresponding sample distribution of calculated values is used to estimate the population distribution. A goal is to choose the sample size large enough so that the probability is high that the quantiles in the sample distribution are close to the quantiles in the population distribution.

For example, it is reasonable to choose the sample size to be large enough that the 95-th sample quantile is close to the 95-th population quantile. For instance, the probability that the 95-th sample quantile is less than the 90-th population quantile should be small (say, less than 5%); that is,

P(95-th Sample Quantile < 90-th Population Quantile) < 0.05

Similarly, the probability that the 95-th sample quantile is greater than the 99-th population quantile should be small (say, less than 5%); that is,

P(95-th Sample Quantile > 99-th Population Quantile) < 0.05.

Inferences may be based on sample quantiles other than the 95-th sample quantile. For instance, the 99-th and 99.9 sample quantiles may be the basis for some inferences. In such cases, it would be nice if the sample size were large enough that all of the following conditions are satisfied:

P(95-th Sample Quantile < 90-th Population Quantile) < 0.05
P(95-th Sample Quantile > 99-th Population Quantile) < 0.05

P(99-th Sample Quantile < 95-th Population Quantile) < 0.05
P(99-th Sample Quantile > 99.9-th Population Quantile) < 0.05

P(99.9-th Sample Quantile < 99.5-th Population Quantile) < 0.05
P(99.9-th Sample Quantile > 99.95-th Population Quantile) < 0.05.

Table 1 indicates how the behavior of the sample quantiles is related to the sample size. For example, a sample size of 5,000 ensures that:

P(95-th Sample Quantile < 90-th Population Quantile) $<3 \times 10^{-38}$
P(95-th Sample Quantile > 99-th Population Quantile) $<1 \times 10^{-92}$

P(99-th Sample Quantile < 95-th Population Quantile) $< 1 \times 10^{-55}$
P(99-th Sample Quantile > 99.9-th Population Quantile) $< 2 \times 10^{-33}$

P(99.9-th Sample Quantile < 99.5-th Population Quantile) $<1 \times 10^{-6}$
P(99.9-th Sample Quantile > 99.95-th Population Quantile) < 0.042.

Roughly speaking, a sample of size 5,000 ensures that the 95-th and 99-th sample quantiles are going to be extremely close to their corresponding population quantiles. Also, if the sample size is 5,000, then there is less than a 1-in-a-million chance that the 99.9-th sample quantile is less than the 99.5-th population quantile, and less than a 5% chance that the 99.9-th sample quantile is greater than the 99.95-th population quantile. Thus, a sample size of 5,000 essentially guarantees that the 99.9-th sample quantile will not appreciably underestimate the 99.9-th population quantile and will not appreciably ove restimate the 99.9-th population quantile more than 5% of the time.

Table 1. Behavior of Sample Quantiles for Different Sample Sizes [1]

Sample Size	P(95-th Sample Quantile < 90-th Population Quantile)	P(95-th Sample Quantile > 99-th Population Quantile)	P(99-th Sample Quantile < 95-th Population Quantile)	P(99-th Sample Quantile > 99.9-th Population Quantile)	P(99.9-th Sample Quantile < 99.5-th Population Quantile)	P(99.9-th Sample Quantile > 99.95-th Population Quantile)
1000	6×10^{-9}	2×10^{-20}	3×10^{-12}	1 E-8	0.04	0.090
2000	2×10^{-16}	1×10^{-38}	4×10^{-23}	6×10^{-15}	0.003	0.080
3000	1×10^{-23}	1×10^{-56}	5×10^{-34}	4×10^{-21}	0.0002	0.066
4000	5×10^{-31}	1×10^{-74}	8×10^{-45}	2×10^{-27}	0.00002	0.052
5000	3×10^{-38}	1×10^{-92}	1×10^{-55}	2×10^{-33}	0.000001	0.042
6000	1×10^{-45}	1×10^{-110}	2×10^{-66}	1×10^{-39}	1×10^{-7}	0.033
7000	7×10^{-53}	2×10^{-128}	4×10^{-77}	9×10^{-46}	9×10^{-9}	0.027
8000	4×10^{-60}	2×10^{-146}	6×10^{-88}	7×10^{-52}	8×10^{-10}	0.021
9000	2×10^{-67}	2×10^{-164}	1×10^{-98}	5×10^{-58}	7×10^{-11}	0.017
10000	1×10^{-74}	2×10^{-182}	2×10^{-109}	4×10^{-64}	6×10^{-12}	0.014

[1] Probabilities are calculated using binomial probabilities and the techniques for determining confidence and probability limits for quantiles as described in Bradley (1968), Hogg and Craig (1970), or Conover (1971).

Thus, a sample of size 5,000 is sufficient for reliably estimating population quantiles by sample quantiles. This suggests that the size of the Reference Population be at least 5,000. In practice, the population quantiles are of interest not only for the U.S. population but also for some subpopulations. Hence, the goal is to make the size of the Reference Population large enough that the sample size for subpopulations of typical interest can be at least 5,000.

The following is a list of some of the subpopulations of the U.S. population that are, separately or in combination, frequently of interest:

Race/Ethnicity:
- White (Non-Hispanic)
- Black (Non-Hispanic)
- Asian
- Native American
- Hispanic

Age/Gender:
- Nursing infant (<1 year)
- Non-nursing infant (<1 year)
- Child (1-3 years)
- Child (4-6 years)
- Child (7-12 years)
- Male (13-19 years)
- Female (13-19 years)
- Male (20-54 years)
- Female (20-54 years)
- Seniors (55+ years).

The goal is to create a Reference Population large enough so that these subpopulations would have a sample size of at least 5,000. A Reference Population of 100,000 was constructed that attains this goal.

2.4 Sample Design

A stratified random sample of 100,000 real people from the 5% PUMS was selected to form the Reference Population.

The stratified random sample was designed to have the following characteristics. The number of people in each of the following age and gender categories is at least 5,000:

Category	**Abbreviation**
Infants	00-00
Ages 1 to 3	01-03
Ages 4 to 6	04-06
Ages 7 to 12	07-12
Males: Ages 13 to 19	Males13-19)
Females: Ages 13 to 19	Females 13-19)
Males: Ages 20 to 54	Males 20-54
Females: Ages 20 to 54	Females 20-54
Ages ≥ 55	55+

In fact the size of the infant population was required to be at least 20,000. This requirement was to chosen so that the expected number of nursing infants would be at least 5,000. This was based on an estimate that approximately 25% of infants are nursing infants. A separate stratum for nursing infants could not be used because the nursing/non-nursing characteristic is not included in the Census.

The number of people in each of the following race/ethnicity categories is at least 5000:

White,
Black,
Asian,
Native American, and
Hispanic.

The stratified sampling design included strata for each the 9 following Census Divisions (a subcategory of Region). The sampling resulted in at least 5,000 people in each of these 9 region/divisions.

Region	Division	Abbreviation	States
Northeast	New England	NE	Maine, New Hampshire, Vermont, Massachusetts, Rhode Island, Connecticut
	Middle Atlantic	MA	New York, New Jersey, Pennsylvania
Midwest	East North Central	ENC	Ohio, Indiana, Illinois, Michigan, Wisconsin
	West North Central	WNC	Minnesota, Iowa, Missouri, North Dakota, South Dakota, Nebraska, Kansas
South	South Atlantic	SA	Delaware, Maryland, District of Columbia, Virginia, West Virginia, North Carolina, South Carolina, Georgia, Florida
	East South Central	ESC	Kentucky, Tennessee, Alabama, Mississippi
	West South Central	WSC	Arkansas, Louisiana, Oklahoma, Texas
West	Mountain	MTN	Montana, Idaho, Wyoming, Colorado, New Mexico, Arizona, Utah, Nevada
	Pacific	PAC	Washington, Oregon, California, Alaska, Hawaii

Tables 2 and 3 indicate the number of people in the Reference Population by age/gender, race/ethnicity, and region/division resulting from the stratified sampling plan. Details of the development of the sampling plan are given in Appendix A.

Table 2. The Number of People in the Reference Population by Age/Gender and Race/Ethnicity

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native American	Hispanic	Other	
Infants 00-00	14,079	2,548	496	236	2,590	54	20,003
01-03	3,229	599	263	322	573	18	5,004
04-06	3,304	580	252	308	547	18	5,009
07-12	4,448	795	437	593	701	18	6,992
Males 13-19	3,284	574	282	328	524	18	5,010
Females 13-19	3,285	608	274	306	518	18	5,009
Males 20-54	12,929	1,424	1,139	1,107	1,444	20	18,063
Females 20-54	13,333	1,817	1,266	1,206	1,428	20	19,070
55+	12,890	1,134	591	594	613	18	15,840
Total	70,071	10,079	5,000	5,000	8,938	202	100,000

Table 3. The Number of People in the Reference Population by Age/Gender, Race/Ethnicity, and Region/Division

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native American	Hispanic	Other	
Infants 00-00	NE 860 MA 2205 ENC 2780 WNC 1272 SA 2211 ESC 807 WSC 1325 MTN 843 PAC 1776 --- 14,079	NE 50 MA 308 ENC 384 WNC 72 SA 851 ESC 287 WSC 358 MTN 32 PAC 206 --- 2,548	NE 20 MA 72 ENC 35 WNC 13 SA 40 ESC 5 WSC 25 MTN 15 PAC 271 --- 496	NE 3 MA 7 ENC 15 WNC 24 SA 12 ESC 3 WSC 36 MTN 76 PAC 60 --- 236	NE 64 MA 283 ENC 163 WNC 35 SA 186 ESC 11 WSC 552 MTN 253 PAC 1043 --- 2,590	NE 6 MA 9 ENC 7 WNC 2 SA 8 ESC 2 WSC 3 MTN 2 PAC 15 --- 54	NE 1003 MA 2884 ENC 3384 WNC 1418 SA 3308 ESC 1115 WSC 2299 MTN 1221 PAC 3371 --- 20,003
01-03	NE 200 MA 501 ENC 627 WNC 288 SA 516 ESC 191 WSC 308 MTN 196 PAC 402 --- 3,229	NE 12 MA 76 ENC 85 WNC 16 SA 201 ESC 66 WSC 87 MTN 7 PAC 49 --- 599	NE 10 MA 37 ENC 21 WNC 8 SA 20 ESC 3 WSC 14 MTN 9 PAC 141 --- 263	NE 4 MA 11 ENC 21 WNC 33 SA 21 ESC 4 WSC 52 MTN 95 PAC 81 --- 322	NE 15 MA 64 ENC 35 WNC 7 SA 41 ESC 2 WSC 124 MTN 56 PAC 229 --- 573	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 2 --- 18	NE 243 MA 691 ENC 791 WNC 354 SA 801 ESC 268 WSC 587 MTN 365 PAC 904 --- 5,004
04-06	NE 199 MA 502 ENC 657 WNC 308 SA 507 ESC 197 WSC 321 MTN 207 PAC 406 --- 3,304	NE 11 MA 70 ENC 81 WNC 16 SA 192 ESC 67 WSC 89 MTN 8 PAC 46 --- 580	NE 10 MA 33 ENC 20 WNC 8 SA 20 ESC 3 WSC 14 MTN 8 PAC 136 --- 252	NE 4 MA 9 ENC 22 WNC 32 SA 20 ESC 5 WSC 50 MTN 89 PAC 77 --- 308	NE 14 MA 59 ENC 33 WNC 7 SA 38 ESC 2 WSC 125 MTN 55 PAC 214 --- 547	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 2 --- 18	NE 240 MA 675 ENC 815 WNC 373 SA 779 ESC 276 WSC 601 MTN 369 PAC 881 --- 5,009
07-12	NE 254 MA 665 ENC 903 WNC 428 SA 668 ESC 281 WSC 440 MTN 289 PAC 520 --- 4,448	NE 14 MA 94 ENC 113 WNC 21 SA 265 ESC 97 WSC 123 MTN 9 PAC 59 --- 795	NE 15 MA 59 ENC 34 WNC 12 SA 37 ESC 5 WSC 26 MTN 13 PAC 236 --- 437	NE 9 MA 19 ENC 46 WNC 62 SA 40 ESC 13 WSC 103 MTN 156 PAC 145 --- 593	NE 18 MA 77 ENC 43 WNC 10 SA 49 ESC 3 WSC 166 MTN 72 PAC 263 --- 701	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 2 --- 18	NE 312 MA 916 ENC 1141 WNC 535 SA 1061 ESC 401 WSC 860 MTN 541 PAC 1225 --- 6,992
Males 13-19	NE 192 MA 516 ENC 662 WNC 295 SA 514 ESC 225 WSC 323 MTN 196 PAC 361 --- 3,284	NE 10 MA 72 ENC 83 WNC 15 SA 189 ESC 72 WSC 86 MTN 7 PAC 40 --- 574	NE 9 MA 40 ENC 21 WNC 8 SA 26 ESC 3 WSC 16 MTN 9 PAC 150 --- 282	NE 5 MA 11 ENC 28 WNC 32 SA 26 ESC 7 WSC 61 MTN 83 PAC 75 --- 328	NE 12 MA 59 ENC 32 WNC 5 SA 41 ESC 2 WSC 123 MTN 50 PAC 200 --- 524	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 2 --- 18	NE 230 MA 700 ENC 828 WNC 357 SA 798 ESC 311 WSC 611 MTN 347 PAC 828 --- 5,010

Table 3. (Continued)

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native American	Hispanic	Other	
Females 13-19	NE 189 MA 511 ENC 662 WNC 293 SA 526 ESC 223 WSC 321 MTN 194 PAC 366 --- 3,285	NE 10 MA 76 ENC 90 WNC 15 SA 205 ES 75 WSC 90 MTN 6 PAC 41 --- 608	NE 8 MA 40 ENC 21 WN 8 SA 24 ESC 4 WSC 15 MTN 8 PAC 146 --- 274	NE 4 MA 10 ENC 24 WNC 28 SA 24 ESC 7 WSC 55 MTN 81 PAC 73 --- 306	NE 13 MA 60 ENC 31 WNC 6 SA 39 ESC 2 WSC 124 MTN 52 PAC 191 --- 518	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 2 --- 18	NE 226 MA 699 ENC 830 WNC 352 SA 820 ESC 313 WSC 607 MTN 343 PAC 819 --- 5,009
Males 20-54	NE 823 MA 2047 ENC 2412 WNC 1039 SA 2173 ESC 790 WSC 1211 MTN 716 PAC 1718 --- 12,929	NE 29 MA 195 ENC 191 WNC 35 SA 487 ESC 146 WSC 195 MTN 20 PAC 126 --- 1,424	NE 37 MA 181 ENC 81 WNC 22 SA 99 ESC 11 WSC 63 MTN 29 PAC 616 --- 1,139	NE 19 MA 49 ENC 94 WNC 91 SA 106 ESC 25 WSC 186 MTN 248 PAC 289 --- 1,107	NE 32 MA 178 ENC 82 WNC 15 SA 143 ESC 5 WSC 295 MTN 128 PAC 566 --- 1,444	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 4 --- 20	NE 942 MA 2652 ENC 2862 WNC 1204 SA 3010 ESC 979 WSC 1952 MTN 1143 PAC 3319 --- 18,063
Females 20-54	NE 859 MA 2128 ENC 2497 WNC 1061 SA 2242 ESC 826 WSC 254 MTN 731 PAC 1735 --- 13,333	NE 35 MA 256 ENC 254 WNC 44 SA 626 ESC 191 WSC 248 MTN 20 PAC 143 --- 1,817	NE 40 MA 190 ENC 90 WNC 25 SA 123 ESC 15 WSC 70 MTN 39 PAC 674 --- 1,266	NE 20 MA 52 ENC 102 WNC 103 SA 114 ESC 26 WSC 199 MTN 283 PAC 307 --- 1,206	NE 36 MA 199 ENC 76 WNC 14 SA 145 ESC 5 WSC 301 MTN 129 PAC 523 --- 1,428	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 4 --- 20	NE 992 MA 2827 ENC 3021 WNC 1249 SA 3252 ESC 1065 WSC 2074 MTN 1204 PAC 3386 --- 19,070
55+	NE 773 MA 2199 ENC 2313 WNC 1119 SA 2298 ESC 782 WSC 1188 MTN 645 PAC 1573 --- 12,890	NE 17 MA 161 ENC 165 WNC 27 SA 379 ESC 136 WSC 158 MTN 11 PAC 80 --- 1,134	NE 13 MA 72 ENC 31 WNC 7 SA 37 ESC 3 WSC 19 MTN 15 PAC 394 --- 591	NE 9 MA 29 ENC 47 WNC 46 SA 52 ESC 12 WSC 125 MTN 124 PAC 150 --- 594	NE 10 MA 82 ENC 26 WNC 6 SA 100 ESC 2 WSC 138 MTN 65 PAC 184 --- 613	NE 2 MA 2 ENC 2 WNC 2 SA 2 ESC 2 WSC 2 MTN 2 PAC 2 --- 18	NE 824 MA 2545 ENC 2584 WNC 1207 SA 2868 ESC 937 WSC 1630 MTN 862 PAC 2383 --- 15,840
Total	NE 4349 MA 11274 ENC 13513 WNC 6103 SA 11655 ESC 4322 WSC 6691 MTN 4017 PAC 8857 --- 70,781	NE 188 MA 1308 ENC 1446 WNC 261 SA 3395 ESC 1137 WSC 1434 MTN 120 PAC 790 --- 10,079	NE 162 MA 724 ENC 354 WNC 111 SA 426 ESC 52 WSC 262 MTN 145 PAC 2764 --- 5,000	NE 77 MA 197 ENC 399 WNC 451 SA 415 ESC 102 WSC 867 MTN 1235 PAC 1257 --- 5,000	NE 214 MA 1061 ENC 521 WNC 105 SA 782 ESC 34 WSC 1948 MTN 860 PAC 3413 --- 8,938	NE 22 MA 25 ENC 23 WNC 18 SA 24 ESC 18 WSC 19 MTN 18 PAC 35 --- 202	NE 5012 MA 14589 ENC 16256 WNC 7049 SA 16697 ESC 5665 WSC 11221 MTN 6395 PAC 17116 --- 100,000

The design above was used to create the Reference Population as a probability sample of 100,000 individuals from the Census/PUMS. The sequential algorithm for the probability minimum replacement (PMR) design described by Chromy (1979) was used to randomly select the desired number of individuals from within each stratum. Individuals within each stratum were sampled with equal probability.

The individuals in the Census have "weights" corresponding to the number of people they represent in the U.S. Population on the basis of the sampling design used to generate the Census. The sampling plan used to generate the Reference Population increases these weights on the average by approximately 120 fold because there are 100,000 people in the Reference Population and 12,240,321 people in the 5% PUMS. Specifically, the weight of an individual in the Reference Population who originally had weight w in the Census and is in the i-th age/gender, j-th race/ethnicity, and k-th Division in the Reference Population is

Individual's Weight in Reference Population

= w / (sampling rate in stratified sample)

$$= w \times \frac{\text{number of people in the (i,j,k) -th stratum}}{\text{sample size for the (i,j,k)-th stratum}}.$$

As expected, the stratified sample used to generate the Reference Population closely parallels the Census. Table 4 shows that the distributions of the numbers of people represented by the Census and by the Reference Population are nearly identical with respect to age/gender, race/ethnicity, and Division. The number of people represented in a Reference Population stratum is the sum of the Reference Population weights for that stratum. Similarly, the number of people represented in a Census stratum is the sum of the Census weights for that stratum. The total weights for both the Reference Population and the Census is approximately 241 million people.

Table 4. Distributions of the Percent of the Total Weight over the Strata for Age/Gender, Race/Ethnicity, and Region/Division in the U.S. Census (5% PUMS) and the Reference Population

	Percent of the Total Weight	
	Census (5% PUMS)	Reference Population
Age/Gender		
Infants	1.32	1.31
Ages 01-03	4.69	4.67
Ages 04-06	4.51	4.53
Ages 07-12	8.82	8.76
Males 13-19	4.83	4.81
Females 13-19	4.63	4.62
Males 20-54	24.74	24.72
Females 20-54	25.66	25.76
Ages 55+	20.81	20.83
Race/Ethnicity		
White	75.90	75.89
Black	11.58	11.60
Asian	2.83	2.84
Native American	0.74	0.74
Hispanic	8.84	8.83
Other	0.10	0.10
Census Division		
New England	5.28	5.26
Middle Atlantic	15.08	15.04
East North Central	16.93	16.97
West North Central	7.07	7.03
South Atlantic	17.50	17.48
East South Central	6.10	6.08
West South Central	10.76	10.84
Mountain	5.51	5.52
Pacific	15.77	15.77

2.5 Advantages of Using the 5% PUMS to Create the Reference Population

A major advantage of using the U.S. Census to create the Reference Population is that the people in the Reference Population are real people. That is, these people's characteristics that are in the Census are real characteristics. This means that a person's combination of characteristics such as age, gender, race, etc. is real and not hypothetical or derived based on multiple assumptions. Because the Census is a random sample from the U.S. population and the Reference Population is a random sample from the Census, the distributions of age, gender, race, etc. are representative of the corresponding distributions in the U.S. population. Not only are the distributions of single characteristics representative, but also the joint distribution of the characteristics in the Census are representative.

Furthermore, because the Census randomly samples people of all ages, the Reference Population accurately reflects people of specific ages. That is, a 60-year-old person in the Reference Population has the characteristics of a real 60-year-old person. There is no derivation of these characteristics or assumptions about how a 60-year-old person would live his life from birth to age 60.

The Reference Population allows a representative sample of people in the U.S. population at a fixed point in time; namely, 1990. This is not a hypothetical cross-section at some point in the future derived on the basis of assumptions about how people will live their lives in the future.

The 5% PUMS represents the largest sample of individuals available as individual records. PUMS is 5% sample ofall households in U.S. In fact, PUMS is really an approximately 30% sample of the 1 out of 6 U.S. households that received the detailed Census 'long -form'. Thus, we have about 1/3 of all the available household data. This translates to approximately 13 million individuals.

PUMS is a valid statistical sample of the U.S. population. PUMS sample individuals have been assigned statistical weights to adjust for the ‘long-form’ sampling design and the 5% PUMS subsampling process. These weights allow for correct extrapolation to the entire U.S. population. Because the PUMS is a 5% sample, the average individual weight is approximately 20. That is, an ‘average’ individual in PUMS represents about 20 individuals in the U.S. population.

PUMS is a sample of complete households. Therefore, the entire array of data on every individual in a selected household is present.

The data are complete for every individual. There are no missing data in the PUMS. The Census Bureau has performed allocation (statistical imputation) on every missing item or non-responding individual.

The PUMS has geographic references down to a specially constructed "Public Use Microdata Area", or PUMA. PUMAs represent areas containing between 100,000 and 200,000 persons that are all completely within a State. In most cases, all of a PUMA is within a county as well. The Census Bureau provides maps delineating each PUMA. If these PUMA were placed into a Geographic Information System (GIS), they could be used to coordinate with microscale areas in other databases. For example, they might be used in conjunction with USGS hydrologic zones ('watersheds') maps.

The data available in PUMS consists primarily of geographic, demographic, and socio - economic information on individuals and households. These include descriptions of housing, occupational information including commuting behavioral patterns, and detailed economic information. Some miscellaneous characteristics such as 'source of household water' (CWS, private well, etc.) are also included.

Since most large-scale surveys include many Census definitions and characteristics, the PUMS provides an excellent common link for joining together multiple sources of data.

The large number of records in PUMS means that it includes many subpopulations that are misrepresented or even missed in smaller surveys. Thus, PUMS is ideal as a 'template' to insure representativeness.

In fact, the PUMS has the potential of calibrating non-statistical 'surveys' (collections of data) during the matching process. Records matched to the PUMS will acquire the representativeness of the PUMS—at least with respect to the Census characteristics that are used in the matching.

3. An Individual's Characteristics

3.1 Characteristics Implied by the Census

An individual in the Reference Population is a real person from the Census. The individual's characteristics identified in the Census are retained. That is, the individual's characteristics identified in the Census are not separated from the individual. The Census characteristics include

a. the number of people in the U.S. population represented by the individual (i.e., the sampling weight)
b. age
c. gender
d. race (including Hispanic origin codes)
e. location: region, division of the region, state, PUMA
f. location: metropolitan area or other
g. number of persons in the individual's household
h. household income indexed to a reference year
i. household income as a percent of poverty level
j. household percent poverty category
k. employment status
l. educational attainment
m. occupation categories
n. ownership status of individual's housing unit
o. household structure characteristics
p. type of household
q. source of water

There are several other characteristics available in the Census record for an individual.

3.2 Vector of Individual Characteristics

The individual's characteristics that are in the Census and used by any component of CARES are saved in a vector of individual characteristics (VIC).

There is a VIC for each individual in the Reference Population. The VIC is a long list of the characteristics of an individual that are used in the calculation of an individual's dietary and/or non-dietary exposures over a year. Basically, the VIC contains all of the available non -chemical specific information about an individual that the dietary and non-dietary exposure equations, models, and algorithms need to know in order to calculate that individual's exposure.

The VIC contains the individual's age, gender, income, residence type, etc. as well as the characteristics derived from this information such as food consumption, frequency and duration of activities leading to exposure, etc.

The two major components of the VIC are the VIC Kernel and the VIC Augmentation.

The VIC Kernel contains the information on the individual that is constant and does not change from one CARES analysis to another. The individual's characteristics from the Census are one part of the VIC Kernel.

Because the Census does not contain all of the information needed to calculate an individual's exposures, doses, and risks, some parts of the VIC Kernel are inferred from databases other than the Census. For example, an individual's food and water consumption is inferred from USDA's Continuing Survey of Food Intakes by Individuals (CSFII) and EPA's Food Commodity Intake Database (FCID).

An individual in the Reference Population is a real individual because he or she is an individual sampled from the U.S. population. The portion of the VIC Kernel equal to the individual's characteristics in the Census is real. The portion of the VIC Kernel originating from another database (such as CSFII or FCID) are also real in the sense that they come from real people; however, the person or person's in the other databases are unlikely to be the same as the Census individual. Therefore, the characteristics in the VIC Kernel originating in a database other than the Census are "attributed" characteristics. Thus, the Reference Population contains real people with some characteristics that are real (the characteristics from the Census) and some characteristics that are attributed (the characteristics originating in a database other than the Census).

The VIC Augmentation is the portion of the VIC added at the time of a CARES analysis. Sometimes individual characteristics not in the VIC Kernel are needed in a CARES module calculating 365-day profiles of food, water, or residential exposures. For example, the individual's body surface area might be needed in the residential exposure module. If that characteristic were needed in any other calculation module, then that characteristic would be added to VIC at runtime as part of the VIC Augmentation.

3.3 Time Series in VIC

Some of the characteristics in the individual's VIC are a time series of values. This time series includes a value for each time interval in a year. The time interval may be as small as needed (a day or an hour is probably the smallest time interval for which good data currently exist). The time intervals collectively cover a calendar year. The extrapolation of database information to cover the time intervals in a year incorporates the ideas of several members of the Technical Committee. For example, Novigen Sciences, Inc., contributed to the development of methods to extrapolate CSFII consumption data from an observed 1 or 2 days for one individual to 365 days. Also, Infoscientific, Inc., developed algorithms for the stochastic allocation of pesticide use events over a year.

The time intervals for different characteristics may be different. For example, if the appropriate data were available, food consumption might be evaluated on an hourly basis whereas residential exposure might be evaluated on a daily basis.

An important responsibility of the Population Generator is that all time series (including both those used in the dietary (food and water) modules and those used in the non-dietary modules) are generated in a mutually consistent fashion. This implies that all of the forecasting and backcasting to fill out the VIC for a year are done in a consistent manner.

3.4 Interdependence Among an Individual's Characteristics

By identifying an individual's vector of individual characteristics (VIC) from databases, the interdependence ("correlation") between many of these characteristics is captured directly. That is, the data in the databases reflect the observed interdependence between multiple characteristics directly, and this observed interdependence is incorporated into the CARES analysis. For example, the data in CSFII reflect the interdependence between the consumption of different types of food. CSFII indicates everything that an individual ate on a day; thus, the CSFII data captures the interdependence between different types of food consumption (e.g., beef and potatoes) without having to infer that interdependence from separate data on each type of food consumption and estimates or assumptions about how these consumptions co-occur.

3.5 Composition of Vector of Individual Characteristics

A general representation of the composition of a VIC for an individual constructed from the Census and any number of additional databases (or surveys) is as follows:

Census

- Census individual identification code
- Number of people in the U.S. population represented by the individual
- A list of values for relevant Census characteristics such as age, gender, race, location, etc.

Database/Survey 1

- Database 1 matched individual identification code
- A list of values for this individual's relevant characteristics (not present in Census)

Database/Survey 2

- Database 2 matched individual identification code
- A list of values for this individual's relevant characteristics (not present in Census or Database 1)

etc.

The values for relevant characteristics allocated from each of the non-Census databases can have a complex structure. For example if the database were the CSFII/FCID, the structure might be

CSFII/FCID

- CSFII/FCID matched individual identification code (a combination of household and sample person codes)
- A list of values for the CSFII/FCID individual's non-time series characteristics (i.e. those that do not change appreciably over a year such as body weight for adults.)
- A complete 365-day food consumption profile constructed for this individual by using consumption information from similar persons. That is,
    - January 1, CSFII Person ID and consumption day used
    - January 2, CSFII Person ID and consumption day used
    - • • •
    - December 31, CSFII Person ID and consumption day used

In the above example, the surrogate CSFII person ID and consumption day values are pointers to an extensive set of food consumption values obtained for that person on that particular day.

This structure is, of course, merely conceptual. When implemented, CARES will use an efficient method of storage and retrieval of the VIC information.

4. Matching a Census Individual to a Person in Another Database

4.1 Objective of Matching

The Census does not contain all of the information needed to complete an individual's vector of individual characteristics (VIC). In order to fill in the VIC for a Reference Population (RP) individual, the information from the Census is pooled with the information from other databases. The portions of the VIC that are in the Census are set equal to those Census values. The portions of the VIC that are not in the Census are filled in with the values for a person in another database who is matched to the RP individual. This raises the issue of "matching" an individual from the Census with an individual in another database.

The information available from the Bureau of the Census intentionally does not allow the user to identify the specific person corresponding to a sample individual. Nor does it provide any detailed geographic information that might allow one to infer a person's identity. Thus, the sample individual's name, complete address, Social Security number, etc. are not identifiable. Even if these identifiers were present they would be of little use. It is unlikely that any two samples from the large U.S. population would contain the same individuals. In addition, for surveys taken at different times, even the same individuals would be at different ages and perhaps at different locations. (In fact, infants and younger children may not even have been born at the time an earlier survey was taken.) Hence, it is impossible to match an individual in the Census with the exact same individual in another database.

It is possible, however, to identify persons in another database that closely match the characteristics of the individual in the RP. For example, it is often possible to find a person (or several people) in a database that has at least some characteristics (e.g., age, gender, race, and region) that are the same as the RP individual.

Of course, the matching between a Census individual and an individual in another database can only be directly based on the characteristics that are in common between the databases. For example, if a person in the Census is matched to a person in CSFII, then the characteristics in common between the two databases include age, gender, race, Region, etc. Here, Census Region is considered to be a characteristic in common even though Region only appears explicitly in CSFII. Sufficient information is available in the Census (namely, the PUMA or, more grossly, the State or Division) to allow a Census individual's Region to be determined. Thus, "characteristics in common" include those that are comparable and those that can be constructed to be comparable. On the other hand, a person's body weight is a characteristic available in the CSFII but not in the Census. Because there is not a way to infer body weight from Census information, body weight is an example of a characteristic that is not in common for these two databases. Appendix B describes the common characteristics used for matching.

4.2 Approach to Matching

When it is not possible to exactly match all of the Census-derived characteristics of a Reference Population individual with those of an individual in another database, a procedure is needed to determine which person is the closest match to the RP individu al.

First, some restrictions to matching were established. Because certain activities of importance in at least some FQPA assessments are unique to females such as pregnancy, surrogate individuals are not allowed to cross gender boundaries. That is, RP females are only matched with females in other databases, and RP males are always matched to males in other

databases. This restriction avoids the complexity of adjusting or inferring purely male or purely female characteristics (e.g. pregnancy, lactation status) if one gender could replace another.

An age restriction to matching was also imposed. For children and adolescents less than 20 years of age, there is a clear relationship between body weight (or height) and age. Since an RP individual inherits his weight and height from the matched CSFII person, mismatching of ages could distort the distribution of these physical characteristics with age. To prevent this potential distortion, RP individual less than 20 years of age were only allowed to match with persons of the same age.

In the CSFII no females less than 15 years old or greater than 45 years old were pregnant or lactating. To maintain this feature in the RP, no female RP individual aged outside the range 15-45 years could match with a pregnant or lactating female in the CSFII.

Apart from the restrictions described above, the general strategy with respect to characteristics other than gender is to match individuals that have similar (if not identical) characteristics. More specifically, the strategy is to determine for each RP individual a measure of how similar each person in the other database is to the RP individual, and then, using the Census-derived characteristics, match the RP individual to a person in the other database on the basis of this similarity measure.

The similarity measure considers relevant characteristics that are in common between the two databases. The similarity measure is a single number obtained by pooling the relative similarity evaluated for each characteristic. For each RP individual, a similarity measure is calculated for each person in the other database.

The similarity measure reflects the objective of the matching. For example, if a Census individual is being matched to a person in CSFII primarily for the purpose of obtaining food consumption information, then the similarity measure reflects the importance of matching characteristics with respect to food consumption. That is, any differences in a characteristic between a Census individual and a person in CSFII are evaluated in terms of the importance of that characteristic with respect to food consumption. For example, Region might be relatively unimportant for food consumption but be more important for residential exposures; so that, the value of the similarity measure might de-emphasize region when matching a Census individual to a person in CSFII but emphasize region when matching a Census individual to a person in a database pertaining to residential exposures. Different values of the similarity measure are obtained when matching different databases for different purposes.

4.3 Matching a Census-derived Reference Population Individual to a Person in CSFII

The similarity measure is illustrated in this section for the case of matching a Census individual to a person in CSFII primarily for the purpose of obtaining information on food consumption. The same general approach can be used for matching Census individuals to a person in another database.

For each Reference Population individual, the value of the similarity measure is computed for each person in CSFII (actually, but equivalently, each person in FCID) that is not restricted. The value of the similarity measure should reflect the impact on food consumption of any differences between the level of a Census-derived characteristic for the RP individual and the level of that same characteristic for the CSFII person. In other words, individual differences in a characteristic should be less important when they have no impact on food consumption. Thus, it seems reasonable that characteristics that are more strongly associated with food consumption differences should ‘count more’ in any measure of similarity. The procedure described here uses the average overall difference in food consumption between subpopulations as a means for calibrating a similarity measure.

The food consumption data used for this process are from the Food Commodity Intake Database (FCID). The USDA and the Environmental Protection Agency's Office of Pesticide Programs have transformed these data from those in the CSFII. Roughly speaking, the FCID expresses the consumption of foods as eaten back into their component agricultural commodities (in mg/kg-day). In the FCID, there are 548 different food commodities represented. Of these, only 465 have any non-zero consumption and could be used. In addition, the large water component of milk ("Milk, water") was excluded because it dominated all other food commodities in the distance measurement. (Drinking water would present the same problem, but it was not one of the 465 commodities.) Thus, there were a total of 464 FCID commodities actually used in this analysis.

These FCID consumption data were then used to determine the impact of each potential matching characteristic. For example, how important is it that Region of the CSFII person matches the Region of the Census individual? (The Census Regions are Northeast, Midwest, South, and West, abbreviated NE, MW, S, and W, respectively.) For each of these four Regions, the average daily consumption of each of the 464 commodities is computed from the food consumption values and the appropriate survey weights in FCID. The result can be represented as follows:

Commodity	**Average Daily Commodity Consumption by Region**			
	NE	**MW**	**S**	**W**
1	Avg. NE(1)	Avg. MW(1)	Avg. S(1)	Avg. W(1)
2	Avg. NE(2)	Avg. MW(2)	Avg. S(2)	Avg. W(2)
3	Avg. NE(3)	Avg. MW(3)	Avg. S(3)	Avg. W(3)
...	...	...	...	...
464	Avg. NE(464)	Avg. MW(464)	Avg. S(464)	Avg. W(464)

A distance (or dissimilarity) measure between regions with respect to their average food consumption can be computed from these region specific average commodity consumption values. The measure used here is the simple Euclidean distance (e.g., Cox and Cox, 1994). For example, the distance between the NE region and the S region with respect to food consumption is:

$$\text{Distance}_{\text{Region}}(\text{NE},\text{S}) = \{ \sum_{r=1}^{464} [\text{Avg. NE}(r) - \text{Avg. S}(r)]^2 \}^{1/2} .$$

The distance provides a quantitative measure based on the object of the matching (here, food consumption) of the similarity between two levels of a characteristic (two levels of region in the above example). As the distance increases, the similarity decreases. Thus, distance and dissimilarity are equivalent terms.

For categorical characteristics such as Region, employment status, etc., distance was calculated as shown above. For quantitative variables such as income, household size, etc., a further refinement was used to insure consistency between adjacent levels. In this second step, the Euclidean distances computed between all pairs of levels (e.g., between each pair of ages) were used to generate a transformed value T_{Age} for each level. This was done using multidimensional scaling or 'MDS' (Cox and Cox, 1994). In the case of age, one-dimensional MDS simply finds for every value of age, the numbers T_0, T_1, …, T_{90}, that can be used to approximate distance. For example, for ages 2 and 24:

$$\text{Distance}_{Age}(2, 24) \approx | T_2 - T_{24} |$$

Then a smooth function Q(A) was fit to these MDS values so that it could be used to compute distance. For example:

$$\text{Distance}_{Age}(2, 24) \approx | Q(2) - Q(24) |$$

The values of distances and functions Q used are given in Appendix C.

The Euclidean distance provides a separate measure of dissimilarity for each matching characteristic. It is then necessary to combine these distances to reflect the similarity between individuals with a set of characteristics. This combined distance will be used to match an RP individual to a person in CSFII. We use Gower's Dissimilarity Index (Gower, 1971; Cox and Cox, 1994) as a simple measure for combining the individual characteristic distances. For the most part, Gower's Dissimilarity is simply an average distance. As Gower's Dissimilarity increases, the similarity decreases. If the j-th person in CSFII is being considered as a match to the i-th RP individual, then Gower's Dissimilarity is:

$$G_{IJ} = \frac{\text{Distance between i and j with respect to characteristic K summed over all comparable characteristics K}}{\text{Number of comparable characteristics}}$$

Any two values of a characteristic are comparable if neither one is missing and both have meaning. For example, it would not be meaningful to compare two individual's occupations if one or both of them were infants. Mathematically, this is expressed as:

$$G_{IJ} = \frac{\sum_K \text{Distance}_K [\, \text{Level}(K,i), \text{Level}(K,j) \,] \times \delta_K [\, \text{Level}(K,i), \text{Level}(K,j) \,]}{\sum_K \delta_K [\, \text{Level}(K,i), \text{Level}(K,j) \,]}$$

where

$\delta_K [\, \text{Level}(K,i), \text{Level}(K,j) \,] = 1$, if Level(K,i) and Level(K,j) are comparable

$\delta_K [\, \text{Level}(K,i), \text{Level}(K,j) \,] = 0$, if Level(K,i) and Level(K,j) are not comparable (e.g., one missing).

Thus, Gower's Dissimilarity measure is the average distance over characteristics that have comparable levels and is a measure of the similarity with respect to food consumption between i-th Census individual and the j-th person in CSFII. As Gower's Dissimilarity Measure increases, the similarity decreases.

For each Census-derived RP individual, the value of Gower's Dissimilarity is computed for each person in CSFII that is in the matching neighborhood (i.e., not restricted from matching) of the RP individual. The M persons in CSFII with the greatest similarity (the smallest values of G_{IJ}) are identified. Then one of these M persons is randomly selected (with probability proportional to the CSFII/FCID survey weight) to be the match with the RP individual. Choosing M=1 would be appropriate if the similarity measure were perfect in the sense that it captured all relevant information about the similarity of two people. On the other hand, choosing M>1 is appropriate if the similarity measure is reasonably accurate in the sense that the similarity measure captured most (but not necessarily all) relevant information about the similarity of two people. The use of M>1 increases the average Gower dissimilarity of matches but increases the expected number of CSFII individuals that could be used in the matching process. This puts more randomness in the process at the expense of similarity. In the extreme, a value of M=21,662 would result in the random match of any CSFII individual to any RP individual without regard to similarity. Clearly, M must remain a small fraction of the total number of CSFII individuals. In this case, a value of M=20 was chosen to allow for some possible imperfection in the similarity measure and to increase the probability that every individual in CSFII can be matched to at least one Census individual. M=20 implies that the Census individual is matched to one of the 20 most similar individuals in CSFII (from among the 21,662 individuals in CSFII). Twenty is less than 0.1% of the total number of people in CSFII.

5. Creating 365-Day Profiles for Individuals in the Reference Population

As described above, each individual in the Reference Population (RP) is sampled from the Census. Following this, each sampled Census individual is matched to a person in the CSFII. The matched CSFII person fills in some parts of the VIC for the RP individual. In particular, the matched CSFII surrogate individual provides any supplemental information that is both (1) day-independent and (2) does not conflict with any Census-supplied characteristics. An example might be the (chronic) health status of an individual. In addition, the surrogate CSFII individual provides day-specific characteristics that are used in the construction of 365-day profiles. Specifically, the matched CSFII person provides body weight, height, and pregnancy status on a single day. In addition, the matched CSFII person provides one or two days of food consumption on specific dates.

The first element in every 365-day profile represents the value of a characteristic on the RP individual's last birthday. By 'last' birthday, we mean the birthday on which he/she attained the Census-provided age. Each successive element in the profile provides the value for the next day at that age. The 365^{th} element will be the value at the day prior to the next birthday. The day-specific characteristics from the CSFII were surveyed on known dates over a 5-year period. For reference purposes, all data were aligned to the Census year 1990. As described in the next section, this alignment process provides consistency. This alignment converts day-specific surveyed characteristics to an equivalent day in 1990. Everyone RP individual will have surveyed 'events' in 1990, but because profiles range from birthday to birthday, they may overlap into 1989 or 1991. While the particular years (1989-1991) are arbitrary, it is still true that the entire set of 100,000 RP individuals in CARES spans three consecutive calendar years. This is important when comparing or constructing time series, such as water concentrations, to c ompare with 365-day profile. In general, a 3-year time series will be needed to contain the profiles of all RP members.

5.1 Converting Sample Dates into Aligned Day-of-Year Values

As described above, each individual in the RP is sampled from the Census and then matched to a sample person in the CSFII. Each matched CSFII sample person provides consumption information for either one or two sample dates, usually, but not always, in the same calendar year. As a whole, however, the CSFII sampling dates spanned the five years 1994-1998 (including a small number in 1997). Thus, to put all the RP individuals on the same footing, all dates were converted to a day-of-year aligned on the 1990 Census year. First, each sampling date was re-expressed as the number of days in the year of the first sampling date. For example, if an individual's intake was surveyed on March 3, 1995, this would correspond to:

Day of Year 1995 = (March 3, 1995) – (January 1, 1995) + 1

= Day 62

We could also consider this to be equivalent to day 62 of the Census year 1990. In this case, day 62 of 1990 would also correspond to March 3, 1990 since neither 1990 nor 1995 are leap years. However, March 3, 1995 falls on a Friday whereas March 3, 1990 was a Saturday. We could reassign this date to March 2, 1990 (day 61), however, and preserve the day-of-week. It is not usually possible to convert the sample intake dates to 1990 while preserving both the same day-of-year and day-of-week. As a result, it was deemed preferable to adjust all day-of-year values to preserve the day-of-week. The following adjustments were made:

Original Year Of 1st Sample	Number of Days Adjustment to Days of Year to Align Days of Week
1994	-2
1995	-1
1996	0
1997	2
1998	3

Note that for 1996, there is no adjustment to day-of-year necessary. Since 1996 is a leap year, however, the calendar dates after February 28 will not match those in 1990. For example, the 129th day of the year is May 8 in 1996 and May 9 in 1990. Both of these dates fell on Wednesdays.

This alignment to 1990 will result in some surveyed event 'dates' falling outside the range of 1 to 365 days. For example, the second date of intake might be recorded in the following year. Re-expression of this date to a day-of-year in 1990 will give a value greater than 365. This should be viewed as a day in 1991. In addition, the alignment process may produce values very slightly less than 1. These should be viewed as dates in 1989.

5.2 Creating Birthdays for Each Individual in the Reference Population

Of primary importance to the creation of 365-day profiles is the generation of a birthday for each RP individual. The birthday is critical since it determines the starting and ending day -of-year for each individual's profile. This birthday must be randomly generated as part of the population generation procedure. The Census provides no information and, hence, no restriction on the birthday. The CSFII does, however, give an age in months for children less than one year of age. Thus, any birthday generated for an infant must be consistent with this value. The CSFII induces another, much subtler, restriction on birthday generation. The CSFII sample person provided consumption information for either one or two days. For the most part, sampling dates

were 3-10 days apart although the separation between survey dates could be as great as 130 days. We have made the necessary assumption that all RP individuals are at their stated age for both sample food intake dates. For RP individuals of one year and older this means that the last birthday must be between

[(Sample Date 2) – 364 days] and (Sample Date 1)

(Note: there were a few CSFII individuals for whom the 'second' sample date was actually earlier than the 'first' date. It was assumed that both dates were correct, but in reverse order. In such cases, the role of date 1 and date 2 above are merely reversed.) When the RP individual has only a single date of intake, then the birthday must be between

[(Sample Date 1) – 364 days] and (Sample Date 1)

These limits merely require that the person's last birthday be on or before the first survey date, but less than a year before the second date, if present. The birthdays for these RP individuals were generated randomly and uniformly between the ranges given above. The birthdays are expressed in days-of-year 1990 and are quite often negative since they occur in 1989.

For RP children less than one year of age, an age-in-months value (A_m) was available from the CSFII and refers to the age at the first sampling date. In these cases, it was necessary to generate birthdays consistent with this characteristic. The concept of an age-in-months presents a messy bookkeeping problem since calendar months have an unequal number of days. For the purpose of this calculation, therefore, a month will be treated as meaning 30 days. When there is only a single sampling date, this implies that the date of last birthday must be between D_{min} and D_{max} where:

$$D_{min} = \text{(Sample Date 1)} + 1 - 30(A_m + 1) \text{ days}$$

$$D_{max} = D_{min} + 29 \text{ days.}$$

For example, if a person is 2 months old at the first sampling date this his birthday could be anywhere from (sampling date – 89 days) to (sampling date – 60 days).

When there are two sampling dates, there is a potential for a logical 'inconsistency' to develop. For example, suppose a person is 11 months old at sample date 1 and there are 90 days until the second day of intake. In this case it would be impossible for a person to be less than one year of age at both sampling dates. In general this situation occurs whenever

$$D_{max} < \text{(Sample Date 2)} - 364 \text{ days}$$

Because we are requiring an individual to remain at the same age (in years) throughout the 365-day profile, the second inconsistent date of consumption is ignored. (It is only excluded, however, for the primary matched CSFII individual. When constructing the 365-day consumption profiles below, this day of consumption is treated as a valid observation for a 1-year old individual.) Whenever

$$D_{max} \geq \text{(Sample Date 2)} - 364 \text{ days}$$

it is then possible to generate a birthday that is consistent with the age-in-months and keeps the individual under one year old for the second sampling date. This is accomplished by redefining D_{min} as (Sample Date 2) – 364. All birthdays for these infants in the RP were generated randomly and uniformly from the limits above. Once the birth dates were generated, the day of the week on which it falls was also determined and saved as part of the VIC. The day-of-week is coded as successive integers from 1 to 7 representing Sunday through Saturday, respectively.

5.3 Converting Sample Dates into Profile Days-at-Age

As described above, the 365-day profile for each RP individual starts at the 'last' birthday—the date on which the individual reaches the nominal RP age. Thus the last birthday is the individual's first day-in-age. The last (or 365th) element of the profile will represent the day before the next birthday. This is day-in-age 365. The one or two food intake survey dates are re-expressed in terms of day-in-age by the relation

Survey Date As Days-in-Age	=	Survey Date as Day-of-Year 1990	–	Birthday as Day-of-Year 1990	+	1

By design, both valid sample intake dates will occur somewhere from day-in-age 1 to day-in-age 365. Because each day-in-age profile starts on the RP individual's birth date, the calendar date of a particular day-in-age will not be directly comparable from individual to individual.

5.4 Creating Gestational Age Profiles for Pregnant Females

Some females in the RP are matched to primary CSFII individuals who are pregnant. For these individuals a 'beginning' date of pregnancy was generated so that a profile of gestational ages and associated weight gains could be generated. CSFII individuals recorded their pregnancy status and, if appropriate, a 'number of months pregnant' (G_m) on the household interview. In most cases, this is approximately the same time as the first sample date. Thus, it was necessary to generate a beginning date of pregnancy consistent with this information. That is, whatever the pregnancy start date, the person should be the correct months pregnant at the first sample intake date.

For simplicity in this implementation of the population generator it is assumed that the period of gestation is a constant 280 days (from date of last menstrual period). As was the case with age-in-months, we assume that gestational age-in-months ('months pregnant') is measured in equal day months of length $365/12 \approx 30$ days. Under this assumption the gestational age in days at sample date 1, G_1, can range anywhere from G_{min} to G_{max}, where:

$$G_{min} = \text{Max}\{1, \text{Round}[P_m (365/12)]\}$$

$$G_{max} = \text{Min}\{280, \text{Round}[(P_m+1)(365/12)] - 1\}$$

The notation Round(x) means rounding x to the nearest integer. For example a woman who claims to be six months pregnant (G_m=6) is assumed to have a gestational age in days between G_{min}=183 days and G_{max}=212 days. The 'number of months pregnant' response was missing for a small number of pregnant females. In this case a value of 280 days was used for G_{max} and G_{min} was set equal to 30 days. (This '1 month' minimum gestational age was used in missing value imputation instead of G_{min}=1. It reflects the belief that women are less likely to claim pregnancy in the survey when they less than a month pregnant.) A random value of G_1 was generated for each pregnant individual using these limits above. The start-day of the pregnancy D_p expressed as days-in-age is then given by:

$$D_p = D_1 - G_1 + 1$$

The last day of pregnancy under the assumption of a 280 days gestation period is D_p + 279 days-in-age. For any days-in-age value, D, the gestational age in days is given by:

$$G = D - D_p + 1$$

If G>280, then pregnancy has terminated.

5.5 Creating a Profile of Pregnancy Weight Gains

Pregnant females will experience an increase in weight as their pregnancy progresses. In this version of the population generation methodology, pregnancy weight gain will be modeled as a deterministic function of gestational age. Thus, females at same gestational age are assigned the same pregnancy weight. The profile of basal body weights created for each individual will represent the amounts that must be added to the 'basal' body weight profile (see below).

Pregnancy weight gain was modeled to be consistent with the guidelines for 'desirable weight gain' for single births published by the Texas Department of Health (Garriott and Morat, 2000). These guidelines recommend a gain of 3.5 lbs during the first trimester and an additional pound per week thereafter. A simple cubic exponential model was fit to these 'data' giving the following computationally convenient formula for weight gain after G days of gestation

$$PWG(G) = S\,[1 - EXP(-B_1G - B_2G^2 - B_3G^3)]$$

Here:
- $PWG(G)$ = the cumulative weight gain in kilograms at G days
- S = 16.36046
- B_1 = 3.804×10^{-9}
- B_2 = 6.9455×10^{-6}
- B_3 = 6.0085×10^{-8}

At G=280 days, this model gives a total weight gain of about 13.8 kg (or 30.5 lbs).

5.6 Imputing Data for Missing Height Measurements

The CSFII database provided both height and body weight data, corresponding to the first date of intake surveyed, for all individuals. Each member of the RP matched to a CSFII individual inherits his/her height (inches) and weight (lbs). This information was ultimately used to generate height and weight profiles (see next section). However, for some CSFII individuals and, hence, for some RP individuals, the weight and/or height was missing. In EPA's FCID database, the body weights have been converted to kilograms and all missing values replaced with imputed body weights. The EPA imputed body weight using means of selected age and gender categories obtained primarily from National Center for Health Statistics 1976-80 anthropometric reference data (NCHS, 1987). To achieve a complete set of physical data it was necessary to impute missing values of height as well. To the extent possible, the imputation of height used the same methodology and data sources used by the EPA for body weight. Table 5 below gives the height values used when the sample person's height was missing.

Table 5. Height (cm) substituted for missing heights in CSFII.

Age in Years	Height (cm) Males	Height (cm) Females	Source
Infants < 6 months	61.1	61.1	*1*
Infants 6-1 months	72.3	70.4	*2*
1	82.4	80.9	*3*
2	91.2	89.7	*4*
3	99.2	97.5	*4*
4	106.0	104.6	*4*
5	112.6	111.6	*4*
6	119.5	118.4	*4*
7	125.1	123.7	*4*
8	129.9	130.2	*4*
9	135.5	134.4	*4*
10	141.6	141.9	*4*
11	146.0	147.0	*4*
12	152.6	154.4	*4*
13	158.9	158.9	*4*
14	167.5	160.8	*4*
15	170.8	163.2	*4*
16	173.8	162.9	*4*
17	175.1	163.5	*4*
18 or greater	175.5	161.8	*5*

Data Sources

1 Mean height for males aged 3 months. NCHS (2001).
2 Mean height for males or females at 9 months. NCHS (2001).
3 Mean height for males or females aged 18 months. NCHS (2001).
4 Age and gender specific means. Table 15, NCHS (1987)
5 Gender-specific means for individuals aged 18-74 years. Tables 16 and 17, NCHS (1987).

5.7 Creating Weight and Height Profiles

After conversion of units and any imputation of missing values, each individual in the RP had a value for both body weight (kg) and height (cm) at the date of first intake sampling. For pregnant women, these body weights were first reduced by any computed pregnancy weight gains that had occurred by this date. For individuals aged 20 years of age or greater, the height and weight values at the date of first sampling were assumed to hold for all 365 days-in-age. For persons less than 20 years old, however, the assumption of no change during a year is not viable. A more complex procedure was used in this case.

The National Center for Health Statistics (NCHS) at the Centers for Disease Control and Prevention (CDC) publishes detailed growth charts and data for persons less than 20 years of age (NCHS, 2000). The NCHS provides Box-Cox transformation parameters (Box and Cox, 1964, Piegorsch and Bailer, 1997) that transform the distributions of heights and weights into those that are approximately normally distributed. This allows the conversion of weights (or heights) into percentiles, and vice versa, for any age-in-months. Given W_m, the body weight at age m months, the quantity:

$$Zm = [(Wm / Mm)L - 1] / (Lm \cdot Sm)$$

may be considered an approximate random variable from a standard normal distribution. The three Box-Cox transformation parameters are the median (M), the standard deviation (S), and the power (L). The number Zm could, if desired, then be converted to an actual percentile of the normal distribution. For example Zm=1.96 would be equivalent to the 97.5th percentile. To generate a weight for another age-in-months, k, in the same year, it is only necessary to invert the transformation above using parameters for individuals at the same sex and at age -in-months k. That is:

$$Wk = Mk (1 + Lk \cdot Sk \cdot Zm)1/Lk$$

This method of filling in monthly weights (as well as height) values assumes that a person remains at the same height and weight percentile for an entire year. While probably not true in every single case, it seems a reasonable approximation.

This constant percentile method of filling in monthly weights and heights could not be used for all RP individuals. The NCHS/CDC transformation parameters will not necessarily provide a good approximation to a normal distribution for extreme heights and weights. When the computed weight or height percentiles are between the 1st and 99th percentiles (i.e., a value of Zm within ±2.3263) then the method above was considered reliable and used to generate monthly data. For more extreme values of Zm, however, an alternative method was used. In this case the weight at age k months would be calculated as:

$$Wk = Wm \cdot (WP,k / WP,m)$$

In the above, WP,m is the P-th quantile of weight at age m months and WP,k is the P -th quantile of weight at k months of age. If Wm is smaller than the 1st percentile of weight then P=1%. If Wm exceeds the 99th percentile of weight then P=99%. This method keeps the weight for all months at the same distance relative to the 1st or 99th percentile—whichever is closer. The same method is used for generating monthly heights when percentiles are extreme.

For any individual, the height and the (basal) weight will remain constant throughout any month. For pregnant women, however, the actual body weight will be increased by the pregnancy weight gain. Since this is a function of gestational age in days, body weight might change for some days within the same month.

5.8 Creating Food Consumption Profiles

As described above, each RP individual has one or two days of food consumption inherited from the matching CSFII person. Following the alignment and birthday generation processes, these consumption dates were then converted into the corresponding days -in-age. This fills at least one, and usually two, elements of the 365-day profile of food consumption for the RP individual. The next task is to fill in the remaining days.

It is not reasonable to assume that the one or two days of inherited food consumption would be repeated over and over again to fill in all 365 days of food consumption. Actual consumption is expected to be more variable over time, especially between seasons, than this approach would reflect. Instead of unreasonably assuming that an individual eats the same things every day of the year or every other day, surrogate person-days of consumption are used to fill in the consumption time series. The pool of surrogates available for this second matching process is the complete set of 42,269 person-days (based on 21,662 persons surveyed) in the CSFII/FCID.

Conceptually the process is straightforward. For each RP individual, the algorithm considers one day-in-age of the profile at a time. It finds the 3-5 person-days in the surrogate pool that are most similar to the RP person and profile day being filled. One of the 3-5 candidate person-days is randomly selected and added to the profile. If there is another person-day for the surrogate person selected, then an attempt is made to add it to the profile as well. All consumption data associated with a surrogate CSFII/FCID person-day is attached to the RP individual's day-in-age.

More specifically, for each RP individual the food consumption imputation algorithm repeats the following steps until the profile of 365 days-in-age is completely filled with CSFII person-days.

1. Pick the next day-in-age, D, *in random order*. If D is already assigned a CSFII person-day and there are unfilled days-in-age remaining, then pick a new day-in-age, D.

2. Construct all matching characteristics that will be used to compare this RP individual and day-in-age with person-days in the CSFII surrogate pool.

3. Identify the matching neighborhood. This is the subset of person-days in the CSFII database that are valid potential matches for this RP individual on this particular day, D. The neighborhood is constructed to have at least 3 person-days.

4. For every potential person-day in the matching neighborhood, compute a Gower dissimilarity value with the RP person on day D. Retain at least 3 but no more than 5 CSFII person-days having the smallest Gower dissimilarities.

5. Randomly select one out of the 3-5 CSFII person-days and assign this CSFII person-day to the consumption profile for day-in-age, D.

6. If there is no second person-day anywhere in the CSFII database corresponding to the same person just selected then continue with the next unfilled value of D at s tep 1.

7. Identify the set of unfilled days-in-age into which the second person-day could 'fit'. If there are no unfilled days-in-age then continue with next unfilled value of D in step 1.

8. If there are potential openings for the second person-day, find the days-in-age that agree closest with the day-of-week for the second CSFII person-day. Randomly select day-in-age D* from among these and assign the second CSFII person-day to it.

The following sections discuss details regarding the implementation of this algorithm.

5.8.1 Finding the Next Day-in-Age to Process

Each day-in-age could be processed in order sequentially from D=1 to D=365. This might, however, result in some systematic bias in the assignment of person-days to the profile. Instead the 365 days-in-age are processed from a list of 365 integers sorted in random order. A different random order is generated for each new RP individual. If any day-in-age, D, has already been assigned a surrogate CSFII person-day (from step 8 below) then this D is skipped.

5.8.2 Constructing Matching Characteristics

The same general procedure for determining the similarity between Census and CSFII persons (i.e., Gower's dissimilarity) is also used here. The major difference, however, is that we compare not persons but RP person-days with CSFII person-days. In other words both person-

specific and day-specific characteristics must be considered. While the relevant day-specific characteristics already exist in the CSFII/FCID data, they need to be constructed for each RP individual.

The person- and day-specific characteristics used are described in Appendix B2. The person-specific set includes most of those characteristics used in matching the PUMS to CSFII plus additional health and diet-related characteristics that each RP individual inherited from the primary matched CSFII person. There are three day-dependent characteristics used in comparing person-days. These are the day-of-week (Sunday, Monday, etc.), pregnancy status for women, and the age in months for infants less than a year old.

5.8.3 Identification of the Matching Neighborhood

The matching neighborhood for a particular RP individual and day-in-age, D, is the subset of person-days in the CSFII database that are valid potential matches. Clearly, there are some person-days in the surrogate pool that would not be appropriate for a particular RP person-day. As was the case with the PUMS-to-CSFII matching, matching is restricted to persons of the same gender. Also RP and surrogate person-days must have the same age if age is less than 20 years. For infants less than one year old, the neighborhood is also restricted to those with the same breastfeeding status. Thus, infants who are nursing could only be matched with other nursing infants. (Note: although breastfeeding status was not used to restrict the neighborhood for older children, this characteristic was used in computing similarity.)

The matching neighborhood of person-days was also restricted to those 'close to' the RP person-day with respect to day-of-year. For the vast majority of RP person-days the valid neighborhood includes only CSFII person-days that are within ±7 days of D. However, the neighborhood was required to have at least 3 potential person-days. Whenever the ±7 day restriction resulted in fewer than 3 candidate person-days, the restriction was relaxed to ±15 days. If this was insufficient, a wider window of ±30 days was used. A window larger than ±30 days was never required.

5.8.4 Choosing the Surrogate Person-day

The Gower dissimilarity index was calculated between the RP person-day and every other CSFII/FCID person-day in the matching neighborhood described in the previous section. Although the characteristics used are somewhat different (see Appendix B2), the formula for the index itself is identical with that used when matching PUMS and CSFII individuals. Also, the method used to obtain numerical distances between any two characteristic values is the same. That is, we used a Euclidean distance between any two levels (of the same characteristic) based on the mean consumption for each the 464 EPA commodities. The distances used are documented in Appendix C2.

When the neighborhood size exceeded 5, then the Gower dissimilarity measure was used to exclude all but the 5 CSFII/FCID person-days in the matching neighbor that are most similar the RP person-day. Each neighborhood contains only 3-5 of the most similar person-days. Finally, only one of these remaining 3-5 person-days is randomly selected as the surrogate.

5.8.5 Using a Surrogate Individual's other Person-day

Most of the individuals surveyed in CSFII provided two non-consecutive days of food intake. Thus, most of the person-days in the surrogate pool are associated with one other person-day. It is desirable to incorporate both members of a person-day pair to some degree. The use of the selected person's second day wherever possible, minimizes the number of different people

contributing to the Census individual's 365-day food consumption profile and maximizes the incorporation of the natural dependence among food consumption days as evidenced in the data.

This is accomplished by first identifying the second person-day coupled to the surrogate just selected in the preceding section. The day-of-year of this second person-day is then converted to days-in-age, D_2, consistent with the profile of the RP individual. A range of potential days-in-age is then defined as $D_2 \pm 7$ days. If all of the potential days-in-age in this range have been assigned surrogates, then this second person-day is not used.

If there are available days-in-age, however, a preferred day-in-age, D*, within that range is found. Here, preferred means with respect to the day-of-week. For each possible day-of-week, a preferred order of matching days-of-week was established. The highest preferred day-of-week was always the same day-of-week. The remaining six days-of-week are 'preferred' in order of increasing Euclidean distances (see Appendix C2). If there is more than one day-in-age with the same preference, only one of these is selected at random as D*. This second person-day is then assigned as the surrogate in the profile for the RP individual on day-in-age D*.

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Development of the Stratified Sampling Plan for the Reference Population

A.1 Initial Trial Sample Sizes

A stratified random sample from the 5% PUMS was used to select the 100,000 real people in the Reference Population. This appendix documents the procedure used to develop the specific stratified sampling plan.

There were 9 age/gender levels, 6 race/ethnicity levels, and 9 Census Division levels. This yields a total of 486 individual PUMS strata. Let NPUMS denote the 12,240,321 people in the 5% PUMS that are not in Group Quarters. (All persons not living in households are classified by the Census Bureau as living in group quarters.) Let NPUMS(i,j,k) denote the number of people in the 5% PUMS who are at the i-th age/gender level (i=1,...,9), j-th race/ethnicity level (j=1,...,6), and k-th Division level (k=1,...,9). The totals by age/gender and race/ethnicity as well as the marginal totals in the 5% PUMS are as shown in Table A.1.

Table A.1 Number of People in the 5% PUMS

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native Amercan	Hispanic	Other	
Infants 00-00	114,171	20,656	4,025	1,911	21,003	419	162,185
01-03	405,884	75,388	17,088	6,787	72,143	1,299	578,589
04-06	399,801	70,108	16,441	6,497	66,290	1,028	560,165
07-12	790,969	141,099	32,090	12,923	124,602	1,710	1,103,393
Males 13-19	430,746	75,446	18,471	6,882	68,786	748	601,079
Females 13-19	409,323	75,931	17,895	6,438	64,474	802	574,863
Males 20-54	2,303,054	253,305	83,714	24,224	256,450	2,035	2,922,782
Females 20-54	2,374,946	322,952	93,042	26,395	253,855	2,124	3,073,314
55+	2,296,105	201,556	43,403	12,995	108,921	971	2,663,951
Total	9,524,999	1,236,441	326,169	105,052	1,036,524	11,136	12,240,321

If each stratum were sampled with probability proportional to the number of individuals in the stratum, a sample of 100,000 people would have:

NTRIAL(1,i,j,k) = NPUMS(i,j,k) x {100,000 / NPUMS }

people at the i-th age/gender level (i=1,...,9), j-th race/ethnicity level (j=1,...,6), and k-th Division level (k=1,...,9). Each NTRIAL(1,i,j,k) value was rounded to the nearest integer. Any value of NTRIAL(1,i,j,k) less than 2 was set equal to 2; so that, each stratum sample had at least 2 people. (It is conventional practice to insure a sample size of 2 per stratum in order that variance estimates can be computed.) The totals of the NTRIAL(1,i,j,k)'s by age/gender and race/ethnicity as well as the marginal totals resulting from this proportional stratified sample are as shown in Table A.2.

Table A.2 Initial Trial Sampling Plan

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native American	Hispanic	Other	
Infants 00-00	932	168	38	23	173	18	1,352
01-03	3,316	617	140	59	590	19	4,741
04-06	3,267	572	133	56	540	18	4,586
07-12	6,464	1,152	262	105	1,018	20	9,021
Males 13-19	3,520	616	151	57	563	18	4,925
Females 13-19	3,343	620	145	55	528	18	4,709
Males 20-54	18,814	2,069	685	198	2,094	22	23,882
Females 20-54	19,403	2,638	760	216	2,074	23	25,114
55+	18,757	1,646	355	105	891	18	21,772
Total	77,816	10,098	2,669	874	8,471	174	100,102

A.2 Revising the Initial Trial Sample Sizes to Reflect Minimum Desired Frequencies

In Table A.2 the row totals for infants is 1,352 which is less than the desired value of at least 20,000 infants. The row totals for ages 1 to 3 (4,741), ages 4 to 6 (4,586), males 13 to 19 (4,925), and females 13 to 19 (4,709) are slightly less than the desired value of at least 5,000. The column totals for Asian (2,669) and especially Native American (874) are considerably less than the desired value of at least 5,000.

The following procedure was used to increase the row and column totals to their desired values.

The cells that were in both rows and columns that were too small were considered first. This is the columns for Asian and Native American and the rows for infants, 01-03, 04-06, males 13-19, and females 13-19.

For Asian infants, Table A.1 implies that the fraction of infants that are Asian in the 5% PUMS is 4,025/162,185. If there are to be at least 20,000 infants, then the number of Asian infants should be at least

(4,025/162,185) x 20,000 = 496.

Similarly, Table A.1 implies that the fraction of Asians that are infants in the 5% PUMS is 4,025/326,169. If there are to be at least 5,000 Asians, then the number of As ian infants should be at least

(4,025/326,169) x 5,000 = 62.

Thus, in order to satisfy both the requirement that there be 20,000 infants and 5,000 Asians, the number of Asian infants should be at least 496.

For Asians ages 1 to 3, the sample size should be the maximum of

(17,088/578,589) x 5,000 = 148 and (17,088/326,169) x 5,000 = 262.

For Asians ages 4 to 6, the sample size should be the maximum of

(16,441/560,165) x 5,000 = 142 and (16,441/326,169) x 5,000 = 252.

For Asian males ages 13 to 19, the sample size should be the maximum of

(18,471/601,079) x 5,000 = 154 and (18,471/326,169) x 5,000 = 283.

For Asian females ages 13 to 19, the sample size should be the maximum of

(17,895/574,863) x 5,000 = 156 and (17,895/326,169) x 5,0 00 = 274.

For Native American infants, the sample size should be the maximum of

(1,911/162,185) x 20,000 = 236 and (1,911/105,052) x 5,000 = 91.

For Native Americans ages 1 to 3, the sample size should be the maximum of

(6,787/578,589) x 5,000 = 58 and (6,787/105,052) x 5,000 = 323.

For Native Americans ages 4 to 6, the sample size should be the maximum of

(6,497/560,165) x 5,000 = 58 and (6,497/105,052) x 5,000 = 309.

For Native American males ages 13 to 19, the sample size should be the maximum of

(6,882/601,079) x 5,000 = 57 and (6,882/105,052) x 5,000 = 328.

For Native American females ages 13 to 19, the sample size should be the maximum of

(6,438/574,863) x 5,000 = 56 and (6,438/105,052) x 5,000 = 306.

Assuming these sample sizes for these 10 Asian and Native American age level strata, the sample sizes for the rest of the strata in these columns are determined so that the column totals for Asians and Native Americans are each 5,000.

For the Asians, with the sample sizes for infants, 01-03, 04-06, males 13-19, and females 13-19 fixed at 496, 262, 252, 283, and 274, respectively, the sum of the sample sizes for the rest of the strata in this column must be at least

5,000 – 496 – 262 – 252 – 283 - 274 = 3,433.

Using the relative population sizes for these strata in Table A.1, the total population size for the rest of the strata in the Asian column is

326,169 – 4,025 – 17,088 – 16,441 – 18,471 – 17, 895
= 252,249,

and the sample sizes for the rest of the strata in the Asian column must be at least

(32,090/252,249) x 3,433 = 437 for ages 07-12,
(83,714/252,249) x 3,433 = 1,139 for males 20-54,
(93,042/252,249) x 3,433 = 1,266 for females 20-54, and
(43,403/252,249) x 3,433 = 591 for ages 55+.

For the Native Americans, with the sample sizes for infants, 01-03, 04-06, males 13-19, and females 13-19 fixed at 236, 323, 309, 328, and 306, respectively, the sum of the sample sizes for the rest of the strata in this column must be at least

5,000 – 236 – 323 – 309 – 328 - 306 = 3,498.

Using the relative population sizes for these strata in Table A.1, the total population size for the rest of the strata in the Asian column is

105,052 – 1,911 – 6,787 – 6,497 – 6,882 – 6,438
= 76,537,

and the sample sizes for the rest of the strata in the Asian column must be at least

(12,923/76,537) x 3,498 = 591 for ages 07-12,
(24,224/76,537) x 3,498 = 1,107 for males 20-54,
(26,395/76,537) x 3,498 = 1,206 for females 20-54, and
(12,995/76,537) x 3,498= 594 for ages 55+.

Assuming these sample sizes for the strata in the Asian and Native American columns, the sample sizes for the rest of the strata in the rows for infants, ages 01-03, ages 04-06, males 13-19, and females 13-19 are determined so that the row total for infants is 20,000 and the row totals for the rest of the rows are each 5,000.

For the infants, with the sample sizes for Asians and Native Americans fixed at 496 and 236, respectively, the sum of the sample sizes for the rest of the strata in this row must be at least

20,000 – 496 – 236 = 19,268.

Using the relative population sizes for these strata in Table A.1, the total population size for the rest of the strata in the infants row is

162,185 – 4,025 – 1,911= 156,249,

and the sample sizes for the rest of the strata in the infants row must be at least

(114,171/156,249) x 19,268 = 14,079 for Whites,
(20,656/156,249) x 19,268 = 2,547 for Blacks,
(21,003/156,249) x 19,268 = 2,590 for Hispanics, and
(419/156,249) x 19,268 = 52 for Other.

For Ages 01-03, with the sample sizes for Asians and Native Americans fixed at 263 and 323, respectively, the sum of the sample sizes for the rest of the strata in this row must be at least

5,000 – 263 – 322 = 4,415.

Using the relative population sizes for these strata in Table A.1, the total population size for the rest of the strata in the infants row is

578,589 – 17,088 – 6,787 = 554,714,

and the sample sizes for the rest of the strata in the Ages 01-03 row must be at least

(405,884/554,714) x 4,415 = 3,230 for Whites,
(75,388/554,714) x 4,415 = 600 for Blacks,
(72,143/554,714) x 4,415 = 574 for Hispanics, and
(1,299/554,714) x 4,415 = 10 for Other.

For Ages 04-06, with the sample sizes for Asians and Native Americans fixed at 252 and 309, respectively, the sum of the sample sizes for the rest of the strata in this row must be at least

5,000 – 252 – 309 = 4,439.

Using the relative population sizes for these strata in Table A.1, the total population size for the rest of the strata in the infants row is

560,165 – 16,441 – 6,497 = 537,227,

and the sample sizes for the rest of the strata in the Ages 04-06 row must be at least

(399,801/537,227) x 4,439 = 3,303 for Whites,
(70,108/537,227) x 4,439 = 579 for Blacks,
(66,290/537,227) x 4,439 = 548 for Hispanics, and
(1,028/537,227) x 4,439 = 8 for Other.

For males 13-19, with the sample sizes for Asians and Native Americans fixed at 283 and 328, respectively, and the sample size for the row fixed at 5,000, the sample sizes for the rest of the strata in this row must be at least

5,000 – 283 – 328 = 4,389.

Using the relative population sizes for these strata in Table A.1, the total population size for the rest of the strata in the infants row is

601,079 – 18,471 – 6,882 = 575,726.

and the sample sizes for the rest of the strata in the males 13-19 row must be at least

(430,746/575,726) x 4,389 = 3,284 for Whites,
(75,446/575,726) x 4,389 = 575 for Blacks,
(68,786/575,726) x 4,389 = 524 for Hispanics, and
(748/575,726) x 4,389 = 6 for Other.

For females 13-19, with the sample sizes for Asians and Native Americans fixed at 274 and 306, respectively, and the sample size for the row fixed at 5,000, the sample sizes for the rest of the strata in this row must be at least

5,000 – 274 – 306 = 4,420.

Using the relative population sizes for these strata in Table A.1, the total population size for the rest of the strata in the infants row is

574,863 – 17,895 – 6,438 = 550,530.

and the sample sizes for the rest of the strata in the females 13-19 row must be at least

(409,323/550,530) x 4,420 = 3,286 for Whites,
(75,931/550,530) x 4,420 = 610 for Blacks,
(64,474/550,530) x 4,420 = 518 for Hispanics, and
(802/550,530) x 4,420 = 6 for Other.

The above combinations of race/ethnicity and age/gender are in rows or columns that have sample sizes that were originally below their desired minimums. The sample sizes for these combinations have been increased to ensure the desired minimums. The total sample size for these combinations is

(14,079+2,547+496+236+2590+52 = 20,000)
+ (3,230+600+262+323+574+10 = 4,999)
+ (3,303+579+252+309+548+8 = 4,999)
+ (437+591 = 1,028)
+ (3,284+575+283+328+524+6 = 5,000)
+ (3,286+610+274+306+518+6 = 5,000)
+ (1,139 +1,107 = 2,246)
+ (1,266 +1,206 = 2,472)
+ (591+594 = 1,185)
= 46,929.

In order for the total Reference Population size to be 100,000, the remaining combinations of race/ethnicity and age/gender must have a combined sample size of approximately:

100,000 – 46,929 = 53,071.

From Table A.1, the total population in the strata for these remaining combinations of race/ethnicity and age/gender is:

790,969 + 141,099 + 124,602 + 1,710
+ 2,303,054 + 253,305 + 256,450 + 2,035
+ 2,374,946 + 322,952 + 253,855 +2,124
+ 2,296,105 + 201,556 + 108,921 + 971
= 9,434,654.

Therefore, allocating the 53,071 to the remaining combinations of race/ethnicity and age/gender in proportion to their respective population sizes in Table A.1 results in the following sample sizes:

(790,969/9,434,654) x 53,071 = 4,449 for Whites ages 07-12,
(141,099/9,434,654) x 53,071 = 794 for Blacks ages 07-12,
(124,602/9,434,654) x 53,071 = 701 for Hispanics ages 07-12,
(1,710/9,434,654) x 53,071 = 10 for Other ages 07-12,
(2,303,054/9,434,654) x 53,071 = 12,955 for White males 20-54,
(253,305/9,434,654) x 53,071 = 1,425 for Black males 20-54,
(256,450/9,434,654) x 53,071 = 1,443 for Hispanic males 20-54,
(2,035/9,434,654) x 53,071 = 11 for Other males 20-54,

(2,374,946/9,434,654) x 53,071= 13,359 for White females 20-54,
(322,952/9,434,654) x 53,071 = 1,817 for Black females 20-54,
(253,855/9,434,654) x 53,071 = 1,428 for Hispanic females 20-54,
(2,124/9,434,654) x 53,071 = 12 for Other females 20-54,
(2,296,105/9,434,654) x 53,071 = 12,916 for Whites 55+,
(201,556/9,434,654) x 53,071 = 1,134 for Blacks 55+,
(108,921/9,434,654) x 53,071 = 613 for Hispanics 55+, and
(971/9,434,654) x 53,071 = 5 for Other 55+.

After revising the initial trial sample sizes to reflect the minimum desired frequencies, the strata sample sizes are as shown in Table A.3.

Table A.3 Revised Trial Sampling Plan

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native American	Hispanic	Other	
Infants 00-00	14,079	2,547	496	236	2,590	52	20,000
01-03	3,230	600	262	323	574	10	4,999
04-06	3,303	579	252	309	548	8	4,999
07-12	4,449	794	437	591	701	10	6,982
Males 13-19	3,284	575	283	328	524	6	5,000
Females 13-19	3,286	610	274	306	518	6	5,000
Males 20-54	12,955	1,425	1,139	1,107	1,443	11	18,080
Females 20-54	13,359	1,817	1,266	1,206	1,428	12	19,088
55+	12,916	1,134	591	594	613	5	15,853
Total	70,861	10,081	5,000	5,000	8,939	120	100,001

Each of the stratum sample sizes in Table A.3 is partitioned over the 9 Divisions in the Census. This partitioning is proportional to the population sizes of the 9 divisions within a stratum. Any partitioned value less than 2 was set equal to 2; so that, each partition had at least 2 people in it, and a within partition variance estimate could be computed. The totals of the partition sample sizes by age/gender and race/ethnicity as well as the marginal totals are as shown in Table A.4. The sample sizes in Table A.4 are almost identical to those in Table A.3. The slight differences are due to rounding of the partition sample sizes and the requirement that a partition sample size be at least 2.

Table A.4 Trial Sampling Plan after the Partitioning by Census Region/Division

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native American	Hispanic	Other	
Infants 00-00	14,079	2,548	496	236	2,590	54	20,003
01-03	3,229	599	263	322	573	18	5,004
04-06	3,304	580	252	308	547	18	5,009
07-12	4,448	795	437	593	701	18	6,992
Males 13-19	3,284	574	282	328	524	18	5,010
Females 13-19	3,285	608	274	306	518	18	5,009
Males 20-54	12,955	1,424	1,139	1,107	1,444	20	18,089
Females 20-54	13,359	1,817	1,266	1,206	1,428	20	19,096
55+	12,915	1,134	591	594	613	18	15,865
Total	70,858	10,079	5,000	5,000	8,938	202	100,077

The overall sample size in Table A.4 is 100,077. In order to achieve the desired sample size of 100,000 without conflicting with the desired minimum row and column totals, the sample size in the three largest cells were reduced by a total of 77(specifically, 26 subtracted from White males 20-54, 26 subtracted from White females, and 25 subtracted from Whites 55+). The final stratified sample sizes are indicated in Table A.5 (and also in Tables 2 and 3).

Table A.5. Final Stratified Sampling Plan for the Number of People in the Reference Population by Age/Gender and Race/Ethnicity

Age/ Gender	Race/Ethnicity						Total
	White	Black	Asian	Native American	Hispanic	Other	
Infants 00-00	14,079	2,548	496	236	2,590	54	20,003
01-03	3,229	599	263	322	573	18	5,004
04-06	3,304	580	252	308	547	18	5,009
07-12	4,448	795	437	593	701	18	6,992
Males 13-19	3,284	574	282	328	524	18	5,010
Females 13-19	3,285	608	274	306	518	18	5,009
Males 20-54	12,929	1,424	1,139	1,107	1,444	20	18,063
Females 20-54	13,333	1,817	1,266	1,206	1,428	20	19,070
55+	12,890	1,134	591	594	613	18	15,840
Total	70,071	10,079	5,000	5,000	8,938	202	100,000

Characteristics Used as the Basis for Matching

B.1 Characteristics Used for Matching PUMS to CSFII

The following is a description of the characteristics that were found and/or constructed to be equivalent in both PUMS (1990 Census 5% Sample) and CSFII/FCID (1994-96, 98). Many other characteristics were examined but were rejected either because they were unreliable, redundant, or had minimal association with food consumption differences. The acronym used for the characteristic, if different from the name itself, is indicated in parentheses.

Region

The U.S. Census Region in which the household is located. Region is computed from the Census Division characteristic (DIVISION) in PUMS as shown below

Region	Code Used	Division
Northeast (NE)	1	1 or 2
Midwest (MW)	2	3 or 4
South (S)	3	5, 6, or 7
West (W)	4	8 or 9

MSA Status (MSAStatus)

MSAStatus is Yes (1) if the household is in a metropolitan area otherwise it is No (2). MSAStatus is derived from the characteristic URB in CSFII/FCID and from the MSAPMSA and RFARM variables in PUMS. As do all geographic characteristics in PUMS, MSAPMSA refers to the location of the PUMA (PUMS area unit) rather than the household specifically. Thus, some PUMAs include both MSA and non-MSA households. The mixed MSA/non-MSA code in PUMS (9997) was approximately resolved by using the urban/rural dichotomy in variable RFARM.

MSAPMSA (PUMS)	RFARM (PUMS)	MSAStatus	Code
≤ 9360 or 9998	any	Yes	1
9999	any	No	2
9997	0	Yes	1
9997	1 or 2	No	2

MSAStatus	Code	URB (CSFII)
Yes	1	1 or 2
No	2	3

Household Size (HHSize)

The number of persons (related or unrelated) in the person's household. This is identical with the CSFII variable HHSize and the PUMS variable PERSONS. In the case of PUMS however, vacant houses (PERSONS=0) and persons in Group Quarters (GQTYPE>0) are excluded.

Sex

The person's gender. The 0/1 coding in PUMS was converted to the 1/2 coding used in CSFII/FCID.

Sex	Code	SEX (PUMS)	SEX (CSFII)
Male	1	0	1
Female	2	1	2

Age

The person's age in years. This characteristic was coded identically in PUMS and CSFII. Age 0 was used for ages less than 1 year and all ages greater than 90 years were top-coded as 90.

Race/Ethnicity Classification (RaceEth)

A combination of race and Hispanic origin developed from the two categorical variables RaceCat and HispCat. In CSFII RaceCat and HispCat are identical with the variables RACE and ORIGIN, respectively. In PUMS, RaceCat was derived from RACE as:

RaceCat	Code	Race (PUMS)
White	1	001
Black	2	002
Asian & Pacific Islander	3	006-036
Native American	4	004, 005, 301-327
Other	5	037

HispCat was derived from the PUMS variable HISPANIC as:

HispCat	Code	HISPANIC (PUMS)
Mexican American	1	001, 210-220
Puerto Rican	2	002, 261-270
Cuban	3	003, 271-274
Spanish & other Hispanic	4	All other
None of the above	5	000, 006-199

For both PUMS and CSFII, RaceEth was then computed as:

RaceEth	Code	RaceCat Code	HispCat Code
White (non-Hispanic)	1	1	5
Black (non-Hispanic)	2	2	5
Asian & Pac. Islander	3	3	5
Native American	4	4	5
Mexican American	5	–	1
Puerto Rican	6	–	2
Cuban	7	–	3
Spanish or other Hispanic	8	–	4
Other	9	5	5

Household Income (Income89)

Annual household income expressed in 1989 dollars. The CSFII incomes were adjusted to 1989 levels using the annual average consumer price index (CPI) from the Bureau of Labor Statistics for the appropriate income year (the year preceding the survey year) as INCOME89 = Income x CPI, where:

Survey Year	Income Year	CPI Used
1990	1989	1
1994	1993	0.85813
1995	1994	0.83671
1996	1995	0.81365
1998	1997	0.77259

All calculated indexed incomes were rounded to the nearest whole dollar and negative incomes (in PUMS) were set equal to zero. In PUMS, no indexing of household income (variable

RHHINC) was necessary since the income year was 1989. Because CSFII incomes were top-coded at $100,000, the 1998 Income89 values were restricted to values of $77,000 or less. For comparability within CSFII and to PUMS, any year's Income89 value greater than $77,000 was set equal to $77,000.

Percent of Poverty Level (PctPov)

Annual income expressed as a percent of the poverty level. Poverty level is based on the CPI adjusted income and household size. The variable PCTPOV in CSFII was used as is. The analogous variable in PUMS (POVERTY) is based on family, not household, size and is thus not comparable with PCTPOV in CSFII. Using the information in the Census documentation, however, a comparable PCTPOV was derived from the PUMS variables RHHINC and PERSONS as:

$$PCTPOV = 100 \times (RHHINC / L),$$

where L is the 1989 poverty level defined as:

PERSONS (PUMS)	1989 Poverty Level (L), $
1	6310
2	8076
3	9885
4	12,674
5	14,990
6	16,921
7	19,162
8	21,328
9 or more	25,480

PCTPOV was rounded to the nearest whole percent and top-coded at 300% to be compatible with CSFII. Negative values (corresponding to negative RHHINC) were set equal to zero.

Poverty Category (PovCat)

A categorization of PCTPOV into three levels:

1, 0 - 130%
2, 131-350%
3, 350% or greater

(Note: 350% of poverty is approximately the median value for US households.) For CSFII, the variable POVCAT was used unchanged. The value of PCTPOV in PUMS was used to assign the categories according to the definitions above. To be consistent with CSFII, POVCAT was computed before the 300% top-coding of PCTPOV was used.

POVCAT was used in addition to PCTPOV in the matching process even though they were related. Because PCTPOV is top-coded at 300% and POVCAT levels 2 and 3 break at 350%, it was felt that both were complementary.

Employment (Employ)

Employment status condensed to match a slight modification of the CSFII variable EMP_STAT.

EMPLOY	CODE	EMP_STAT (CSFII)	AGE (PUMS)	HOURS (PUMS)	RLABOR (PUMS)
Full Time	1	1 & Age≥16	≥16	≥ 35	
Part Time	2	2 & Age≥16	≥16	1-34	
Absent Last Week	3	3 & Age≥16	≥16	0	1, 2, 4, or 5
Unemployed	4	4 & Age≥16	≥16	0	3
Age<16	5	Age<16	0-15		0
Missing (CSFII only)	9	9 & Age≥16	≥16		

Education Level (Educ)

Maximum educational attainment level for those persons 15 years or older. This variable was derived from the PUMS variable YEARSCH or the CSFII variable GRADE.

Educ	Code	YEARSCH (PUMS)	GRADE (CSFII)
Age<15	0	Age<15	Age<15
Kindergarten at most	1	01, 02, 03	0
Grades 1-4	2	04	1, 2, 3, or 4
Grades 5-8	3	05	5, 6, 7, or 8
Grade 9	4	06	9
Grade 10	5	07	10
Grade 11	6	08	11
HS or GED	7	09 or 10	12
1-4 years college	8	11, 12, 13, or 14	13, 14, 15, or 16
5+ years college	9	15, 16, 17	17
Missing (CSFII only)	99		99

Tenure (HUTenure)

Ownership status of individual's housing unit derived from the PUMS and CSFII variables TENURE as follows:

HUTenure	Code	TENURE (PUMS)	TENURE (CSFII)
Own or purchasing	1	1 or 2	1
Renting	2	3	2
Occupying, not paying rent	3	4	3
Missing (CSFII only)	9		4 or more

B.2 Person-Day Matching Characteristics Available for Imputing 365-day Food Consumption Profiles

All of the variables described in the section above were also used for the imputation of 365-day food consumption profiles. Additional person-specific and day-specific characteristics, most derived from the primary CSFII person matched to the RP, were included as well. In general, a characteristic was included if there were a substantial number of persons in the survey who differed on this characteristic and it was associated with food consumption patterns. Each of these matching variables is described below with the CSFII acronym for the variable in

parentheses. Unless noted otherwise, all characteristics were obtained from the Sample Persons data file in CSFII (record type 25). Because both the RP and CSFII person-days obtained characteristics from the same source, very little adjustments, if any, were needed to make them comparable.

Food Sufficiency (FOODDESC)

This characteristic was obtained from the CSFII Household data file (Record Type 15). It is an assessment of the overall type and amounts of food eaten in the household during the past three months. This categorical variable is coded as

Food Sufficiency	CSFII Code	Code Used
Enough of kinds of food desired	1	1
Enough, but not always of kinds	2	2
Sometimes not enough to eat	3	3
Often not enough to eat	4	4
Don't Know, Missing	8 or 9	9

Health Status (HEALTH)

This characteristic is a self-reported assessment of general health. For matching purposes, it is treated as a quantitative variable. This variable is coded as

Health Status	CSFII Code	Code Used
Excellent	1	1
Very good	2	2
Good	3	3
Fair	4	4
Poor	5	5
Don't Know, Missing	8 or 9	•

Smoking Level (SMK)

This derived characteristic is a self-reported assessment reflecting the quantity of cigarettes smoked per day. It was derived from the responses to three CSFII questions:

- SMK_100 Have you smoked 100 cigarettes during your entire life?
- SMK_NOW Do you smoke cigarettes now?
- SMK_DAY On average, how many cigarettes per day do you smoke?

These questions were only asked of persons 12 years of age or older. For matching purposes, smoking level is treated as a quantitative variable with missing values (•) implying non-comparability. SMK is coded as:

Current Smoking Level	SMK_100	SMK_NOW	SMK_DAY	SMK Code Used
None or <100 in lifetime	2	–	–	0
	1 or 8	2	–	
	1 or 8	1	0	
1-20 / day	1 or 8	1	1-20	1
21-40 / day	1 or 8	1	21-40	2
Over 40 / day	1 or 8	1	41-110	3
Missing	7 or 9	–	–	•
	1 or 8	7 or 9	–	
	1 or 8	1	997, 998, 999, or blank	

Vegetarian (VEGET)

This characteristic is a self-reported claim of vegetarian status. This categorical variable is coded as

Vegetarian?	CSFII Code	Code Used
Yes	1	1
No	2	2
Don't Know, Not Ascertained	8 or 9	9

Diabetic (DOCTOR1)

The respondent was asked "Has a doctor every told you that you have diabetes?" This categorical variable is coded as

Diabetic?	CSFII Code	Code Used
Yes	1	1
No	2	2
Don't Know, Not Ascertained	8 or 9	9

Low Calorie Diet (DT01_YN)

This is a characteristic specifying whether or not the sample person is on a low calorie diet. This categorical variable is coded as

DT01_YN	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Low Fat Diet (DT02_YN)

This is a characteristic specifying whether or not the sample person is on a low fat or low cholesterol diet. This categorical variable is coded as

DT02_YN	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Low Salt Diet (DT03_YN)

This is a characteristic specifying whether or not the sample person is on a low salt or sodium diet. This categorical variable is coded as

DT03_YN	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Low Sugar Diet (DT04_YN)

This is a characteristic specifying whether or not the sample person is on a low salt or sodium diet. This categorical variable is coded as

DT04_YN	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Diabetic Diet (DT07_YN)

This is a characteristic specifying whether or not the sample person is on a diabetic diet. This categorical variable is coded as

DT07_YN	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Milk Allergy (ALLERG02)

This is a characteristic specifying whether or not the sample person has an allergy to cow's milk. This categorical variable is coded as

ALLERG02	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Egg Allergy (ALLERG03)

This is a characteristic specifying whether or not the sample person has an allergy to eggs. This categorical variable is coded as

ALLERG03	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Fish/Shellfish Allergy (ALLERG04)

This is a characteristic specifying whether or not the sample person has an allergy to fish and/or shellfish. This categorical variable is coded as

ALLERG04	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Peanut Allergy (ALLERG06)

This is a characteristic specifying whether or not the sample person has an allergy to peanuts. This categorical variable is coded as

ALLERG06	CSFII Code	Code Used
Yes	1	1
No	2	2
Not Applicable	blank	2
Don't Know or Not Ascertained	8 or 9	9

Breastfeeding Status (BF_STAT)

This is a characteristic specifying whether or not the sample person (infant, child) is breastfeeding. This question was not asked if the child was over three years old. This categorical variable is coded as

BF_STAT	CSFII Code	Code Used
Breastfeeding	1	1
Not Breastfeeding	2	2
Over 3 Years Old	3	9

Lactation Status (LAC)

This is a characteristic specifying whether or not the sample person is lactating. This characteristic was determined from the pregnancy/lactation status characteristic (PL_STAT) asked of women between 10 and 55 years old. This categorical variable is coded as

PL_STAT	CSFII Code	Code Used
Pregnant	1	2
Lactating	2	1
Pregnant and Lactating	3	1
Not pregnant or lactating	4	2
Not female 10-55	5	9

Pregnancy Status (PRG)

This is a day-specific characteristic specifying whether or not the sample person is pregnant on this particular day. This characteristic was determined from the pregnancy/lactation status characteristic (PL_STAT) asked of women between 10 and 55 years old. For those records in the CSFII database this categorical variable for the first sampling date is coded as

PL_STAT	CSFII Code	Code Used
Pregnant	1	1
Lactating	2	2
Pregnant and Lactating	3	1
Not pregnant or lactating	4	2
Not female 10-55	5	9

For the second sampling date, the sampling gap in months was computed as (number of days between sampling dates)/30. If the stated months pregnant (PRG_MON) plus the sampling gap exceeded nine months, then PRG=2 for the second date. Otherwise PRG=1 for both dates.

For RP individuals, this characteristic is determined to some extent by the particular day-in-age, D, being considered. Males and females not within the range 10-55 have PRG=9. For pregnant females, the PL_STAT value of the matched CSFII person must be coded a 1 or a 3 and the gestational age, G, at the current day-in-age, must be between 1 and 280 days. If so, then PRG=1 and otherwise PRG=2.

Age-in-Months (AGM)

This is a day-specific quantitative characteristic specifying the sample person's age in months on this particular day. It is only used for matching infants less that one year old. For person-days in the CSFII surrogate pool, this characteristic was determined from the variable

AGE_M and the number of days between the sampling dates. AGE_M provided the age-in-months for the first sampling date. For the second sampling date, the sampling gap in months was computed as (number of days between sampling dates)/30. This gap was added to AGE_M to get AGM for the second date. If the computed value of AGM for the second date exceeded 11 months, then AGM was reduced by 12 months and the AGE for the second date was changed from 0 years to one year.

For RP individuals, AGM is determined by the particular day-in-age, D, being considered. AGM is computed simply as

$$AGM = \text{Floor}\ [\ (\ D - 1\ )\ 12 / 365\ ]$$

(The function Floor(x) means rounding down an integer.)

Day-of-Week (DOW)

This is a day-specific characteristic specifying the day-of-week of this particular day. For the CSFII surrogate pool of person-days, this characteristic was determined from the two variables D1_DAY and D2_DAY for the first and second sampling dates, respectively. For those records in the CSFII database this categorical variable for the first sampling date is coded as

D1_DAY or D2_DAY	CSFII Code	Code Used
Sunday	1	1
Monday	2	2
Tuesday	3	3
Wednesday	4	4
Thursday	5	5
Friday	6	6
Saturday	7	7

For RP individuals, this characteristic was determined in part by the particular day-in-age, D, being considered. It is also a function of the day-of-week on which his/her birthday falls, DOWBD. Since the calendar date of a birthday is expressed relative to January 1, 1990. From these two variables the day-of-week on day-in-age D is simply

$$DOW = (\ D - 2 + DOW_{BD}\ ) \bmod 7$$

Distances for Matching Characteristics

As discussed in the text, the Gower distance (or dissimilarity) measure, G is used for all comparisons between individuals I and J. Mathematically,

$$G_{IJ} = \frac{\sum_K \text{Distance}_K [\text{Level}(K,i), \text{Level}(K,j)] \times \delta_K [\text{Level}(K,i), \text{Level}(K,j)]}{\sum_K \delta_K [\text{Level}(K,i), \text{Level}(K,j)]}$$

Where:

$\delta_K [\text{Level}(K,i), \text{Level}(K,j)] = 1$, if Level(K,i) and Level(K,j) are comparable

$\delta_K [\text{Level}(K,i), \text{Level}(K,j)] = 0$, if Level(K,i) and Level(K,j) are not comparable (e.g., one missing).

Individuals I and J can be in the same or in different databases. The components of the Gower dissimilarity function are the distances computed for each separate characteristic K. All distances were derived from the respective target database.

C.1 Distances for Characteristics Used in Matching PUMS to CSFII

Distance components used to match PUMS to CSFII/FCID used the vector of 464 commodity consumption values available for each person who had two days of consumption information. For any categorical character (e.g. Region) the distance between any two levels i and j was computed as:

$$\text{Distance}(i,j) = \{ \sum_{R=1}^{464} [\text{AvgCons}_R(i) - \text{AvgCons}_R(j)]^2 \}^{1/2}.$$

Here, $\text{AvgCons}_R(j)$ denotes the weighted average consumption of commodity R for those individuals having level j of the characteristic. All averages were computed using the appropriate survey weights. Tables C.1.1 through C.1.7 contain the distance matrices for the 7 categorical characteristics. Since these distance matrices are symmetric only the lower triangular portions are shown.

For any quantitative characteristic, X (e.g. age), a smooth function Q(X) was fit to the one-dimensional representation of the characteristic. The method of multidimensional scaling (Cox and Cox, 1994) was used to obtain an optimal representation of X based on all pair-wise distances. The function Q(X) is used to calculate the distance between any two values of X. Thus for values X_1 and X_2, the distance would be calculated simply as:

$$\text{Distance}(X_1, X_2) = | Q(X_1) - Q(X_2) |$$

The 4 quantitative characteristics used in matching PUMS to CSFII were Age, Household Size (HHSize), Household Income 1989 dollars (Income89), and Percent of Poverty Level (PctPov). The distance calculations for these are as follows:

Age

$$\text{Distance}(X_1, X_2) = | Q(X_1) - Q(X_2) |$$

Where:

$$Q(X) = (-0.13772922947)\, X + (0.00223710794)\, X^2 + (-0.00001392305)\, X^3$$

Household Size

$$\text{Distance}(X_1, X_2)$$

$$= 0.317505 \, | X_1 - X_2 |, \quad \text{if } X_1, X_2 \leq 9$$

$$= 0.317505 \, | X_1 - 9 |, \quad \text{if } X_1 < 9 \leq X_2$$

$$= 0, \quad \text{if } X_1, X_2 \geq 9$$

Household Income

$$\text{Distance}(X_1, X_2) = 0.00001309 \, | X_1 - X_2 |$$

Percent of Poverty Level

$$\text{Distance}(X_1, X_2)$$

$$= 0, \quad \text{If } X_1 = X_2 = 0$$

$$= 0.60051 \, | \ln(X_1) - \ln(X_2) |, \quad \text{if } X_1, X_2 > 0$$

$$= 0.60051 \, | \ln(2) + \ln(X_2) |, \quad \text{if } X_2 > 0, X_1 = 0$$

Table C.1.1 Distance matrix for characteristic Census Region (Region)

Region	Region Code	Region Code 1	2	3	4
NE	**1**	0			
MW	**2**	0.722	0		
S	**3**	0.767	0.356	0	
W	**4**	0.669	0.501	0.493	0

Table C.1.2 Distance matrix for MSA Status (MSAStatus)

MSA Status	MSA Status Code	MSA Status Code 1	MSA Status Code 2
MSA	**1**	0	
Non-MSA	**2**	0.465	0

Table C.1.3 Distance matrix for Poverty Category (PctPov)

PovCat	PovCat Code	PovCat Code 1	PovCat Code 2	PovCat Code 3
<130%	**1**	0		
131% - 350%	**2**	0.451	0	
>350%	**3**	0.748	0.392	0

Table C.1.4 Distance matrix for Housing Unit Tenure (HUTenure)

HUTenure	HUTenure Code	HUTenure Code 1	HUTenure Code 2	HUTenure Code 3	HUTenure Code 9
Own	**1**	0			
Rent	**2**	0.449	0		
Occupy	**3**	0.498	0.498	0	
Missing	**9**	NC	NC	NC	NC

NC = Not comparable

Table C.1.5 Distance matrix for Race/Hispanic Origin (RaceEth)

RaceEth	RaceEth Code	1	2	3	4	5	6	7	8	9
White	**1**	0								
Black	**2**	0.655	0							
Asian	**3**	1.829	1.729	0						
Native Amer.	**4**	1.062	0.930	1.842	0					
Mex. Amer.	**5**	0.984	0.962	1.662	0.878	0				
Puerto Rican	**6**	1.505	1.180	1.673	1.331	1.370	0			
Cuban	**7**	1.493	1.528	1.561	1.747	1.5610	1.831	0		
Other Hispanic	**8**	0.850	0.677	1.453	0.800	0.619	0.995	1.370	0	
None ofabove	**9**	1.371	1.194	1.760	1.039	1.176	1.185	1.826	1.003	0

Table C.1.6 Distance matrix for Employment Status (Employ)

Employ	Employ Code	Employ Code 1	2	3	4	5	9
Full time	**1**	0					
Part time	**2**	0.279	0				
FT/Absent	**3**	0.240	0.350	0			
Unemployed	**4**	0.349	0.443	0.365	0		
Age < 16	**5**	NC	NC	NC	NC	NC	
Missing	**9**	NC	NC	NC	NC	NC	NC

NC = Not comparable

Table C.1.7 Distance matrix for Educational Level (Educ)

Educ	Educ Code	Educ Code 0	1	2	3	4	5	6	7	8	9	99
Age <15	**0**	NC										
K or less	**1**	NC	0									
Grade 1-4	**2**	NC	0.980	0								
Grade 5-8	**3**	NC	1.190	0.516	0							
Grade 9	**4**	NC	1.450	0.990	0.597	0						
Grade 10	**5**	NC	1.520	1.020	0.621	0.419	0					
Grade 11	**6**	NC	1.649	1.229	0.832	0.407	0.466	0				
HS/GED	**7**	NC	1.311	0.738	0.330	0.455	0.441	0.628	0			
College	**8**	NC	1.322	0.894	0.559	0.488	0.650	0.675	0.434	0		
Post Graduate	**9**	NC	1.377	1.078	0.850	0.814	0.992	0.990	0.787	0.4034	0	
Missing	**99**	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC

NC = Not comparable

C.2 Distances for Characteristics Used in Matching Person-days from the RP to those in CSFII/FCID

The 11 variables and distances described in Sections B.1 and C.1 above were also used when matching RP person-days to the pool of CSFII surrogate person-days. In addition, the 19 characteristics described in B.2 were also incorporated into the calculation of Gower distance. Of these new characteristics only three, AGM, HEALTH, and SMK were treated as quantitative and required distance functions. The other 16 are considered categorical and distances between any two of their levels are represented as elements in a distance matrix. As was the case in Section C.1, two levels of a characteristic could be non-comparable. When this occurs, the Gower function ignored the characteristic.

The distance function developed for **Health Status (HEALTH)** is

$$\text{Distance}(X_1, X_2) = 1.388 \mid \log(X_1 / X_2) \mid$$

If either X_1 or X_2 are missing, then this distance component is considered non-comparable.

For **Age-in-Months (AGM)** the distance function is

$$\text{Distance}(X_1, X_2) = 1.601 \mid X_1 - X_2 \mid$$

If the RP individual is at least one year old then this distance component is considered non-comparable.

For **Smoking Level (SMK)** the distance function is

$$\text{Distance}(X_1, X_2) = 0.412 \mid X_1 - X_2 \mid$$

If either X_1 or X_2 are missing, then this distance component is considered non-comparable.

Of the 16 categorical characteristics, 14 have only two comparable states (yes or no). When comparable, the distance between X_1 and X_2 will simply be 0 whenever $X_1=X_2$ and some positive constant otherwise. Table C.2.1 summarizes the distance values for these two-level characteristics.

The final two characteristics, Food sufficiency and Day-of-Week, have multiple levels. In their case, the distance between any pair of levels is more easily indicated by the corresponding element of a distance matrix. The distance matrix for Food Sufficiency is shown in Table C.2.2 and that for Day-of-Week in Table C.2.3. Because distance matrices are symmetric, only the bottom left portion of each is shown.

Table C.2.1. Distance calculations for the five new two-level characteristics used in computing Gower's dissimilarity.

Characteristic	Distance when $X_1 \neq X_2$	Non-comparable when
Vegetarian	0.904	$X_1=9$ or $X_2=9$
Diabetic	1.152	$X_1=9$ or $X_2=9$
Lactation Status	0.778	$X_1=9$ or $X_2=9$
Breastfeeding Status	4.893	Age<1* or Age>3
Pregnancy Status	0.736	$X_1=9$ or $X_2=9$
Low Calorie Diet	0.600	$X_1=9$, $X_2=9$, or Age=0**
Low Fat Diet	0.519	$X_1=9$, $X_2=9$, or Age=0**
Low Salt Diet	0.531	$X_1=9$, $X_2=9$, or Age=0**
Low Sugar Diet	0.713	$X_1=9$, $X_2=9$, or Age=0**
Diabetic Diet	0.662	$X_1=9$, $X_2=9$, or Age=0**
Milk Allergy	0.695	$X_1=9$ or $X_2=9$
Egg Allergy	0.758	$X_1=9$ or $X_2=9$
Fish/Shellfish Allergy	0.745	$X_1=9$, $X_2=9$, or Age=0**
Peanut Allergy	0.469	$X_1=9$, $X_2=9$, or Age=0**

* For Age=0, nursing and non-nursing infants are prohibited from matching.
**CSFII has no variation for this characteristic at Age=0

Table C.2.2. Distance Matrix for Food Sufficiency.

Food Sufficiency	Code	Code				
		1	2	3	4	9
Enough	1	0				
Enough quantity, but not of kinds	2	0.344	0			
Sometimes not enough	3	0.590	0.610	0		
Often not enough	4	1.218	1.373	1.037	0	
Unknown	9	*NC**	*NC*	*NC*	*NC*	*NC*

NC = Not comparable

Table C.2.3. Distance Matrix for Day-of-Week.

Day Of Week	Code	Code						
		1	2	3	4	5	6	7
Sunday	1	0						
Monday	2	0.312	0					
Tuesday	3	0.383	0.211	0				
Wednesday	4	0.340	0.166	0.132	0			
Thursday	5	0.344	0.190	0.194	0.146	0		
Friday	6	0.345	0.300	0.284	0.235	0.245	0	
Saturday	7	0.248	0.323	0.419	0.361	0.363	0.337	0

Appendix C – Residential White Paper

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α-CARES

RESIDENTIAL (NON-DIETARY) MODULE

CARES White Paper

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RESIDENTIAL (NON-DIETARY) MODULE

Executive Summary

The objective of this document is to provide the methodological framework for the alpha CARES (Cumulative and Aggregate Risk Evaluation System) "residential (non-dietary) module." As part of this objective, this document will serve to communicate technical issues, facilitate consensus-building, consolidation and resultant recommendations, and provide the basis for the design of the alpha CARES Residential Module and associated documentation.

This document includes the following:

1) Overview of current regulatory agency guidance and practices for residential exposure assessment;
2) Framework for the alpha CARES Residential Module;
3) Scientific rationale for the framework and associated underlying methods in the context of overarching, "state-of-the-science" issues related to residential exposure assessment specifically, and aggregate and cumulative exposure modeling in general;
4) Meta information from currently available public and proprietary data sources supporting the alpha CARES Residential Module;
5) Vector (or dictionary) of "individual characteristics" used in the alpha CARES Residential Module;
6) Documentation for residential exposure scenario-specific algorithms implemented in the alpha CARES residential module; and
7) Approach for "calendar-based" residential exposure modeling as part of the alpha CARES Residential Module.

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Table of Contents

[Editor's Note: Page numbers have been adjusted to fit this document.]

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List of Tables

List of Figures

List of Appendices

[Editor's Note – These appendices not included in the CARES Technical Manual.]

1. Residential Exposure Assessment: Current Guidance and Practices

1.1 Background

The passage of the Food Quality Protection Act (FQPA) in 1996 mandated the U.S. Environmental Protection Agency (EPA) to immediately begin considering aggregate exposure to pesticides. Aggregate exposure includes pesticides in food and drinking water, as well as non-dietary, non-occupational pesticide exposures for the general population. The latter type of exposure can occur, for example, in a residential setting (or other areas frequented by the general population). These exposures may include breathing vapors while inside a treated home, exposures to children playing on a treated lawn, or exposures attributable to the mouthing behaviors of infants and children. Prior to the passage of FQPA, the Office of Pesticide Programs (OPP) addressed these kinds of exposures on a case-by-case basis, typically in the Special Review process. Other regulatory agencies, e.g., California's Department of Pesticide Regulations (DPR), had also developed approaches to evaluating, measuring, and modeling potential residential exposures prior to FQPA (Ross et al. 1990, 1991, 1992; McKone, 1991).

In response to FQPA, OPP developed *Standard Operating Procedures (SOPs) For Residential Exposure Assessments* (EPA 1997), which it first brought before the Federal Insecticide, Fungicide and Rodenticide Act (FIFRA) Scientific Advisory Panel (SAP) for review on September 9, 1997. The intent of the SOPs was to provide a means for consistently calculating single pathway, screening level exposures and not to provide guidance on other related topics such as aggregate exposure assessment (EPA 1999a, 1999b). The SOPs became the backbone of the Agency's current approach for completing conservative, deterministic (point estimate-based), "Tier I" or "screening-level" residential exposure assessments. However, as acknowledged by OPP (EPA 1999a, 1999b), the state-of-the-art and -science has changed since the release of the original document in 1997 and attention has necessarily focused on scientific and policy issues and the corresponding need for implementation of a more realistic basis for estimating potential residential exposures under the FQPA.

Residential exposure and risk assessment issues have also been raised before OPP's SAP at meetings convened to review the following: Series 875, Post-Application Exposure Monitoring Guidelines (1998); dichlorvos-specific exposure assessment approaches (1998); and application of the FQPA Uncertainty Factor (1998, 1999). [Note: All of these referenced reports and accompanying documents are available from the Internet at http://www.epa.gov/pesticides/SAP.] OPP has also received numerous comments, petitions, and responses to chemical-specific risk assessments that focused on general risk assessment procedures and many of the same issues raised in these previous SAP meetings. As a result, OPP has made a commitment to revise its SOPs periodically to reflect the most recent and best science available.

1.2 Overview of Residential Exposure Assessment

This section provides an overview of the approach that has been used by the EPA to complete residential exposure and risk assessments. This approach is described in recent documentation provided to the FIFRA SAP (EPA 1999b) to supplement the existing SOPs (EPA 1997). Key elements of the process as well as some of the underlying factors are discussed.

1.2.1 Scope

The first step in assessing residential exposure and risk assessment is determining the scope of these types of assessments. The term "residential" refers to the generic umbrella of non-occupational exposures, regardless of where they occur. The term "general population exposure" could be easily substituted. If exposures occur as a result of activity directly related to an application, they are referred to as "handler" exposures (e.g., one who mixes or applies a pesticide product). On the other hand, if exposures occur as a result of activities in a previously treated area, they are referred to as "post-application" exposures. The other distinction that is made by the EPA is the one between the terms "residential" and "homeowner." The term homeowner is used to refer to that segment of the population who purchase pesticides and make their own applications. Conversely, it is possible to have a routine residential post-application exposure scenario that results from the occupational use of a chemical. For example, if a lawn care company or a structural pest control company treats a lawn or a house, the residents can be exposed through their normal activities inside and/or on the treated turf.

Given the above definitions, the Agency currently categorizes exposures in the following manner when completing a residential risk assessment:

- **Homeowner, Handler Exposures** result from an individual, not as a condition of his/her employment, applying a pesticide.

- **Residential, Post-Application Exposures** result from entry and activity in an environment previously treated with a pesticide. These exposures may result from both occupational or homeowner applications and may occur in a variety of settings including homes, schools, day care facilities, and other public places (e.g., parklands).

All exposure scenarios currently addressed in the EPA's SOPs are non-occupational in nature. Exposures that can occur to bystanders of occupational applications or from bring-home events to children (e.g., drift and residue track-in) are also being considered by OPP as they may cause exposures to those individuals not involved in the occupational activity (e.g., children of a farm-worker or pest control operator).

The toxicity of pesticides also determines how the EPA completes its risk assessments. For example, the effects associated with a pesticide can differ based on how it enters the body (e.g., different effects can occur based on whether it is absorbed through the skin or is inhaled). The Agency structures assessments based on the toxicological effects associated with each pesticide and the potential for exposures related to each route of exposure and the registered uses of the products.

1.2.2 Exposure/Risk Assessment Approach

In order to illustrate the critical issues pertaining to the *SOPs For Residential Exposure Assessments* and refined alternatives, it is necessary to summarize the current practices and how the current efforts to refine the assessment approaches are consistent with sound exposure assessment practices.

The risk assessment approach used by the Agency is rooted in the mandate of the Food Quality Protection Act (FQPA) amendments to the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) and the Federal Food, Drug, and Cosmetic Act (FFDCA). The current approach is also consistent with the Agency-wide guidance for exposure assessment detailed in the document *EPA Exposure Assessment Guidelines* (U.S. EPA, 1992). FQPA requires the Agency to address aggregate exposures as follows:

1. Section 408(b)(2)(A)(ii) defines "safe" to mean that "there is a reasonable certainty that no harm will result from aggregate exposures to the pesticide's chemical residue from all anticipated dietary sources as well as all exposures from other sources for which there are reliable information."

2. Section 408(b)(2)(C) requires EPA to give special consideration to infants and children by requiring "that there is reasonable certainty that no harm will result to infants and children from aggregate exposure to the pesticide's chemical residues...."

When FQPA was passed, the Agency had to interpret these mandates and determine how to implement them. The Agency believed that the "reasonable certainty of no harm" could only be established for food use pesticides by conducting appropriate risk assessments. Moreover, the Agency decided that such risk assessments had to routinely include non-occupational (residential) exposures as well as the usual dietary exposures. Finally, the Agency concluded that the procedures developed for these assessments must be adequately protective. These decisions provided the genesis of the *SOPs For Residential Exposure Assessments* (U.S. EPA, 1997).

In order to ensure that the standard of "there is a reasonable certainty of no harm" was established in the risk assessments completed by the Agency, the original *SOPs For Residential Exposure Assessments* document were developed using a deterministic, assumptive approach to exposure assessment that intentionally produced bounding estimates. This approach is based on conservative estimates and results in exposure estimates for a single exposure pathway that are protective and result in a "reasonable certainty of no harm." The Agency, in taking this "precautionary principle" approach, intended to be consistent with its peer-reviewed *Exposure Assessment Guidelines* in that the values calculated resemble the TUBE (or Theoretical Upper Bounding Estimate) of exposure described in the guidelines. TUBE values were to be calculated in lieu of more refined chemical- and scenario-specific data (U.S. EPA, 1992). The following, excerpted from the guidelines, describes the use of TUBE estimates of exposure:

From Section 5.3.4.1 of the U.S. EPA Exposure Assessment Guidelines - - Preliminary Evaluation and Bounding Estimates: "The first step that experienced assessors usually take in evaluating the scenario involves making bounding estimates for individual exposure pathways. The purpose of this is to eliminate further work on refining estimates for pathways that are clearly not important. The method used for bounding estimates is to postulate a set of values for the parameters in the exposure or dose equation that will result in an exposure or dose higher than any exposure or dose expected to occur in the actual population. The estimate of exposure or dose calculated by this method is clearly outside of (and higher than) the distribution of actual exposures or doses. If the value of this bounding estimate is not significant, the pathway can be eliminated from further refinement. The theoretical upper bounding estimate (TUBE) is a type of bounding estimate that can be easily calculated and is designed to estimate exposure, dose, and risk levels that are expected to exceed the levels experienced by all individuals in the actual distribution. The TUBE is calculated by assuming limits for all variables used to calculate exposure and dose, that, when combined, will result in the mathematically highest exposure or dose. It is not necessary to go to the formality of the TUBE to assure that the exposure or dose calculated is above the actual distribution, however, since any combination that results in a value clearly higher than the actual distributions can serve as a suitable upper bound."

It has been pointed out by the EPA (EPA 1999b) that the procedures outlined in the original document were also *not meant to be aggregated* without a definitive characterization by the assessor because it violates the basic tenets of exposure assessment by adding highly conservative estimates of exposures that result in "bounding, unrealistic estimates of exposure" (U.S. EPA, 1992).

The current focus of the Agency is to develop more sophisticated exposure and risk assessment methodologies that are required to complete more refined, aggregate exposure analyses. This

initiative also concurs with the guidance provided in the *EPA Guidelines for Exposure Assessment* (U.S. EPA, 1992). On this matter, the *EPA Guidelines for Exposure Assessment* provide the following guidance:

Section 5.3.4.2 - - Refining the Estimates of Exposure and Dose: "For those pathways not eliminated by bounding estimates or judged trivial, the assessor will then evaluate the resulting exposure or dose. At this point, the assessor will make estimates of exposure or dose that are designed to fall on the actual distribution. The important point here is that unlike a bounding estimate, these estimates should focus on points in the actual distribution. Both estimates of central tendency and estimates of the upper end of the distribution curve are useful in crafting risk descriptors."

Section 5.3.5.1 - - Individual Exposure, Dose, and Risk: "If almost no data are available, it would be difficult, if not impossible, to estimate doses in the high end. One method that has been used, especially in screening-level assessments, is to start with a bounding estimate and back off the limits used until a combination of parameter values is, in the judgment of the assessor, clearly in the distribution of exposure or dose."

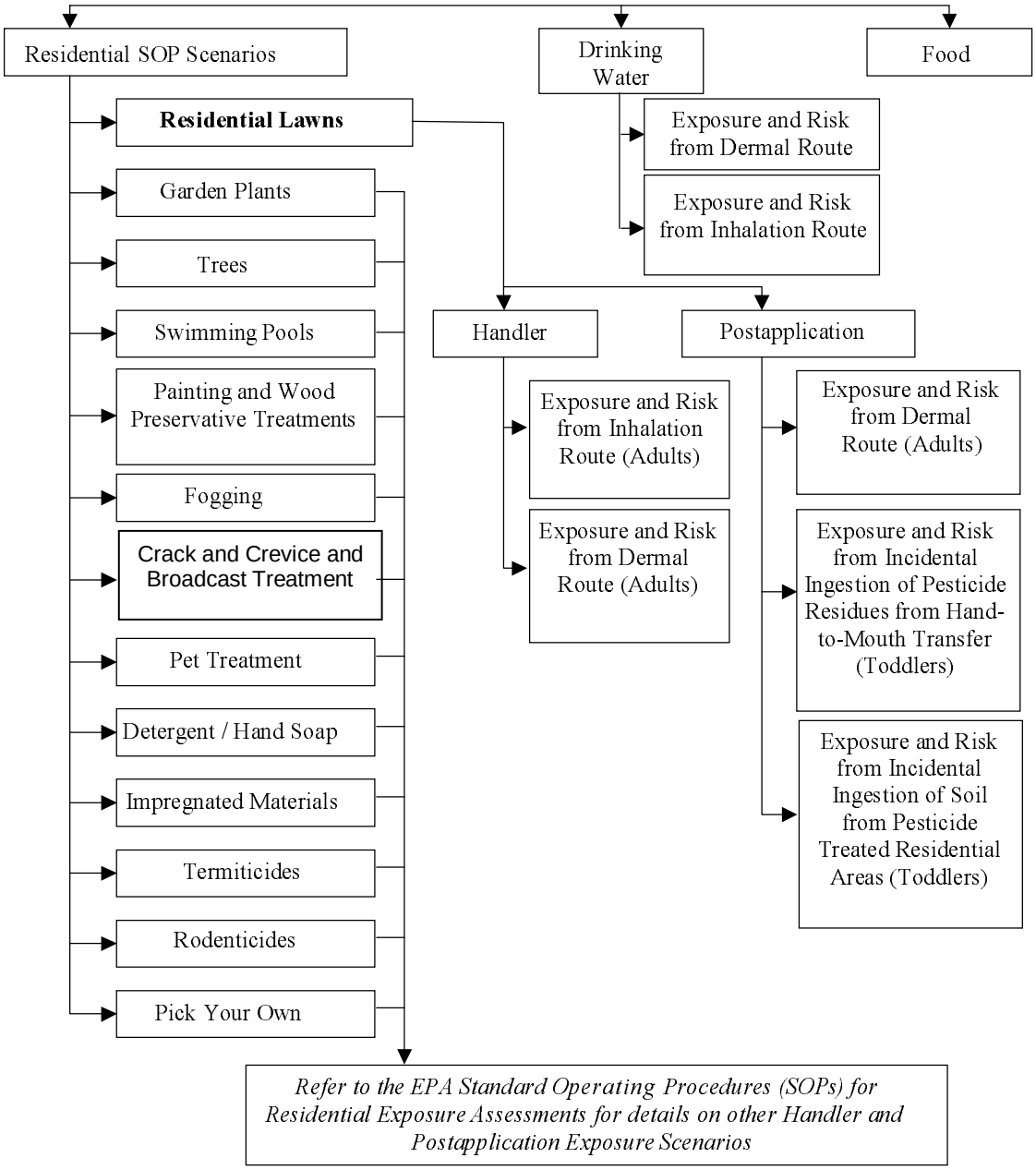
At present, the SOPs identify 16 common pesticide use patterns/use sites (e.g., residential lawns, ornamental plants, crack and crevice treatment, etc.) that may result in exposures to consumer applicators and as the result of post-application activities in proximity to treated areas. Thus, each of these 16 exposure scenarios is further divided into "handler" or mixer/loader/applicator and post-application categories. These are then further divided by age group (e.g., adult female, toddler, etc.), route (inhalation, dermal, oral) and specific activity or pathway (e.g., incidental ingestion from hand-to-mouth transfer). Figure 1 illustrates exemplary scenarios, pathways and routes included in EPA's current SOPs (EPA 1999b).

In summary, the EPA's Office of Pesticide Programs (OPP) currently uses the *Draft Standard Operating Procedures (SOPs) for Residential Exposure Assessments* (EPA 1997) for conducting screening-level, deterministic evaluations. The draft SOPs are being updated (EPA 1999b) in a periodic manner. The exposure assessment methods provided in the SOPs require refinement, particularly with respect to input variable default point values (by replacing with data-driven, alternative point values or distributional data whenever available) prior to incorporation into multi-source (residential, dietary, drinking water) aggregate and cumulative risk analyses. In addition, the SOP methods must be supplemented with explicit consideration (and associated modeling framework) to address temporal, spatial and demographic specificity in a manner consistent with dietary and drinking water exposure analyses. A temporal consideration, for example, is providing in the modeling framework the current understanding of how pesticide products use events occur over time (e.g., across the calendar year) and the likelihood of co-occurring product use events (and potential exposures) during toxicologically relevant time domains (24-hour period, one week, one month, or one year). Allocation of residential pesticide product use events across time must address the positive or negative correlations between one or more products (e.g., flea infestation may result in a higher likelihood of treating infested pets with one product and surfaces, such as carpets and rugs, with another in a short time period, i.e., co-occurring product usage). Conversely, products may serve essentially the same purpose, such that the use of one will almost certainly preclude the use of another. This temporal framework must also address, for example, seasonal use patterns associated with preventative maintenance applications in and around the home and application events resulting from situational pest pressures.

The fundamental difference between the current SOPs and the modeling framework required for aggregate and cumulative modeling is the principle that exposure may occur to each individual (and their respective demographic, behavioral, and spatial characteristics) in the population as a function of time, individual by individual, ultimately representing a probabilistic assessment of exposures across heterogeneous individuals in the reference population (EPA 1997a, 1999b, 2000). EPA's current aggregate (EPA 1999b) and cumulative (EPA 2000) guidance and other

publications (ILSI 1998, 1999) provide useful discussions of the fundamental elements of aggregate and cumulative modeling frameworks and some of the unique aspects of estimating potential exposures associated with pesticide products used in the residential environment. Based in part on the concepts described in some of the documents and publications mentioned above (EPA, 1997, 1999, 1999b, 2000, ILSI 1998, ILSI 2000; OTT, 1985; Paustenbach, 2000), the next section of this document provides an overview and diagrammatic representation of the residential exposure assessment framework for the alpha CARES Residential Module.

Figure 1 RESIDENTIAL LAWNS: Pathways and Routes to be Considered in an Aggregate Exposure/Risk Assessment



2. Alpha CARES Residential Module Framework

An overview of key elements that must be addressed in a residential exposure modeling framework to support aggregate and cumulative risk analyses is presented in Figures 2 and 3. These elements include demographics, lifestyle characteristics (e.g., activity and product use patterns), environmental media, and residential factors (e.g., housing type and air exchange rates, surface types such as carpet, hardwood, turf, pets). These dynamic, time-dependent elements and sub-elements (some of which can be represented as "objects" in the context of object-oriented programming) are designed into the residential module framework as simplified, but discrete parts of the real world in a manner that reflects how they "interact" to result in potential pathway and route-specific exposures.

Figure 4 provides an overview of the conceptual framework included in the alpha CARES Residential Module. Figures 5, 6 and 7 provide more detailed conceptual flow diagrams.

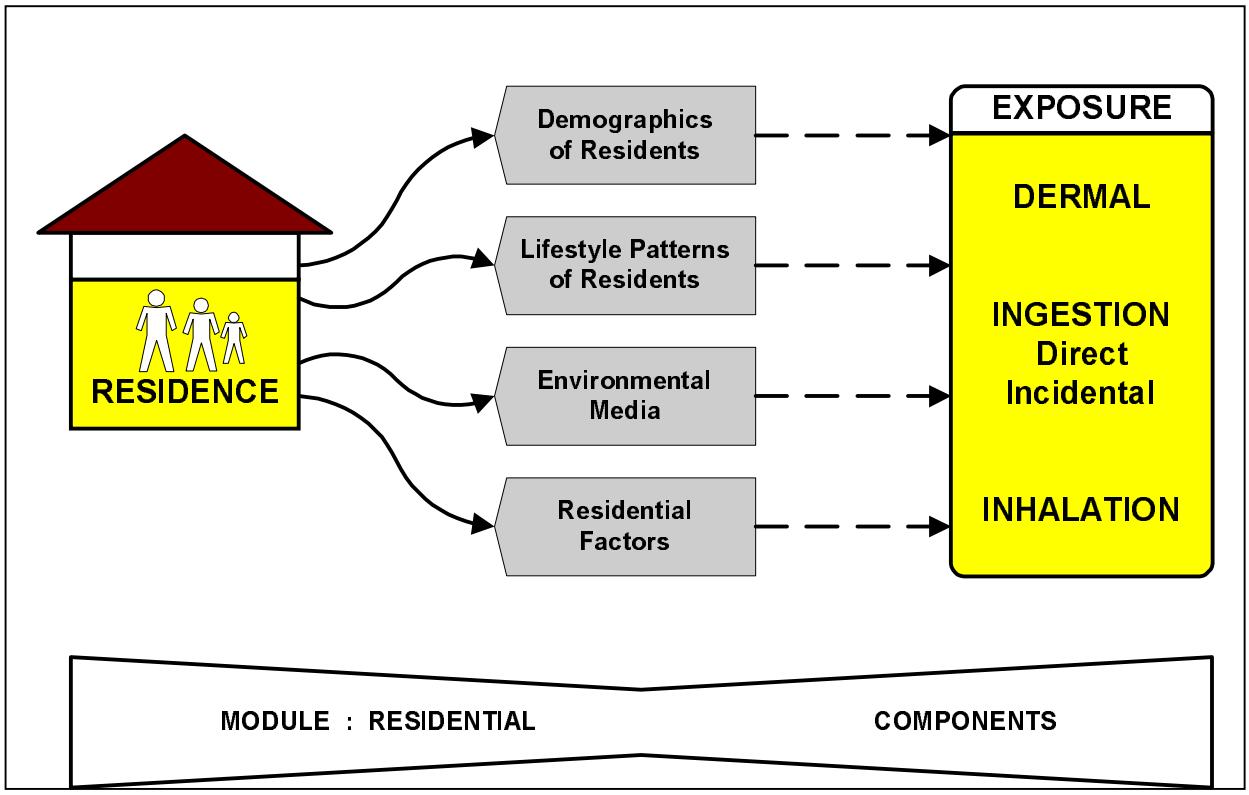


Figure 2 CARES Residential Module Components.

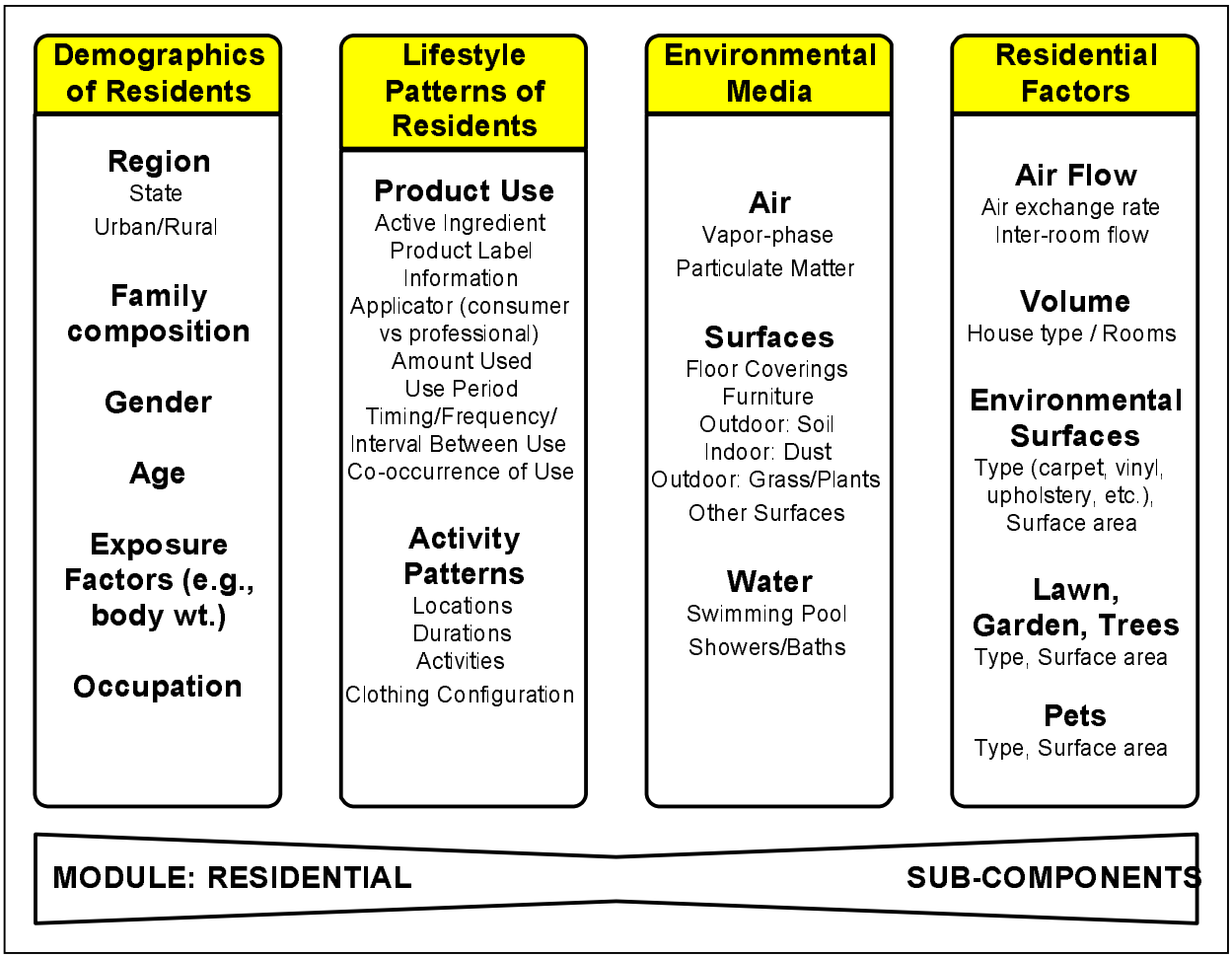


Figure 3 CARES Residential Module Subcomponents

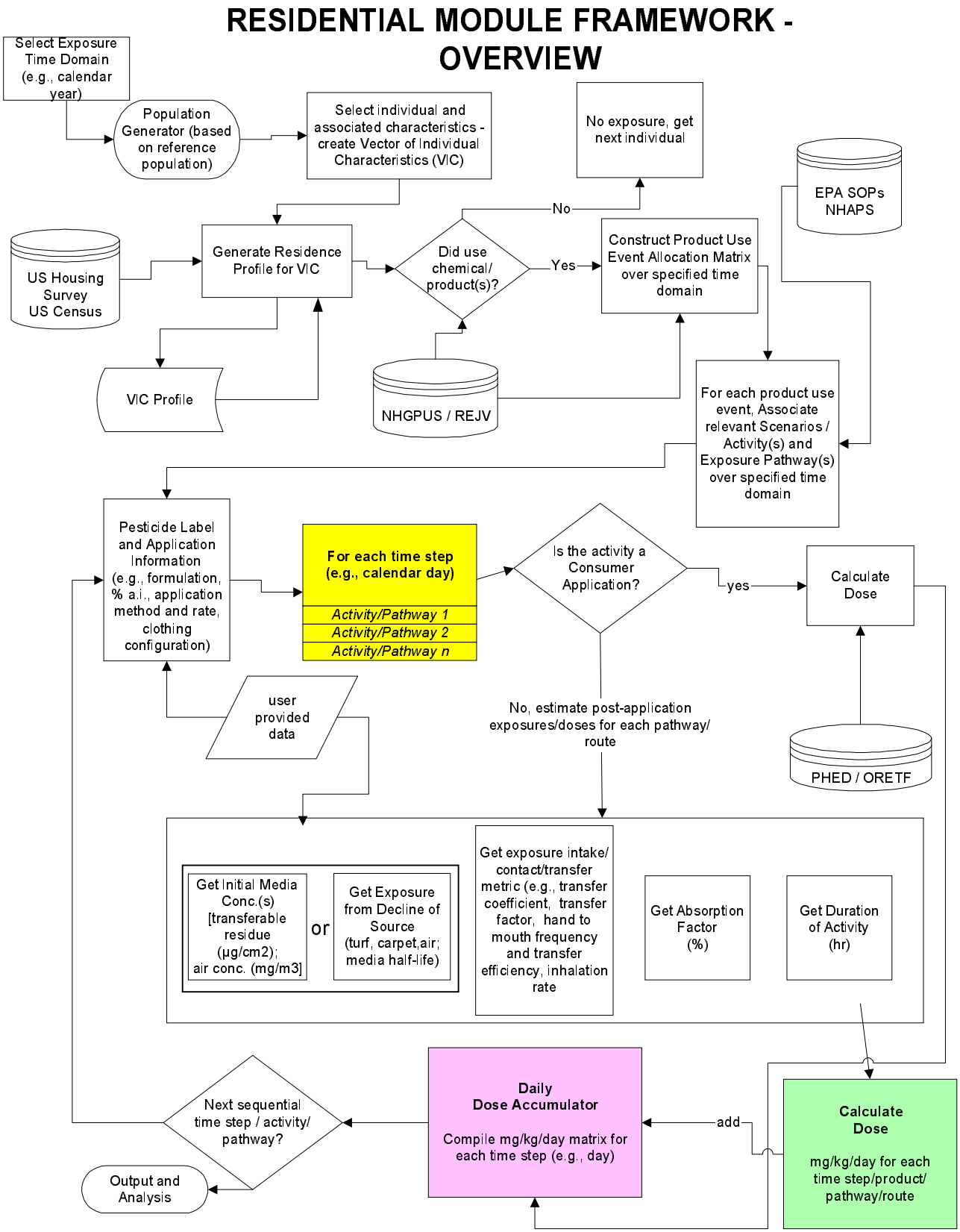


Figure 4 CARES Residential Module Framework

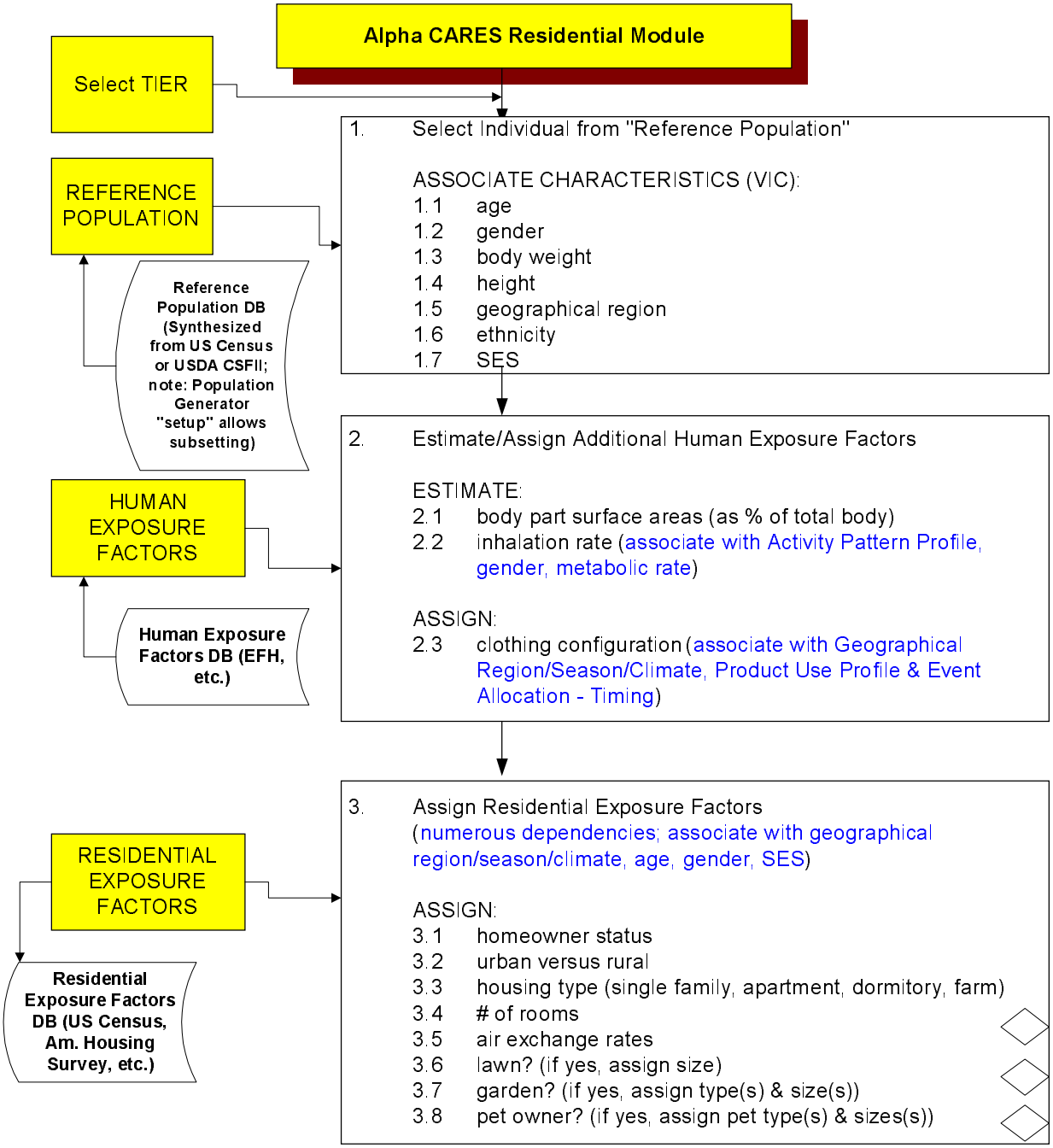
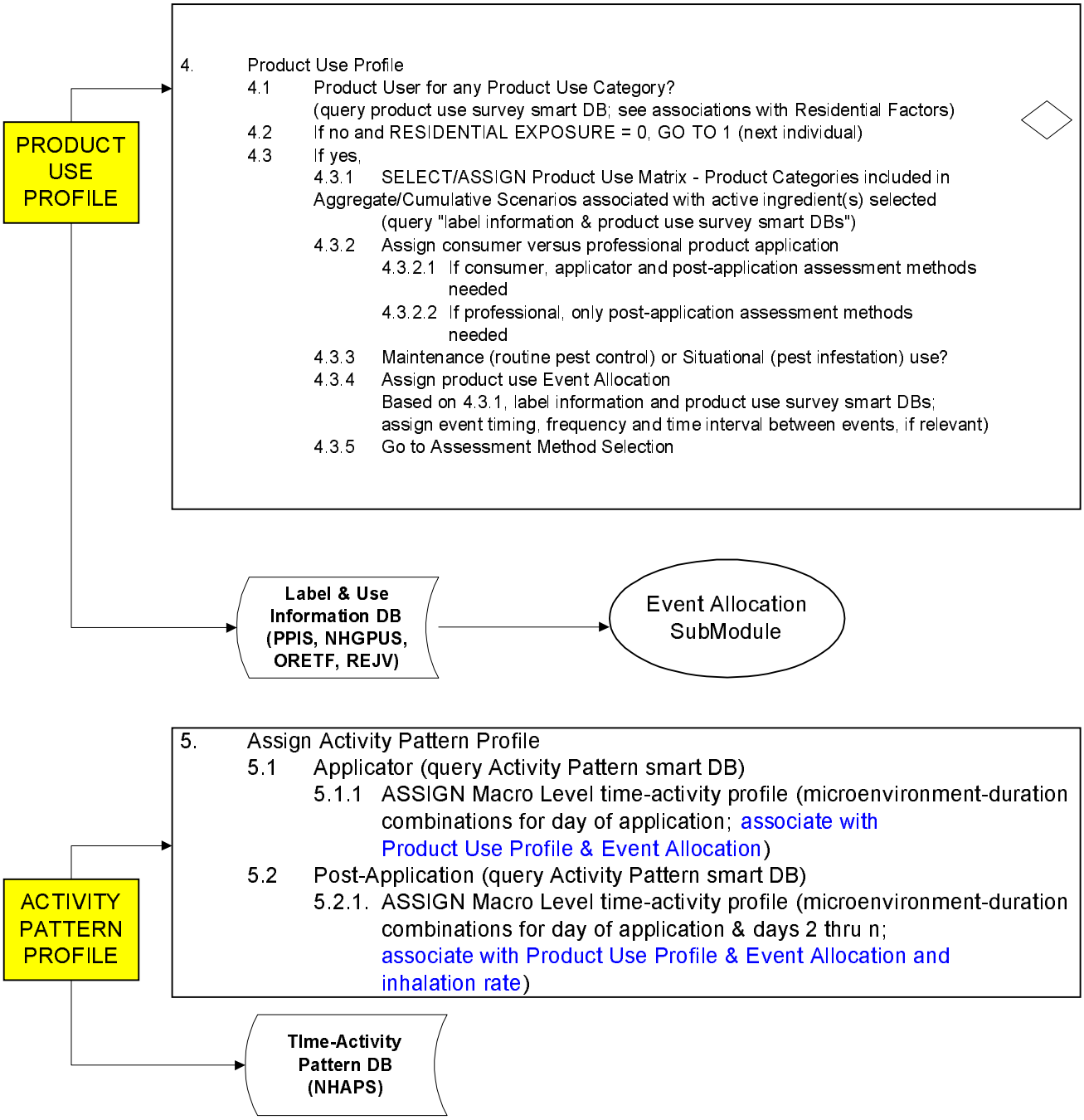
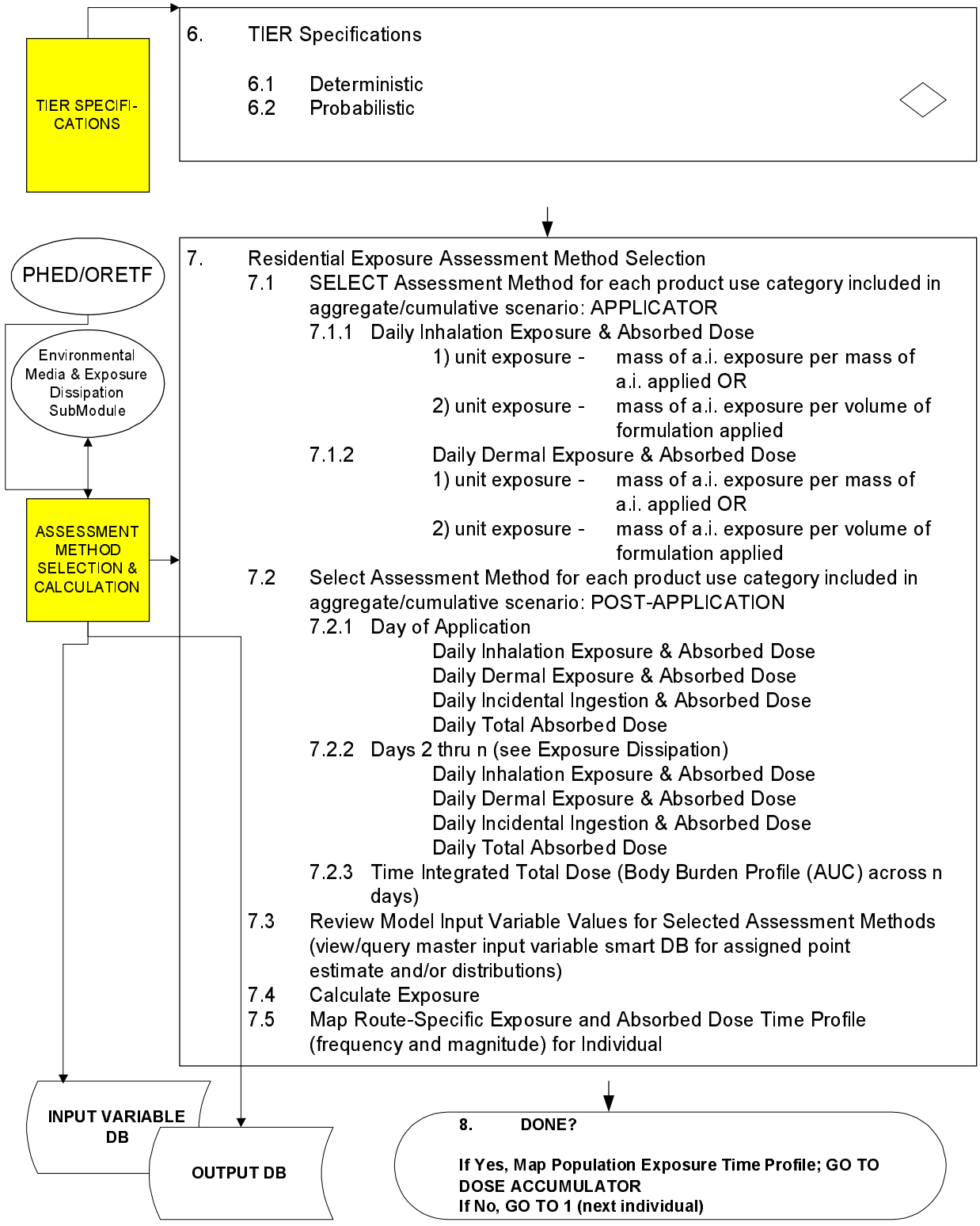


Figure 5 CARES Residential Module Conceptual Flow Diagram.





3. Key Issues Related To Improving Residential Exposure Assessment

This section presents a discussion of key issues related to improving or advancing residential exposure assessment methods for purposes of either deterministic or probabilistic modeling. Each key issue is identified followed by a discussion of the interim solution / approach selected for the alpha version of the CARES Residential Module.

3.1 Tiered Approach

A number of federal regulatory agency offices, including the EPA's OPP use quantitative risk assessment as part of their regulatory decision-making process. The anatomy of a risk assessment includes combining hazard (toxicity) information with exposure information to determine the nature and magnitude of risk to public health and the environment from a particular situation.

Estimating or modeling potential indoor and outdoor residential exposures is a complex task and it requires the use of available exposu re monitoring data in conjunction with label and use information. Further, evaluation of uncertainty and validation of predictive models is important to establish scientific credibility. Residential exposures are typically estimated for adult applicators and for both adults and children during post-application activities. Depending on the toxicological effect being evaluated, route-specific exposures may be calculated separately, or a total absorbed dose may be estimated. In the case of children, total absorbed dose may include contribution from the dermal and inhalation routes, and from incidental ingestion (such as from hand to mouth contact). Typical residential exposures assessments address:

1. Potential consumer applicator exposure (dermal and inhalation);
2. Potential post-application inhalation exposure;
3. Potential post-application dermal exposure; and
4. Potential post-application ingestion exposure.

The models and methods used for purposes of estimating potential residential exposure (and absorbed dose) continue to be refined and validated as new monitoring studies become available. The goal is to simulate actual exposure conditions as closely as possible. The following sections present an example of a simplistic screening-level exposure assessment calculation for a consumer product, followed by a discussion how more refined, probability-based or uncertainty analysis methods can be used. Screening-level methods typically include conservative bias in the form of “default” assumptions that are used in the absence of directly relevant and robust exposure monitoring data and other information. These methods can be used to predict potential exposure; however, it may be necessary to refine the screening-level assessment, if excessive health risk is suggested, to determine more realistic estimates of the potential distribution of exposures and corresponding health risks. As noted above, this is often referred to as the “tiered” approach to exposure and risk analysis. Initial tier calculations can typically be characterized as highly conservative, sometimes even as “theoretical upper-bound estimates.” The overall conservatism results from a variety of sources including the use of studies based on human activities (e.g., Jazzercise™) that overestimate exposures associated with more typical residential activities (e.g., walking, crawling, sitting), the use of conservative “clothing scenarios” (e.g., no clothing being worn by infants and children), the use of conservative methods for estimating the transport and fate, and relative bioavailability of chemical residues on days following application, etc.

It is desirable to also develop, as part of higher Tiers, distributional expressions of input variables and output, e.g., exposures and absorbed doses, to more accurately reflect the underlying mathematical variability and uncertainty associated with key variables included in the analysis and to determine how conservative the initial screening-level estimate is, i.e., what percentile it represents (e.g., 75th, 95th, etc.). This latter representation of exposure and absorbed dose more adequately characterizes the overall uncertainty and conservatism in the inherent assessment and provides more information to the risk manager for decision-making purposes.

In recent years, EPA has adopted the use of a "tiered" approach to risk assessment. In a tiered approach, an initial, screening level risk assessment is conducted using conservative default assumptions. In the case of residential exposure assessments, this is accomplished using the SOPs (EPA 1997). If the situation being investigated does not show an unacceptable risk under the screening assessment conditions, no further analysis is conducted. However, if the conservative screening risk assessment determines that the situation under consideration does exceed an unacceptable risk threshold, then further, more in-depth analyses are undertaken.

While conceptually appealing, this approach has several drawbacks. First, the initial screening level risk assessment typically is so conservative that very few situations pass this initial screen. This has proven to be the case in a number of residential risk assessments included as part of the EPA, OPP Registration Eligibility Decision (RED) process. As a result, the screening level assessment is often a low value effort since the uncertainty factors applied to result in a conservative risk assessment combine to produce a result that is difficult to interpret. Second, if the screening level assessment determines that the potential for unacceptable risk exists, this result can then become "public", and the agency and the regulated community are in the unenviable position of having to explain to other stakeholders why an unacceptable risk appears to exist, when this may not actually be the case. The fact that the screening level analysis was conducted using conservative and perhaps unrealistic assumptions can be lost on a non-technical audience, precipitating an unnecessary risk communication challenge. Finally, by using all default inputs in the screening analysis, it is more difficult to focus subsequent data collection efforts, as the initial screening does nothing to determine which variables contribute the greatest degree of uncertainty to the analysis.

In light of the above, groups such as the former American Industrial Health Council (AIHC) have recommended that a policy be adopted by regulatory agencies which promotes the use of a "continuum" of inputs to the risk assessment process, including the use of all credible, readily-available, situation-specific data early in the analysis. This recommendation is substantiated in the case of conducting residential exposure/risk analyses, particularly for aggregate and cumulative assessments. In these situations, there is no apparent benefit to conducting a screening analysis using default inputs in the EPA SOP algorithms merely for the sake of conducting a screening assessment, when relevant and credible data are available and when, in the case of aggregate and cumulative modeling, compounding conservatism renders the output unreliable for supporting decision-making. The initial assessment should acknowledge the actual potential for human and environmental exposure, rather than merely assuming that such exposure occurs.

If a "continuum-of-input" approach is adopted, the following tangible benefits to the use of risk assessments in regulatory decision-making will emerge:

- The utility of existing data will be optimized, through its early incorporation in the risk assessment process.
- A potentially unnecessary screening step will be eliminated; and, as such,
- A meaningful risk assessment result that can form the basis of a regulatory decision can be arrived at sooner.

- Unnecessary risk communication hurdles could be eliminated by avoiding the generation of screening level risk assessment results that may be divorced from reality.

- The overall credibility of both the agency, and the risk assessment process as a basis for decision-making, will be enhanced.

3.2 Use Of Reliable Information / Data

As described in detail in Section V of this document, a number of "reliable" information / data sources exist to support advanced, probabilistic residential exposure and risk analyses. Further, many of the personal exposure monitoring approaches and exposure assessment methods developed historically can be applied to pesticides. The availability of adequate data is a prerequisite to support scientifically credible calendar-based, probabilistic exposure/risk assessments and to support necessary uncertainty analyses. The definition of reliable information/data must be developed in this context. Thus, to support probabilistic analyses data can be considered reliable if they meet the following criteria:

1. Relevant to the chemical, products and exposure scenario(s) being evaluated (either directly or as a reliable surrogate);
2. Provide an adequate representation of variability and uncertainty (include a sufficient number of replicates that meet quality assurance benchmarks such as recovery efficiency); and
3. Can be adequately stratified with respect to minimally necessary demographic characteristics, i.e., age, gender, geographic area (national).

Evaluation of data sources with respect to "reliability" should include the following elements, where relevant::

I GENERAL INFORMATION
STUDY TITLE:
AUTHOR(S):
DATE:
SOURCE (CITATION):

II CORE CRITERIA (TIER I)

PRODUCT USE SCENARIO(S):
MODEL INPUT VARIABLES ADDRESSED:
META INFORMATION & DEMOGRAPHIC CHARACTERISTICS:
FORMULATION TYPE:
APPLICATION METHOD:
SITE OF APPLICATION:
ACTIVITY DESCRIPTION & CONDITIONS:
APPLICATION REGIMEN:
CLOTHING CONFIGURATION:
SAMPLING & ANALYTICAL METHODS:
DETECTION LIMIT:
    Limit of Detection
    Limit of Quantification
RESULTS & CONCLUSIONS:

III OTHER CONSIDERATIONS (TIER II)

QUALITY ASSURANCE DATA:
ANALYTICAL RECOVERIES:
RECOVERY EFFICIENCY CORRECTION:
FIELD FORTIFICATION SAMPLES:
NUMBER OF REPLICATES:
STATISTICAL & OTHER ANALYSES (analytical correction factors for recovery efficiency, distributional representations of empirical data sets, subpopulation representativeness, e.g., statistical weighting in surveys, etc.):

3.3 Temporal, Spatial And Demographic Resolution

Aggregate and cumulative exposure and risk analyses must explicitly maintain appropriate temporal [e.g., timing, duration and frequency (including seasonal dependencies) of exposure, co-occurrence of exposures from different sources over specified time intervals], spatial (e.g., location and type of home, urbanization), and demographic (e.g., age, gender) specificity. Residential exposure assessments that are part of overall aggregate or cumulative assessments, are developed for hypothetical in dividuals with pre-defined demographic characteristics (age, gender) over specified time intervals (short-term time periods such as day of application during seasons of product use) and geographic locations (e.g., national scale or geo-regions where specific product types are used for a given pest). The degree of temporal, spatial and demographic resolution is dependent upon underlying data sources and their corresponding "common denominators" in this regard. Typically, in the case of residential exposure modeling, many exposure scenarios and associated algorithms and underlying data sets for input variables can be considered conservatively biased and thus, likely to overestimate actual distributions of exposure for a given time period, within and across relevant demographic strata and geographic regions. In contrast, some exposure scenarios, such as turf product application and reentry, and reentry following termiticide application, have a more refined matrix of underlying data sets that reflect different geographic locations and environmental (temperature, humidity, indoor air exchange) conditions. Available human exposure monitoring studies generally reflect label-based application methods and reentry conditions and include multiple replicates involving adult volunteers, representing both male and female genders. In contrast, limited monitoring data exist for teenagers and children (toddlers and infants). Often adult monitoring data and adjunct measurements (e.g., air monitoring at breathing zone levels of children) are used in conjunction with allometric scaling factors to estimate potential exposures to non-adult subpopulations for a given time period and geographic region (which is often assumed to adequately represent upper-bound point estimates or distributions of exposure for the overall U.S. population).

As indicated in part, in current EPA guidance for cumulative risk assessments (EPA 2000), the following considerations should be addressed when considering temporal, spatial and demographic resolution:

1. As data permit, exposures from a variety of plausible (but prioritized) subset of residential sources, pathways and routes should be addressed (and combined if co-occurrence may exist) over a relevant time frame;
2. Generalized, time-related, residential exposure decline following product use as a function of data from both media-specific residue decline measurements (e.g., indoor carpet, outdoor turf) and available temporal passive dosimetry data sets that are developed and incorporated into modeling constructs should include a discussion of limitations and assumptions [e.g., existing data require use of the general exposure decline functions for different demographic strata (e.g., adults, children) and geographic regions (urban, rural)];

3. An individual's temporal residential exposure profile should be matched with relevant characteristics of the toxicological endpoint of interest, e.g., route and duration, time to effect or appropriate time-averaging period;
4. The integrity of the exposure concerning the hypothetical individual should be maintained throughout the simulation (assessment), i.e., the same individual, at the same time, in the same setting, in the same location);
5. Uses among products (and product categories or types) should reflect plausible dependencies (e.g., use of a given product increases the likelihood or probability of using one or more additional products during a relevant time period to address an insect infestation for example; or use of a given product excludes the use of other products);
6. Uses of products over time should reflect, where relevant, known seasonal dependencies and associated geographic distribution;
7. Exposure estimates should by tracked for each relevant route to understand contribution to total exposure over time; and
8. Appropriateness of using short-term data sets to back cast or forecast across longer-term time intervals.

As data sets are developed with prior consideration of temporal, spatial and demographic characteristics, model evaluation can be undertaken to investigate the relative importance (sensitivity) of extrapolation of product use, human activity patterns and other variables across time, geographic location and demographic characteristics. As discussed in Section V data sets that can assist in investigating aspects of temporal, spatial and demographic domains are available from recent residential product use surveys and to a more limited extent, from previously conducted product use and time-activity surveys.

3.4 Individual-, Household-, Subpopulation- And Population-Level Exposure Simulation

Current residential exposure simulations address exposures to individuals in the constructed reference population (e.g., U.S. Census) but do not include potential correlations amongst members of a household. In the alpha version of the CARES residential module, households are not treated as "exposure units" and individuals within each household tracked accordingly. If a product use event occurs in a given household, all residents are potentially exposed as a function of their respective time-activity patterns. However, in the context of probabilistic aggregate and cumulative modeling, if an adequate number of simulations for individuals within a reference population are included, all possible permutations of exposure frequency, magnitude and duration within and across households should be adequately represented. In an analogous manner, exposures within subpopulations and across the entire reference population will be represented. It is anticipated that future versions of the CARES residential module can explore tracking exposures at the household level provided datasets used to construct the "reference population" contain household-level information.

3.5 Macro- Versus Micro-Activity Exposure Simulation

To illustrate residential modeling constructs, Appendix B provides general algorithms associated with two approaches for estimating potential dermal and nondietary ingestion exposure, referred to as the microactivity and macroactivity approaches (Hubal et al., 1999, 2000) (Appendix C provides the macro-activity-based algorithms used in the CARES residential module). In the microactivity approach, exposure is modeled as a series of mass transfers or removals resulting from each discrete dermal contact event (e.g., right hand contacting toy for 10 sec, fingers contacting mouth for 3 sec). In the macroactivity approach, dermal exposure is modeled using empirically derived transfer coefficients or factors to lump the mass transfer associated with a

series of contact events in a pre-specified time domain (Hubal et al., 1999, 2000; ILSI, 1998). The Residential Exposure Assessment Spreadsheet Tool (REx) and the CARES residential module employ the macroactivity method while the EPA's Office of Research and Development's Residential-Stochastic Human Exposure and Dose Simulation (SHEDS) model for residential exposures currently uses the microactivity approach (Zartarian et al. 2000).

In SHEDS, for example, sequential dermal and nondietary ingestion exposure and dose time profiles are simulated by combining measured surface residues and residue transfer efficiencies with actual micro-level activity data quantified from videotapes (Zartarian et al. 2000). Given that the sequence of dermal loading and removal processes is ca ptured from videography data, such exposure profiles can be used to generate hypotheses regarding time-dependent dermal exposure and absorption, which have traditionally assumed a fixed concentration at the skin surface. In contrast the CARES residential module aggregates the micro-events into transfer factors (or coefficients) based on evidence of dermal equilibrium with surfaces contaminated with dry surface residues (ORETF 2000, Ross et al., 1990 and 1991; ILSI, 1998). With both dermal modeling constructs, information on frequency and duration of hand-to-mouth activities can then be used as the basis for estimates of ingested residues. Further, in both cases exposure and dose profiles can also be developed for different time domains based on the toxicological metrics of interest (e.g., daily, subacute or subchronic time-weighted averages). Further, these modeling tools are useful to evaluate the apparent relative contribution of different exposure pathways and routes. When combined with product use information and time-activity data, temporal exposure and dose profiles can also be used to construct "calendar" views of exposure events, cumulative dose and how exposures can be mitigated, if deemed necessary. The design of the CARES residential module (and the overall software platform) will allow for future additions and modifications such that micro-activity-based algorithms and other features and can be easily accommodated.

3.6 Conditional Exposure Variables

Temporal approaches to residential exposure assessment require simplification of the complexities associated with human behavior / activity patterns that may occur as a function of time and geographic region in and around the home. Further, numerous dependencies (e.g., conditional relationships, correlations) may exist, all of which cannot be accommodated in a practical manner. The patterns of use for pesticides in residential, non-occupational and institutional settings are highly dependent upon location, season, dwelling type and a myriad of other factors that impact the behavior of a potential pesticide user. However, key dependencies that are indicated by existing time-activity surveys, product use surveys and other data sources will be addressed in the CARES residential module.

For example, the observed correlation between body weight and body surface area has been evaluated (Phillips et al. 1993, Burmaster et al. 1994, 1998; Costeff, 1966). An example of a conditional relationship is clothing configurations (what people are wearing during application and reentry of pesticide-treated areas) as a function of climate. This conditional relationship can potentially be addressed in the case of consumer applicators for a variety of products used outside the home based on survey data collected by the Outdoor Residential Exposure Task Force (ORETF). The ORETF survey asked participants to record what clothing was being worn by household member-applicators. In the alpha version of the CARES residential module, clothing configuration options will be provided to the users; however, the user will be required to justify selections for subpopulations in different geographical regions.

Other conditional relationships that will be addressed in the residential module include obvious relationships such as lawn exposures only being relevant for the percentage of home having turf grass, amount of product applied to lawns being proportionate to lawn size, pet care product

exposures only be relevant for the percentages of homes having pets, amount of product applied to pets being proportionate to pet size, etc.

Age/gender/pathway conditional relationships should reflect known behaviors of individuals. Young children may be exposed to pesticide residues due in part to developmental behaviors. For example, videography data suggest that young children engage in more hand-to-mouth activity (potential non-dietary ingestion) than adults. Some national surveys of home and garden pesticide usage suggest that more males than females treat lawns while females are more likely to treat the interior of the house. Consideration of data of these types aid in developing reasonable and realistic exposure and risk assessment scenarios that reflect conditional relationships.

As noted previously, to the extent possible, the assessment of residential, non-occupational and institutional use patterns should characterize seasonal and geographic variations. Although residential uses may not result in residues that are as highly localized as residues in drinking water, these types of uses cannot be assumed to track with the large regional breakouts currently used in the food exposure assessment arena. For instance, a regional food exposure assessment will cover the entire Pacific Northwest region of the U.S. However, the coastal regions of Washington and Oregon are more humid and have a milder temperature regime than would be found in Idaho. Residential uses of pesticides would likely differ considerably between these two areas because of differences in pest pressure even though they are within the same "region." Aggregate and cumulative risk assessments should reflect use patterns and practices on a scale sufficient to capture the variability in pesticide use. In addition, a natural overlay of market share by region may help to direct the assessment on a geographic basis. An example of the incorporation of this type of data into the assessment is the very localized use of temephos for mosquito control in parts of southern Florida. This pesticide should have only limited consideration in the cumulative assessment of other organophosphate pesticides including those used for mosquito control.

A key set of conditional relationships are involved in estimating the probability of co-occurring product use during toxicologically relevant time periods and within and across different geographic locations or regions. For example, the frequency of product application as a function of season during the calendar year, and corresponding pest pressures, in the CARES residential module will be based on empirical survey data from ORETF, REJV and other sources. Additional discussion of the conditional probability matrix associated with product use event allocation during the calendar year is presented in Section VIII.

3.7 Guiding Principles for Conducting Probabilistic Assessments of Residential (Non-Dietary) Exposures

Currently little guidance exists regarding the preparation and conduct of a probabilistic exposure assessment to assess either operator or residential exposures. The United States Environmental Protection Agency (EPA) has developed a policy guidance document on the use of probability analyses in risk assessments (U.S. EPA, Office of Research and Development) and the EPA's Office of Pesticide Programs has issued draft guidance on the use of probabilistic assessments for pesticides (U.S. EPA, Office of Pesticide Programs). Both documents provide sound guidance on the critical area regarding the development of a probabilistic exposure assessment for operators or residential pesticide uses. These documents can provide the foundation for the development of a global guidance document that can provide harmonized principles and guidance for non-dietary probabilistic risk assessments.

The EPA has established eight conditions for acceptance of probabilistic analysis. These conditions are relevant to operator and residential risk assessments as well as dietary

assessments and assessments of exposure to non-pesticidal chemicals in the environment. The eight conditions or guiding principles are:

1. Define the purpose and scope of the assessment,
2. Document the methodology of analysis,
3. Include a sensitivity analysis,
4. Discuss the presence or absence of moderate to strong correlations and dependencies between variables,
5. Include information describing each input distribution and the output distribution,
6. The stability of the central tendency and the higher end of the distribution of the output are to be discussed,
7. Provide a deterministic exposure and risk assessment for comparative purposes, and
8. Assure that those exposure assumptions such a body weights or exposure duration are consistent with the toxicity metrics.

3.7.1 Define the purpose and scope of the assessment

A clear and unambiguous statement of the purpose and scope of the assessment is necessary to define the boundaries of the assessment and analysis of the output. This assessment is important in defining the population of concern for which the exposure assessment is being prepared. The EPA's Office of Pesticide Programs has provided some guidance in this area in regard to probabilistic dietary exposure assessments (U.S. EPA, OPP, 14 Nov 98, U.S. EPA, OPP, 19 January 1999) regarding the defining of highly exposed subpopulations for acute assessments. However no guidance was evident for issues related to operator and residential probabilistic exposure assessments.

A key issue that requires discussion and guidance development revolves around the fundamental differences between the target of concern with an acute (or short-term) assessment and a chronic assessment. With a chronic assessment our interest is focused on the results of multiple exposures over an extended period of time that usually exceeds six months. Here the variability in use practices such as application rates, use of competing products, and use of engineering controls can come into play as one assesses the chronic exposure to a target population.

Contrast this to a short-term assessment where the focus is now on the end result of a single exposure. Here the issue becomes the potential exposure distribution to a homeowner resulting from one potential use. "Either/or" variability is less important as the emphasis is assumed to shift toward defining a "reasonable upper-bound" but plausible individual. In the home setting this may be a person who treats multiple sites around the home during one day. Precedence for this was set in the EPA's first aggregate assessment of non-dietary exposure under the Food Quality Protection Act (FQPA) in which a deterministic non-dietary exposure assessment was prepared for the synthetic pyrethroids using the "flea infestation scenario." Here the scope was defined as an assessment to a homeowner with a flea infestation who would treat the lawn, indoor carpet, and the pet with a synthetic pyrethroid pesticide. This scenario was considered plausible because the labels permit such applications and the risk assessors involved agreed that greater use during a single day was unlikely. Because the deterministic exposure and risk assessment demonstrated adequate safety, further refinement in the assessment was unnecessary. Knowledge of the position of the "reasonable upper-bound" individual will be required to interpret the probabilistic output of a short-term probabilistic exposure assessment. For example, survey data showing that 2% of a product's users will actually treat three separate sites around the home during one day will be necessary to understand and interpret the distribution variability around the exposure to this individual who is already in the upper 2% of users of the product.

3.7.2 Document the methodology of analysis

This guiding principle is really not different from the current situation required during the preparation of deterministic operator or residential non-dietary exposure assessments. The key question in the preparation of any submission is, "Can the reviewer of my document understand what I did, why I did it, and independently reproduce my assessment?" Discussions on the methodology used must include the model and software used to generate the analysis. A corollary of this is that the model must be transparent so that the reviewer can understand the model's manipulation of the input data. An issue that also needs to be addressed in regards to model selection is the use of proprietary models that require the reviewer to expend significant funds to obtain the model for the purpose of independent validation of the submitted exposure assessment. Regulatory agencies must be sensitive to the use of proprietary models that require the regulated community to purchase such models at significant costs.

3.7.3 Include a sensitivity analysis

A sensitivity analysis should be conducted and the results presented and discussed in the analysis of the probabilistic exposure assessment. The sensitivity analysis permits an evaluation of how individual inputs affect the overall exposure distribution. Such an analysis has potential important impacts on the interpretation of the output distribution and defining potential variables for exposure mitigation that may be necessary. An example of the use of sensitivity analysis in an operator exposure assessment is determining that approximately the upper 30% of the distribution have unacceptable risk for a short-term exposure scenario involving open-pour mixing/loading and open-cab tractor application. The sensitivity analysis indicates that the area treated per day is a major determinant in the exposure distribution. Analysis of the use information indicates that the subpopulation treating large areas are custom applicators or large agribusiness operations that primarily utilize closed loading systems and enclosed cab tractors. This use of the sensitivity analysis provides information with important implications for exposure mitigation, allowing the user to identify those characteristics that may be associated with the highest potential exposures and to refine the exposure assessment based on potential mitigation options.

Comments have been provided to the OPP draft guidance document (Sielken, 16 February 1999) emphasizing the importance of the sensitivity analysis in determining if limited data sets or default assumptions are driving the exposure assessment. Such knowledge is critical in the interpretation of the output and decision-making. Such a sensitivity analysis indicates that regulatory decisions may be premature and that a focused effort to refine the limited data or default would be the logical next step.

3.7.4 Discuss strong correlations or dependencies

The presence or absence of moderate to strong correlations or dependencies between input variables is to be included in a submission and discussed. The effects of these correlations or dependencies should also be included. Depending on the scope of the assessment certain correlations will exist such as formulation type and exposure potential. These correlations are important to understand but are fundamental to an assessment of exposure to a population in which several formulations may be utilized. An example is a homeowner applying a granular formulation to the lawn and a liquid formulation of the same active substance to the vegetable garden on the same day.

Certain other correlations or dependencies may exist in the assessment that require linkage to eliminate nonsensical situations. Postapplication exposure is an example where body surface

area distributions and body weights are dependent and must be linked. The absence of linkage would permit the model to randomly select a large body surface area simultaneously with a small body weight or visa versa. Therefore, some dependencies must be linked in the variable selection to avoid errors in the exposure calculations.

3.7.5 Provide information on input and output distributions

Each submission should provide information regarding the selection of the input data used in the probabilistic exposure assessment. Key variables that would be expected to contain distributional data are the exposure data, application rates, area treated, and body weights. Documentation of the source of the information utilized to obtain the distributions for the variable is critical to provide the opportunity to individuals reviewing an assessment. The submission should provide a discussion of the rationale used to select a distribution and the descriptive parameters such as mean, median, and standard deviation that were used to define the selected distribution. Consideration should be given to using the discrete values of a data set in place of a continuous distribution when it is not possible to determine how well the data conform to some theoretical distribution. When a continuous distribution is used that can mathematically continue to infinity, such as a lognormal distribution, the distribution must be truncated. Examples of variables requiring truncation at the upper tail and possibly the lower tail include body weight distributions and exposure distributions. A rationale must be provided as to the justification of the selection of the maximum and minimum values. Such selections can be based on the upper and lower values of the data set or a set number of standard deviations, above and below the mean.

Discussion of the input data sets must include some discussion of the variability and uncertainty surrounding the data sets. The variability is important since it defines the true heterogeneity in the population. Prior experience with non-dietary exposure data has shown that significant variability exists in the exposure potential resulting from the use of pesticide products; this is evidenced by the broad range of exposures to applicators documented in EPA's Pesticide Handlers Exposure Database. Uncertainty refers to the lack of knowledge about specific factors and is an area that has not been routinely addressed in worker and residential non-dietary exposure assessments to date. Uncertainty exists from taking distributions from survey data that inherently have a sampling error. It also comes from systematic errors that may occur from combining similar data into exposure databases in which the data were collected using different sampling techniques. Differentiation between uncertainty and variability is important. Variability is not usually reduced by additional data development whilst uncertainty can be reduced by additional data development.

3.7.6 Discuss the stability of the output distribution

The numerical stability of the output distribution's central tendency and upper tail are important to the interpretation of the output. This process was found useful in the development of the OP Case Study Group's Residential Exposure Model or Rex (FIFRA SAP Meetings, September 26-29, 2000; http://www. epa.gov/scipoly/sap/). During initial model case study simulations significant instability was found in the upper 10% of the distribution. Such instability was determined to result from not truncating the upper end of some of the parametric input distributions. Refinements such as placing bounds on the input distributions provided stability in the model output to beyond the 99th percentile.

The potential selection of upper percentiles for use in acute non-dietary exposure assessments makes an *a priori* discussion of upper tail stability and relevance critical. The EPA has generated significant controversy with its use of the 99.9th percentile of the dietary output distribution for acute risk assessment. It is unlikely that most of the data sets utilized in non-dietary exposure assessments will be of sufficient size to measure the 99.9th percentile of each input variable with

any certainty. Therefore, the 99.9th percentile will incorporate compounded uncertainty that surrounds the upper-ends of each input variable distribution. Decisions regarding the selection of an appropriate percentile for risk assessment must be made in the context of an understanding of the nature of non-dietary exposures and the populations being assessed.

3.7.7 Provide a comparative deterministic assessment

A deterministic exposure or risk estimate gives perspective to the more refined probabilistic assessments. When providing a comparison it is important to note whether the data and exposure methods used in the deterministic and probabilistic assessments were comparable. Unless the two assessments used similar data sets and assumptions a comparison may be difficult. If the two assessments used the same data sets and basic assumptions with the difference being the utilization of parametric or empirical distributions for the input variables, then a comparison of the point estimate with the probabilistic exposure assessment is possible.

Recognizing that single point estimates of exposure are more familiar to risk assessors than parametric or empirical distribution information, the point estimate provides an important frame of reference. Typically in a probabilistic worker exposure assessment the point estimate is around the 70th percentile if the point variables were based on central tendencies and above the 85th percentile if maximum values were used. Such an exercise is important in explaining the effect of multiple conservative assumptions on the final exposure estimate.

3.7.8 Ensure consistency with toxicity metrics

The toxicity endpoints selected for the risk assessment should be consistent with the duration of exposure being modeled. In addition, selection of route-specific toxicity endpoints would reduce some of the uncertainty incorporated into the risk assessment process. For example, evaluating risks from dermal exposures by comparing estimated dermal absorbed doses to a No-Observed-Adverse-Effect-Level (NOAEL) from an oral toxicity endpoint incorporates uncertainty attributed to different metabolic pathways of the active ingredient from the different routes of exposure, and uncertainty associated with the fraction of the dermal exposure that is absorbed versus the oral absorption fraction.

The nature of the toxicity endpoint may also influence the type of input data used in preparing the probability assessment. A developmental toxicity endpoint is relevant to females of childbearing age. In this instance the scope of the assessment could be limited to this subpopulation and distributional data specific to the subpopulation rather than the population as a whole.

3.8 Good Exposure Assessment Practices

Expanding on the previous guidance for probabilistic residential exposure analyses, the following section provides an overview of guiding principles for "good exposure modeling practices" in the context of an exposure assessment in general. The guidance is based in part, on concepts and principles described by Hawkins et al. (1992), the American Industrial Health Council (AIHC, 1994) and EPA (1992 and 1997) regarding "good exposure assessment practices." Good exposure assessment practices incorporate "good exposure mode ling practices," given that exposure modeling represents a core component of the overall exposure assessment process. The use of good exposure modeling practices facilitates providing an acceptable level of documentation, validation and characterization of the variability and uncertainty associated with a given model and how it is used in the context of an exposure assessment.

Exposure assessments are often based on predictive modeling methods, which incorporate the results of a variety of estimated or measured variables, e.g., emission rates, media concentrations (airborne levels, transferability from treated surfaces, etc.), degradation, etc., for the chemical of interest, if available, or for valid surrogates. In some cases, these models are extended beyond estimates of external exposure, to include varying degrees of information and sophistication regarding route-specific absorption, distribution, metabolism and elimination. Further, in the absence of "real-time" personal monitoring data (particularly longitudinal measurements), it is often necessary to integrate the results of multiple "sub-models" to obtain estimates of potential "total exposure" from multiple pathways, routes and/or sources. This integration process can include models that predict source term characteristics (e.g., release/emission rate into residential indoor air, e.g., g/hr), fate and transport processes (e.g., deposition rate of aerosols emitted into the air onto surfaces) and human (receptor) characteristics (e.g., demographic, behavioral, physiological). This process is intended to result in plausible combinations of potential aggregate multi-pathway/multi-route exposures to chemicals as a function of time and space. The major factors in this process can be summarized as follows:

- *Source characteristics* -- e.g., method of application, formulation type, rate of release
- *Fate & transport processes* -- time-related movement and dissipation/degradation of the chemical(s); and
- *Receptor and environmental characteristics* -- demographic, behavioral, physiological, spatial, temporal and environmental factors that determine exposure pathways and routes (and absorbed dose) for a specific subpopulation/location/time

As described in the EPA's Exposure Assessment Guidelines (1992), a tiered approach to exposure assessment and the underlying exposure modeling, provides a means for time-efficient and cost-effective utilization of resources for decision-making purposes. The quality of scientific information/data, the kind and degree of professional judgments/assumptions, and the level of sophistication (e.g., deterministic, point estimates versus probability-based simulation) that are incorporated into tiered exposure assessments and modeling processes should be appropriate to the purpose for which the assessments will be used. The table presented below provides some exemplary model "selection criteria" recommended in the EPA's Guiding Principles for Monte Carlo Analysis (EPA 1997a) to facilitate appropriate matching of the exposure assessment's objectives to the capabilities and degree of uncertainty provided by available models.

Some Considerations in the Selection of Models

- appropriateness of the model's assumptions *vis-à-vis* the analysis objectives
- compatibility of the model input/output and linkages to other models used in the analysis
- the theoretical basis for the model
- level of aggregation, spatial and temporal scales
- resolution limits
- sensitivity to input variability and input uncertainty
- reliability of the model and code, including peer review of the theory and computer code
- verification studies, relevant field tests
- degree of acceptance by the user community
- friendliness, speed and accuracy
- staff and computer resources required

Deterministic exposure assessments intended for "screening-level" purposes will tend to overestimate potential exposures because of the use of conservative assumptions and values for multiple variables. The combination of multiple conservative assumptions and overly simplistic models often results in exposure estimates that are in the high-end (i.e., greater than the 95th percentile) of the actual exposure distribution or even higher than the maximum expected value. The latter estimate is referred to as a Theoretical Upper-Bound Estimate (TUBE). Thus, deterministic (point estimate) exposure assessments intended for "screening-level" purposes will often be significantly influenced by uncertainties and assumptions that bias towards "high-end exposures" such that the resulting estimate represents either a theoretical upper-bound or an upper percentile of the actual distribution of potential exposures. In the context of a "tiered approach" to exposure assessment, if conservative screening-level estimates are "safe," then the assessment may not require additional refinement. However, if the screening-level assessment suggests that exposure levels may not be considered "safe," then the assessor should carefully evaluate the modeling approach used and should consider the use of more realistic assumptions, alternative models, data quality objectives and appropriate uncertainty analyses. Following this, the assessor should consider the use of more advanced analysis methods (e.g., probability-based methods, more sophisticated/rigorous models) and focused data collection efforts to facilitate the development of a modeling approach that will result in estimates that are more representative of the actual exposure distribution. In the case of data collection, additional studies may be justified by the reduction in uncertainty of the model estimates.

Regardless of the level of sophistication, an exposure model(s) used for a given purpose/situation should be accompanied by sufficient documentation and reporting, so that the assumptions, underlying mathematical and statistical procedures, data quality and transformations, input and output, validation procedures, minimally required data, and intended use and limitations are transparent and clearly defined. These are essential components of good exposure modeling practices. These practices ensure an appropriate level of understanding can be achieved by users and individuals making decisions based on the results of a given model. The following components have been adapted, in part, from recommendations of the AIHC (1994) to provide adequate documentation for models used in the context of exposure assessments:

PROTOCOL / USER'S GUIDE

Every exposure assessment should have a protocol written before its initiation. The protocol should first state the purpose of the exposure assessment and the model(s) used therein. It should also include the variables to be evaluated (i.e., a clearly defined assessment endpoint), the level of detail needed, how uncertainty will be addressed, and the relationship of uncertainty to the conclusions that may be drawn. Further, the protocol should describe each of the other principles of practice noted below in sufficient detail so that the assessment is clearly adequate for the purpose. Similarly, exposure models used in assessments should be accompanied by adequate documentation regarding procedures for using the model, the minimum information that is required as input data and software references and computer system requirements.

GENERAL DESCRIPTION OF EXPOSURE MODEL

The model or set of models used in the exposure assessment to relate the presence of a substance to human exposure/absorbed dose should be stated. The model's general description should provide enough detail so that the user or reviewer understands the input variables, underlying mathematical algorithms and data transformations and output/results, such that the model can be easily compared to other alternatives. The basis for each model, whether deterministic, empirical, or statistical, should be described. The statement of the model should include which variables are measured and which are assumed. A description should be provided of how uncertainty in parameters and the model itself are to be evaluated and treated.

DETAILED DESCRIPTION OF MODEL INPUTS & OUTPUTS

Descriptions of model input variables, e.g., data collection methods, analytical methods, and data transformation procedures, should be stated. Further, appropriate statistical measures should be included for both input variables and model results (output) to facilitate qualitative and quantitative evaluations of uncertainty and appropriate interpretations.

EXPOSURE MODEL VALIDATION

Validation of an exposure model involves two primary processes: 1) verifying the underlying mathematical and statistical procedures and 2) evaluating the model's overall predictive accuracy and precision through comparisons to relevant empirical data. In the absence of adequate empirical data, statements should be made regarding the absence of model validation studies and any plans for future validation should be described.

QUALITY ASSURANCE PRACTICES

Procedures should be established and recorded to ensure that an acceptable quality level is associated with input data extraction and use, model execution and validation procedures. The procedures described by the EPA's Good Automated Laboratory Practices (GALP) should be considered, where applicable.

ARCHIVING

Model protocol/procedures, inputs and outputs, and other relevant information/documents should be retained so that they are retrievable for a specified period.

In addition to the exposure model "documentation components" noted above, AIHC (1994) and EPA (1997) have recommended general principles for exposure assessments, particularly those based on Monte Carlo simulation, that are also relevant for simulation models used as part of the overall assessment process. The EPA has also issued guidelines for data quality assessment relevant to model documentation. Some of these principles are listed below; more details are provided in EPA (1997) and AIHC (1994; see also Burmaster and Anderson, 1994).

1. Describe all formulae and validation procedures;
2. Calculate and present deterministic point estimates (based on regulatory agency recommended methods) in contrast to distributional representations;
3. Present the results from univariate (or multivariate) sensitivity analyses of the deterministic calculations to identify the inputs suitable for probabilistic treatment, and then discuss any variables not included in the sensitivity analysis;
4. Consider restricting the use of probabilistic techniques to the most significant exposure pathways/routes;
5. Provide detailed information on the input distributions selected;
6. To the extent possible, describe how the input distributions (and their parameters) capture and represent both the variability and the uncertainty in the input variables;
7. Use measured data to inform the choice of input distributions whenever possible, after making sure that the data are relevant and representative of the demographic, spatial and temporal situation;
8. Discuss the methods and report the goodness-of-fit statistics for any parametric distributions for input variables that were fit quantitatively to measured data;
9. Discuss the presence or absence of moderate to strong correlations between or among the input variables;
10. Provide detailed information and graphs for each output distribution;
11. Perform probabilistic sensitivity analyses for all of the key inputs represented by a distribution in the Monte Carlo analysis in such a way as to distinguish the effects of variability from the effects of uncertainty in the inputs;

12. Investigate the numerical stability of the (1) central moments (mean, standard deviation, skewness, and kurtosis) and (2) the tails of the output distribution of the simulation;
13. Present the name and the statistical quality of the random number generator used; and
14. Discuss the limitations of the methods and of the interpretation of the results; include the source, the nature, and the possible effects of any unresolved sources of bias not explicitly included in the analysis, and indicate where additional research or measurements could improve the analysis; a sensitivity analysis should be performed to assess the influence of the input parameters on the exposure assessment; it can also be used to illustrate the effect of subjective judgments on the exposure assessment (including Delphi-derived information).

Finally, validation of the results of the modeling can be compared to concurrent biomonitoring data for a surrogate chemical. For example, stochastic simulations based on the comparison of available exposure measurements such as surface residue transferability and passive dosimetry can be compared to biomonitoring results in individuals following broadcast carpet treatment in homes. These comparisons are usually based on data for adults or adult volunteers simulating the activities of infants and children (e.g., playing with blocks, crawling on the floor).

4. Sources of Reliable Information/Data

4.1 Ideal Matrix of Integrated Data Sources

The "ideal" matrix of integrated data sources includes the following:

- An electronic database of pesticide label information, market share proportions and predicted product lifespans indexed by EPA registration number;
- An electronic database of temporal (multiple years to reflect pest population dynamics) product use survey diaries for U.S. households (indexed on EPA registration number) that are statistically weighted for a variety of "matching" strata across and within national, regional (based on climate and pest incidence), and urbanization zones;
- An electronic database of matched human and residential exposure factors;
- An electronic database of matched human time-activity data;
- An electronic database of matched exposure monitoring data (scenario-specific passive dosimetry data with concurrent environmental media measurements and biological monitoring data) (Adgate et al, 1998); and
- An electronic database of matched population-based biomonitoring data for a variety of index chemicals to compare to aggregate and cumulative model simulation results;

The “ideal” data matrix or meta data are stratified and matched in an identical manner for temporal, demographic, and geographic characteristics, supporting either deterministic or stochastic modeling that can be temporally, demographically and spatially resolved. Given an absence of the above idealized suite of integrated data, data sources (many of which are described below) require statistical matching criteria and back casting and forecasting estimation methods to achieve a credible approximation or characterization of residential exposures to a reference population across time (e.g., calendar year), stratified to common denominators with respect to demographic and geographic (spatial) characteristics. The section that follows presents summary information regarding currently available data sources and their role in the CARES residential module.

4.2 Currently Available Data Sources, Relevant Meta Information, and Their Role in the Alpha CARES Residential Module

4.2.1 Public Data Sources

PESTICIDE HANDLERS EXPOSURE DATABASE (PHED)

Exposures associated with application of consumer products containing pesticides in and around the home can be estimated using data from the EPA database known as the Pesticide Handlers Exposure Database (PHED) developed by the Office of Pesticide Programs. The primary source of exposure monitoring data in PHED is industry-sponsored studies. Normalized exposures for the relevant application scenario(s) addressed in PHED have been summarized by EPA (see Appendix D) based on measured values for surrogate chemicals. PHED is commonly used by registrants and government agencies to supplement and validate field exposure studies, and as

an evaluation tool for analysis of field exposure data. PHED contains over 1,700 records of data on measured dermal and inhalation exposures, as well as accompanying data on parameters that may affect the magnitude of exposures. Relevant data can also be extracted from PHED and used in probabilistic analyses. ORETF (see discussion below) has also developed proprietary mixer/loader/applicator exposure data for a variety of outdoor residential products, which can support deterministic or probabilistic assessments.

NATIONAL HUMAN ACTIVITY PATTERN SURVEY (NHAPS)

The NHAPS study was designed to be used in the assessment of personal exposure to pollutants in air and water systems with which people in the United States come into contact throughout their typical daily routine. The complete data-collection methodology (including example questionnaires) can be obtained from EPA's Office of Research and Development. Carried out between October 1992 and September 1994, NHAPS is an extensive data resource, containing geographic (EPA region, U.S. Census region, state, zip code, etc.) socioeconomic (gender, age, race, education, etc.) and time/season (quarter, month, day of week, etc.) information on 9,386 different respondents (*i.e.*, respondents were never re-interviewed in the study) distributed over 8 seasonal quarters throughout the entire nation. Table 1 provides a summary of the NHAPS features.

Table 1 Summary of the National Human Activity Pattern Survey (NHAPS) Features

Characteristic	Description
Dates of Data Collection	October 1992 through September 1994 (8 three-month seasonal quarters)
Data Collection Instrument	Telephone interviews using a Random-Digit Dial (RDD) method and Computer Assisted Telephone Interviewing (CATI)
Data Types	(1) 24-hour diaries with beginning and ending times at minute resolution, (2) demographic questions, and (3) 175 follow-up questions on medical background, housing characteristics, and exposure to chemicals
Number of Total Respondents	9,386
Response Rate	63% (65% for last seven quarters; first quarter was 46% from difficulties in procedure and training schedules)
Cooperation Rate	Excluding those respondents not contacted (or because they were not interviewed for other factors) the cooperation rate was over 75%
Geographic Coverage of Respondents	The 48 contiguous United States, *i.e.*, excluding Alaska and Hawaii, by state, EPA region, U.S. Census region, telephone area code, working postal zip code, and residential postal zip code
Socio-economic Coverage of Respondents	Ages 0 to 93, gender, race, education, employment status, etc.
Emphasis of 175 Follow-up Questions	Personal exposure to contaminants in air and water from household sources
24-Hour Diary Location Categories	82 categories arranged by Own House, Friend's/Other's House, Traveling, Other Indoor, and Other Outdoor

Characteristic	Description
24-Hour Diary Activity Categories	91 categories arranged by Non-Free Time (Paid Work, Household Work, Child Care, Obtaining Goods/Services, Personal Care) and Free Time (Educational, Organizational, Social, Recreational, Communications)
Diary Variables for each Microenvironment	date (month, day and year), starting time, ending time, elapsed time (duration), presence of a smoker, heavy breathing activity (yes or no), location category, and activity category
Total Diary Records (Microenvironments)	157,234
Number of Different Microenvironments Per Person	Range = 1 to 59; Mean = 17

Detailed minute-by-minute 24-hour diaries were collected for each respondent containing 82 different possible locations (Residence-Kitchen, Residence-Garage, Office, School, Bar-Restaurant, Automobile, etc.), 91 different activities (Cleaning, Food Preparation, Bathing, etc.), and whether a smoker was ever present or not. Additionally, respondents were asked some fraction of 175 exposure-related follow-up questions (focused on air and water pathways) on specific pollutant sources (paint, glue, etc.) or prolonged background activities (gas heaters, wood smoke, etc.).

The interviews began with random selection of a respondent from the selected household. Saturdays and Sundays were over-sampled to insure an adequate weekend sample size. The interviews lasted an average of 23 minutes with most beginning between 6:00 and 9:00pm. If the respondent chosen was a child too young to provide responses, an adult (18 and older) in the household gave a proxy interview. Since either an adult or a child could have been chosen from the household, and their probability of selection depends on the number of adults/children in the household and the criteria used for selection, a compensating weight was created. This weight was combined with the probability of household selection based on the number of non-business phones in each household (Table 2) to produce the weighting variable (WEIGHT). In this report WEIGHT was used to calculate a joint frequency table across various subgroups (age, gender, day of week, season), which was then used to create an overall weighting variable WEIGHT4 that improved the representativeness of the NHAPS sample with respect to these subgroups using 1990 Census data.

Each of the 9,386 persons interviewed was asked to recount their entire daily routine from midnight to midnight on the day preceding the day that they were interviewed. The beginning and ending times of each microenvironment in these diaries were recorded with a time resolution of one minute in the “diary” data file (Table 2). Together, the set of beginning and ending times for each microenvironment spanning one day comprise a comprehensive, sequential account of a person’s locations, activities, and proximity to smokers.

Table 2 Description of the two NHAPS Data Files

File Name	Description
MAIN.XXX 455 Variables 9,386 records	Main file containing household and identification information (respondent ID #, length of interview, etc.), demographic background information (region, gender, age, etc.), temporal information (day of week, month, year, etc.), responses to the 175 exposure follow-up questions, and frequencies in each location and activity diary category for all 9,386 respondents.
DIARY.XXX 16 variables 157,234 records	Diary file containing multiple-record 24-hour diaries for each of the 9,386 respondents. The variable set of records corresponds to all the different microenvironments each respondent visited and include the location, activity, and smoker-present codes, and the beginning and ending times for each microenvironment.

Note: Each file has a variable containing a unique identification code for each respondent that can be used to link the information in the two files.

The NHAPS study did not collect any minute-by-minute diary data on the respondents' proximity to specific pollutant sources (besides a smoker). For example, there are gaps in the source type such as cleaning agent, pesticide, solvent, or stove, and in their method of use. Minute-by-minute categories for housing characteristics such as windows open or heat on, and types of exercise such as running or hiking are also missing.

After the 24-hour diaries were collected each respondent was asked follow-up questions on personal exposure, household characteristics, and medical background, which were stored in the "main" data file. The follow-up questions were placed on questionnaires (version A, B or both) and given to a nationally representative number of respondents (4,723 for A only and 4,663 for B only). The main file also contains all the demographic, respondent identification, and time variables (e.g., respondent ID #, interview date, time interview began, duration of interview, number of phones in household, type of interview, age, race, etc.). In addition to "yes or no" questions on specific exposure issues (e.g., do you use a humidifier?, does your house have a basement?, etc.), many of the follow-up questions concerned the frequency and duration of exposure events (e.g., how many cigarettes do you smoke?, for how many minutes did you take a shower?, etc.).

The microenvironment is the basic building block of NHAPS diaries and is defined by the time period that some combination of exposure events (an activity occurring in a particular location) -- called an *episode* -- occurs. Analyses using NHAPS data have typically split the microenvironmental concept into a *microenvironmental-factor* component (location, activity, and smoker-present categories by themselves or in combination) and a time component (beginning and ending times over the 24-hour diary day or -- for time-of-day analysis -- equal time intervals such as a minute or 3-hours). See Appendix E for a discussion of the microenvironmental concept and its use in human exposure modeling.

In the context of the CARES residential module, time spent in relevant microenvironments for various age groups, seasons of the year, geographic regions (e.g., time spent indoors by different age/gender subgroups, time spent outdoors for different age/gender subgroups, time spent by children playing outdoors, time spent by children on grass, time spent in living room/family room, etc.; see examples in Table 3 below) will be extracted from NHAPS as percentile distributions and used for the "duration" input variables in scenario-specific algorithms where they occur (see Appendix C). For example, percentile distributions for time spent indoors during a 24-hour period can be used for estimating potential inhalation exposures associated with a 24-hour, time-weighted average indoor air concentration (across multiple indoor zones, or rooms) for a given airborne pesticide. In the case of the dermal and incidental ingestion routes, duration (hr) input variables used with contact rate metrics (e.g., transfer coefficients (cm^2/hr); hand-to-mouth events/hr) will be based on NHAPs percentile distributions for time spent in relevant

microenvironments and other data sources (e.g., children's videography). For, example the duration input variable associated with reentry onto a treated lawn, can be based on an age-specific 50th percentile value for time spent on grass or a percentile distribution (in the case of probabilistic modeling). Similarly, for an indoor fogger exposure scenario, reentry duration could be based on the reported time spent in family/living room areas of homes, or more conservatively, on the reported non-sleeping time indoors as reported by NHAPs respondents.

As noted above, supplemental time-activity data sources (children's videography studies) will be used for specific purpose such as percentile distributions for frequency and duration of hand-to-mouth and object-to-mouth activities for children in relevant developmental age groups (Groot et al. 1998, EPA 1999b, EPA 2000).

Table 3 The Weighted Percentages of Time Spent in Each Location on the Diary Day Across Various Subgroups*

Percentage	Residential - Indoors	Residential - Outdoor	In Vehicle	Near Vehicle	Other Outdoor	Office/ Factory	Mall/Other Store	School/ Public Bldg.	Bar/ Restaurant	Other Indoor
Overall	68.73	3.69	5.52	1.7	2.19	5.39	2.26	6.61	1.84	2.07
Males	64.79	4.49	5.94	2.49	2.96	6.46	1.85	6.53	1.94	2.55
Females	72.47	2.93	5.12	0.94	1.45	4.38	2.65	6.68	1.75	1.63
0-4	84.08	5.38	3.14	0.56	0.96	0.05	1.39	3.45	0.57	0.42
5-7	67.81	5.05	4.29	1.41	2.83	0.18	1.15	15.33	0.76	1.18
17-64	64.71	2.93	6.43	2.06	2.33	8.42	2.77	5.19	2.43	2.74
65+	80.84	4.48	4.17	0.99	1.27	1.18	1.89	2.83	1.27	1.07
Northwest	68.77	3.25	5.57	1.78	2.02	5.9	2.34	6.66	1.65	2.05
Midwest	68.22	3.41	5.62	1.51	2.26	5.27	2.05	7.24	2.18	2.24
South	68.75	4.03	5.57	1.64	2.05	5.49	2.29	6.63	1.64	1.91
West	69.24	3.89	5.25	1.93	2.48	4.88	2.4	5.77	1.96	2.19
Weekday	66.91	3.12	5.35	1.89	1.87	7.02	2.15	7.86	1.65	2.17
Weekend	73.26	5.12	5.93	1.2	2.97	1.34	2.54	3.5	2.31	1.84
Winter	71.2	1.71	5.34	1.45	1.27	5.37	1.95	7.48	1.97	2.24
Spring	66.76	5.33	5.76	1.67	2.33	5.5	2.29	6.77	1.77	1.85
Summer	67.27	5.18	5.39	1.89	3.42	5.44	2.4	4.98	1.8	2.22
Fall	69.68	2.54	5.57	1.77	1.72	5.26	2.41	7.21	1.83	1.99

*Subgroups are for gender, age, U.S. Census region, day of week, and season.

NATIONAL HOME AND GARDEN PESTICIDE USE SURVEY (NHGPUS)

The NHGPUS is a cross-sectional survey of the uses of pesticides in and around homes in the U.S. sponsored by the EPA. Research Triangle Institute located in North Carolina conducted the survey from August to September 1990. The survey was designed as a national, probability-based sample of households with interviews conducted in person at the sample residences. The dwellings in the target population are housing units, which are defined by the U.S. Census as a room or groups of rooms occupied or intended for occupancy as separate living quarters in which the occupants: 1) live and eat separately from any other persons in the building and 2) have direct access from the outside of the building or through a common hall. The survey included the 48 coterminous States and the District of Columbia that are occupied as primary residences (a person's primary residence is defined as the home where the person lives for half the year or more). The survey excluded institutions, group quarters (housing units occupied by 10 or more unrelated family units), military reservations and Indian reservations.

The following types of data were collected by the NHGPUS regarding use of pesticides by the households in the target population (pesticides that were used solely for crops or livestock grown for sale were excluded from consideration):

1. Which pesticides were used;
2. What were they used for;
3. How often were they used;
4. How they were applied, including safety precautions;
5. How unused portions were stored and disposed of;

6. How product containers were disposed of;
7. How child resistant packaging was used;
8. How effective the pesticides were judged to be; and
9. Which pests were major problems (either treated or untreated).

Most data were collected for a 12-month reference period (on a recall basis) ending on the date of the interview. Because pesticides tend to be used more in the summer than during the winter, data collection was performed late in the summer (August and September 1990) to temper the effects of these limitations.

The NHGPUS was not designed to collect quantitative usage data (i.e., estimates of aggregate quantities of pesticides actually used for a specific purpose over a period of time). However, the frequency of application data collected in the NHGPUS are helpful in some aspects of product use event allocation over time based on recall estimates provided for frequency of and intervals between applications.

The sampling design for the NHGPUS can be summarily described as a stratified, three-stage probability sampling approach. The areas selected at the first two stages of sampling were selected with probabilities proportionate to estimates of the numbers of housing units currently in defined areas. Fifty-eight sample counties located in 29 different States were selected at the first stage of sampling. Approximately five subcounty areas defined by Census blocks and enumeration districts were selected at the second stage of sampling within each sample county for a total of 298 sampled subcounty areas, called sample segments. A sample of 2,674 housing units were selected, of which 2,447 housing units were eligible for the NGHPUS (i.e., occupied primary residences). Of these 2,447 eligible households, 2,078 participated in the survey for a response rate of 84.9 percent (2,078/2,447). Because of the high response rate, the potential for non-response bias affecting the survey statistics is low.

Appendix F provides selected tables from the NHGPUS reports (RTI 1992a, 1992b, 1992c, 1992d). Table 1.1 in Appendix F, for example, provides the percentage of homes (weighted form the overall U.S.) that are in urban versus rural areas, have private lawns, swimming pools, fruit and nut trees, engaged in growing vegetables, and engaged in growing roses. The percentages can be used for conditional probability sampling and as part of the vector of individual characteristics in the CARES residential module (see Section VI). Percentages of households in different U.S. Census regions are presented in Table 2.3 of Appendix F. Table 2.37 in Appendix F presents the percentage of households using products with specified frequencies by type of pesticide and site of application.

It is important to recognize that the NHGPUS was designed to provide defensible national inferences, not regional inferences. Regional inferences would require a much larger sample size. A sample of approximately 30 or more counties per region would be necessary. Because the NHGPUS is based on a sample of 60 counties, no more than limited inferences for two regions that each contains approximately 30 counties are supported.

EXPOSURE FACTORS HANDBOOK (EFH)

The EPA's Exposure Factors Handbook (EFH) is currently available on CD ROM (EPA/600/C-99/001; February 1999). The National Center for Environmental Assessment (NCEA) of the Office of Research and Development (ORD) prepared the handbook to address factors commonly used in exposure assessments. The handbook was first published in 1989 in response to requests from many EPA Program and Regional offices for additional guidance on how to select point values (e.g., central tendency estimates) or use distributions in deterministic and probabilistic exposure simulations, respectively.

The current EFH includes exposure factor data and recommendations for the following subject areas:

1. Guidance regarding characterization of variability and uncertainty;
2. Drinking water intake;
3. Soil ingestion and pica;
4. Inhalation-related factors (e.g., activity-level-specific inhalation rates);
5. Dermal-related factors (e.g., body part surface areas, soil adherence)
6. Body weight distributions;
7. Life expectancy;
8. Fruit and vegetable intake;
9. Fish and shellfish intake;
10. Meat and dairy product intake;
11. Grain product intake;
12. Intake rates for various home produced food items;
13. Breast milk intake;
14. Time-activity factors and population mobility;
15. Consumer product-related exposure factors (e.g., frequency of use of household solvents, spray paint usage by gender); and
16. Residential building characteristics (e.g., room volumes, air exchange rates).

Tabular data from the EFH will be used in the CARES residential module for general and scenario-specific input variable values (point estimates and distributions) where relevant. The source of the data used will be documented as part of the CARES residential module quality assurance features.

CHILD-SPECIFIC EXPOSURE FACTORS HANDBOOK (C-SEFH)

EPA (ORD) has recently developed a draft "Child-Specific Exposure Factors Handbook" (http://www.epa.gov/nceawww1/csfh2.htm). Appendix G provides the draft introduction section the handbook, which includes the table of contents. The C-SEFH was developed by EPA's ORD, NCEA, in part, as the result of the April 1997 "Executive Order to Protect Children from Environmental Health Risks and Safety Risks" issued by President Clinton. The handbook is intended to support EPA's efforts to improve exposure and risk assessments for children. The handbook is a compilation of available data from a variety of sources. Most of these data in the C-SEFH have been described in detail in the EPA EFH, but data that have been published subsequent to the release of the EFH are also presented.

The introductory chapter to the C-SEFH (see Appendix G) provides useful considerations and approaches for reviewing exposure factor data sources and recommending point estimates and distributions for use in exposure assessments involving children. Considerations include level of peer review, accessibility, reproducibility, focus on the exposure factor of interest, data pertinent to the U.S., primary data availability, current information, adequacy of data collection period, validity of approach, representativeness of the population, variability in the population, minimal (or defined) bias in study design, and minimal (or defined) uncertainty in the data. For purposes of illustration, Chapter 6 of the C-SEFH is included in Appendix G; this chapter addresses factors for estimation of potential exposures to environmental contaminants such as pesticides from non-dietary ingestion pathways including hand-to-mouth and object-to-mouth activities. Data from the C-SEFH will be used in the CARES residential module in a manner similar to data from the EFH; i.e., for general and scenario-specific input variable values (point estimates and distributions) where relevant.

NATIONAL HUMAN EXPOSURE ASSESSMENT SURVEY (NHEXAS)

The National Human Exposure Assessment Survey (NHEXAS) was developed by the Office of Research and Development (ORD) of the U.S. Environmental Protection Agency (EPA) early in the 1990s to provide critical information about multipathway, multimedia population exposure distribution to chemical classes (http://www.epa.gov/her1/nhexas.htm). The first phase consisted

of three pilot studies with the objectives of (1) evaluating the feasibility of NHEXAS concepts, methods, and approaches for the conduct of future population-based exposure studies; (2) evaluating the utility of NHEXAS data for improved risk assessment and management decisions; (3) testing the hypothesis that the distributions of exposure given by modeling and extant data do not differ from the measurement-based distributions of exposure; (4) defining the distribution of multipathway human exposures for a relatively large geographic area; and (5) stimulating exposure research and forging strong working relationships between government and nongovernmental scientists. NHEXAS began before the enactment of the Government Performance and Results Act (GPRA), which was written to ensure accountability in the use of resources. Thus, a "new" objective was added in the form of the hypothesis: NHEXAS approaches can be used to develop a "GPRA Report Card" on the efficacy of EPA's regulations to reduce exposure.

NHEXAS studies conducted to date include approximately 550 people in three areas of the United States (http://www.epa.gov/her1/nhexas.htm). The data collection phase of NHEXAS was completed recently, the initial data analyses are being published in the Journal of Exposure Analysis and Environmental Epidemiology (JEAEE) and the principal investigators have additional analyses under way. Appendix H presents a NHEXAS Workshop report that has the goal of obtaining a wide range of expert opinion on which research projects best would ensure the utility of the NHEXAS data. The report provides an overview of the workshop, and as described therein, the workshop projects will be used as information in developing the ORD strategy for analysis of the NHEXAS pilot data.

In the context of the CARES residential module (and overall CARES aggregate and cumulative model), NHEXAS data, when quality assured, peer reviewed data are available, may serve to assist in evaluating CARES simulation output.

MISCELLANEOUS SOURCES

The Organophosphate Case Study Group's Non-Dietary Committee has reviewed a substantial number of published (scientific, peer-reviewed journals and government agency reports) applicator and post-application exposure monitoring studies relevant to a variety of residential exposure scenarios. These reviews, which were conducted using a Standard Operating Procedure, can be used in the context of the CARES residential module for identifying and documenting scenario-specific input variable values, where relevant.

4.2.2 Proprietary Data Sources

OUTDOOR RESIDENTIAL TASK FORCE (ORETF)

Over the past several years the Outdoor Residential Exposure Task Force (ORETF) has developed data to improve the characterization of residential exposure to turf pesticides. These data and analyses include:

1. Development of methodology for the collection of transferable turf residue (TTR) data; Analysis of standard Jazzercise routines using the Stanford videography techniques;
2. Analysis of children's activity patterns on turf using computer techniques developed at Stanford University to quantify the videotapes of children playing outdoors for frequency and duration of contact;
3. Analysis of TTRs and Transfer Factors (TFs) from four proprietary Jazzercise turf reentry studies;
4. Measurement of exposures of professional Lawn Care Operators and homeowners during the mixing, loading and application of residential pesticides to turf, gardens and ornamentals; and

5. Collection of survey information on residential use and application of outdoor pesticides.

The proposed uses of these data in the CARES residential module are as follows:

- TTR data. Day 0 (day of application) turf transferable residues, expressed as a percentage of the application rate have been shown to be comparable within a given formulation type (e.g., liquid, granular); thus, the "formulation-type-specific" range of TTR values can be used as surrogates for predictive modeling.

- Dermal Post-Application TFs (or Transfer Coefficients, i.e., TCs). Transfer Factors or Coefficients derived from the ratio of "Jazzercize"-based, body-part-specific dermal loading, as measured on human volunteers wearing passive dosimeters, to the concurrent TTRs measured during these studies result in distributions of TFs or TCs that can be used as surrogates to estimate Day 0 (day of application) post-application dermal exposures (Jazzercize-equivalent exposures represent a likely upper-bound dermal exposure due to the high surface contact involved in the choreographed routine).

- Consumer Mixer/Loader/Applicator Unit Exposure Metrics (µg/lb active ingredient handled). Exposure monitoring studies involving products used on treated lawns and ornamentals provide distributions of Mixer/Loader/Applicator unit exposure values that can be used in a surrogate manner, categorized by formulation type and method of application, for estimating potential homeowner exposures.

- Outdoor Lawn & Ornamental Product Use Survey - The Outdoor Residential Pesticide Product Use Survey data are organized in the following six data files:
    1. Demographics
    2. Applicator: Professional/Landlord
    3. Applicator: Household member/Relative/Neighbor
    4. Application: General
    5. Application: Equipment Used
    6. Application: Clothing/Protection Worn

The organization in infoscientific.com's NOTITIA™ is based on three different categories: Demographics-related, Applicator-related and Application-related. The Demographics-related category has one data file (number of records = 2709), which provides demographic information on the 2709 respondents who participated in the three "waves" (each wave represents a different time period during which a two month recall questionnaire was administered; i.e., product use from April to May, June to July, and August to September).

The Applicator-related category has two data files, one related to hired professional or landlord as applicators and the other related to relative, neighbor or household member as applicators. The Applicator: Professional/Landlord data file has 886 records and the Applicator: Relative/Neighbor/Household member data file has 1889 records.

The Application-related category has three data files, each with 4934 records. The Application: General data file has general application-related information. The Application: Equipment Used data file has information related to the type(s) of equipment used during each application. And, the Application: Clothing/Protection Worn data file has information related to the type(s) of clothing and protection worn during each application.

Information from the Gallup Poll, provided to the National Gardening Association, is organized in a separate data file. This information is based on 1522 respondents and it specifically provides data on garden sizes.

Demographic information categories associated available from the survey are shown in Table 4. Other data file meta information is included in help files within the database; information categories relating to clothing configuration is presented in Table 5.

Table 4 ORETF Product Use Survey: Demographic Information Categories.

Variable	Description
ID	Respondent's Identification Number (as specified in survey)
County	Respondent's Country (United States / Canada)
State	Respondent's State (US only)
Region	Respondent's Region (6 in United States, 3 in Canada)
Wave	Survey Wave (1 = April & May, 2 = June & July, 3 = August & September)
Hired Professional	Whether person who applied product was a Hired Professional
Landlord	Whether person who applied product was a Landlord
Relative	Whether person who applied product was a Relative
Neighbor	Whether person who applied product was a Neighbor
Household Member	Whether person who applied product was a Household Member
Residence	Respondent's Type of Residence
Urban	Whether Respondent's Residence in Urban, Suburban or Rural setting
Number of Children	Number of Children less than 18 years of age in Respondent's Household
Age (1st child)	Age of 1st child over 18
Age (2nd child)	Age of 2nd child over 18
Age (3rd child)	Age of 3rd child over 18
Age (4th child)	Age of 4th child over 18
Age (5th child)	Age of 5th child over 18
Age (6th child)	Age of 6th child over 18
Age (7th child)	Age of 7th child over 18
Age (8th child)	Age of 8th child over 18
Age	Respondent's Age
Gender	Respondent's Gender
Years in School	Number of years of School Respondent completed
Occupation	Respondent's Occupation
Weighting Factor	Survey Weights (to translate data for entire population)

Table 5 ORETF Product Use Survey: Information Categories Regarding Clothing/Protection Worn During Application.

Variable	Description
ID	Respondent's Identification Number (as specified in survey)
Relative	Whether applicator was a Relative
Neighbor	Whether applicator was a Neighbor
Household Member	Whether applicator was a Household Member
Product Type	Type of pest control product applied
Site Type	Site in respondent's outdoor residence that was treated with pest control product
Application ID	Application ID distinguishes "row" data when Respondent ID, Product Type, and Site Type are the same
Number of Clothing	Number of different types of clothing worn while applying product
Hat/Cap	Whether applicator wore Hat/Cap (Head)
Goggles/Safety Glasses	Whether applicator wore Goggles/Safety glasses (Head)
Dust Mask	Whether applicator wore Dust Mask (Head)
Head: Don't Know	Whether applicator did not know what was worn on the Head
Shoes/Sneakers	Whether applicator wore Shoes/Sneakers (Feet)
Boots	Whether applicator wore Boots (Feet)
Sandals	Whether applicator wore Sandals (Feet)
Socks	Whether applicator wore Socks (Feet)
Feet: Nothing	Whether applicator wore Nothing (Feet)
Feet: Other	Whether applicator wore Other (Feet)
Feet: Don't Know	Whether applicator did not know what was worn on the Feet
Rubber Gloves	Whether applicator wore Rubber Gloves (Hand)
Leather Gloves	Whether applicator wore Leather Gloves (Hand)
Cloth Gloves	Whether applicator wore Cloth Gloves (Hand)
Hand: Other	Whether applicator wore Other (Hand)
Hand: Don't Know	Whether applicator did not know what was worn on the Hand
Short Sleeves Shirt	Whether applicator wore Short Sleeves Shirt (Upper Body)
Tank Top	Whether applicator wore Tank Top (Upper Body)
Long Sleeves Shirt	Whether applicator wore Long Sleeves Shirt
Upper Body: Swimsuit	Whether applicator wore Swimsuit (Upper Body)
Upper Body: Nothing	Whether applicator wore Nothing (Upper Body)
Upper Body: Don't Know	Whether applicator did not know what was worn on the Upper Body
Shorts	Whether applicator wore Shorts (Lower Body)
Long Pants	Whether applicator wore Long Pants (Lower Body)
Dress/Skirt	Whether applicator wore Dress/Skirt (Lower Body)
Lower Body: Swimsuit	Whether applicator wore Swimsuit (Lower Body)
Lower Body: Don't Know	Whether applicator did not know what was worn on the Lower Body

NON-DIETARY EXPOSURE TASK FORCE (NDETF)

Passage of the Food Quality Protection Act in 1996 (FQPA) in the United States has increased the importance of quantitative characterization of indoor residential exposure to pesticides. Due in part to the demands of FQPA, the Non-Dietary Exposure Task Force (NDETF), government agencies and the general scientific community have initiated research programs to develop relevant data to produce estimates of potential residential exposure (e.g., dermal, hand-to-mouth-based incidental ingestion) (Barnes, 1990; Camann et al 1995a, 1995b, 1996; Davis, 1995; Fenske and Lu, 1994; Geno et al, 1998; Gregory et al, 1995; Groot et al, 1998; Mills and Tyler, 1992; NRC, 1993; Ruscioni et al, 1994; Simon, 1998) to adults, and particularly to children, during and following the use of pesticide products inside the home. This need has been acknowledged by medical professionals, toxicologists and other scientists, some of who participate in scientific advisory boards for the U.S. Environmental Protection Agency and other international, national and state government organizations (EPA 1999a, 1999b).

Regulatory agencies and the regulated community have used existing human exposure data from monitoring studies with concurrent environmental measurements (e.g., transferable pesticide residues from indoor treated surfaces, such as carpet) in conjunction with state-of-the-art behavioral analysis to estimate children's indoor residential exposure. This approach is consistent with the premise that the most accurate estimates of human exposure are those made from direct measurement in or on humans (Krieger et al., 1999; Lu and Fenske, 1999; Woolen, 1993; Brouwer et al., 1999; 1996b; Geno et al., 1996; Vaccaro et al., 1996; Lewis et al., 1994; Ross et al., 1990; Ross et al., 1991; Bradman, 1997; Hill et al.; 1995; Zartarian, 1995; Zartarian, 1998; Versar, 1997; Zweig et al, 1983). However, the variability and uncertainty associated with available data and modeling assumptions requires that additional studies be conducted involving human volunteers under well-defined experimental conditions that are relevant to the residential environment.

Although it has been assumed that dermal transfer of residues to a person from environmental surfaces is linear over time, several recent studies suggest that this transfer process is rapidly saturable, reaches an effective equilibrium, and is non-linear (Spencer et al., 1995; Brouwer et al., 1999; Lu and Fenske, 1999; EPA, 1996, 1997; Versar, 1997). The duration or frequency of contact required to reach equilibrium in transferring environmental residues to the body was not explored until recently, and much of this work involves transfer to hands. However, a well-defined empirical relationship between dermal mass transfer from treated surfaces to skin, as a function of skin surface area contacted, and the number, duration and force of sequential contacts has not been characterized. The NDETF's studies provide a means for characterizing transferable residues from hard (vinyl) and soft (carpet) surfaces following application of common liquid (aqueous-based) formulations and Day 0 (day of application) dermal loading (particularly to hands given the relevance to hand-to-mouth incidental ingestion exposure estimation) under conditions relevant to the residential environment (e.g., as a function of duration of contact, contact pressure, wet versus dry hands, hand surface area, single versus repeat contact). Further, these studies are specifically designed to be used in refined residential exposure models to reduce the current uncertainty associated with pesticide exposure (dermal and incidental oral) estimation. Similar to post-application exposure data collected by ORETF, the NDETF database can be used as surrogate information for predictive modeling (particularly for Day 0).

RESIDENTIAL EXPOSURE JOINT VENTURE (REJV)

The Residential Exposure Joint Venture (REJV) is an industry Task Force that is sponsoring the prospective collection of temporal (diary instrument) pesticide product use information from a statistically representative sample of the U.S. population. A 3-month pilot study has been completed with a sub-sample of U.S. households to evaluate the survey instrument for use in a 12-month (one calendar year) survey. The primary purpose of the survey is to obtain the necessary information regarding the timing and frequency of product use events (and related ancillary information) to permit more realistic calendar-based aggregate and cumulative exposure

modeling. As described previously, aggregate and cumulative exposure modeling require demographic, geographic and temporal specificity. Further, the central issue of establishing a temporal profile of exposures based on the timing and frequency of product use is critical to scientifically credible aggregate or cumulative exposure assessments. For example, what is the likelihood that a given individual is going to use two or more products that contain a given pesticide during a time period that is toxicologically relevant (e.g., one day, one week, one month)? The REJV survey is designed to answer this question. Participants in the REJV survey can be statistically matched with demographically "equivalent" individuals in the CARES reference population and information that is being collected from the REJV survey for each individual can be used directly in the residential module's "event allocation" algorithms (see "Calendar-Based Residential Exposure Modeling" section of this document). The information required for stochastic calendar-based product use event allocation includes the following: product inventory, product identification (by EPA Registration No.), date of product use, applicator identification (consumer or professional), applicator demographic information (e.g., age, gender), method of application, season of application (month), day of week that product is applied, re-entry interval, co-occurrence of other product use events (captured in diary), and annual number of uses.

Supplemental demographic information (e.g., geographic region, household size, income level) specifically collected from participants in the REJV survey is presented below:

5. Vector of Individual Characteristics

5.1 Conceptual Approach

The primary “Vector of Individual Characteristics” (VIC) used in CARES is a set of static characteristics associated with each individual in the "reference population". These demographic characteristics are matched across data sources (e.g., U.S. Census, CSFII) that comprise the reference population. Each member of the CARES reference population includes the following "primary" VICs (note, additional characteristics that can be associated with the primary VIC include for example, Pregnancy Status, Lactation Status, Nursing Infants):

- Age
- Gender
- Geographic Location
- Urbanization
- Ethnicity
- Body Weight
- Height
- Surface Area (estimated)
- Socio-Economic Status (SES)

All data sources used within CARES must be evaluated with respect to the availability of the primary VICs so that the information can be appropriate "matched" to relevant individuals within the reference population. Table 6 provides a list of key data sources proposed for use in CARES residential module and comments of the level of information available fo r primary VIC matching. With the exception of time-activity and product use survey data, most data sources provide only age/gender specificity (i.e., no additional demographic details, no geographic specificity and often only single day time domains)

Table 6 Availability of Desired Primary VIC Characteristics from Key Residential Module Data Sources.

DATA SOURCE	DATA STATIFICATION LEVEL
PHED	Generic distributions of dermal and inhalation unit exposure distributions across all applicators (no age or gender stratification)
ORETF	Generic distributions of dermal and inhalation unit exposure distributions across all applicators (no age or gender stratification)
NHAPS	Age/gender subgroups (additional demographic and geographic information available)
NHGPUS	Age/gender subgroups
EFH	Age/gender subgroups
C-SEFH	Age/gender subgroups
NHEXAS	Age/gender subgroups
Published Scientific Literature (exposure monitoring studies)	Age/gender subgroups (geographic location available in some studies)

DATA SOURCE	DATA STATIFICATION LEVEL
ORETF & NDETF turf transferable residue data	Generic across all age/gender groups
NGA survey	Household-level demographic information
ORETF product use survey	Individual participant demographic and geographic information available; time-related information is based on short-term recall
NDETF indoor surface transferable residue data	Generic across all age/gender groups
REJV Product Use Survey	Individual participant demographic and geographic information available; prospective temporal diary-based product use information available
Chemical-Specific Residue Dissipation Studies	Generic across all age/gender groups
Children's Videography Data	Age/gender subgroups

In contrast to the primary VIC, module-specific VICs are also integrated into the CARES program to facilitate analyses unique to each module and to accommodate the dynamic nature of the module-specific characteristics. In the case of the CARES residential module, module-specific VICs include characteristics associated with product use event allocation. In addition, other ancillary characteristics such as inhalation rate and clothing configuration are associated with a given individual person's VIC profile based on geographic location and season of the year.

5.2 Specification of Individual Characteristics for the CARES Residential Module and Integration Across Other CARES Modules

Table 7 presents many of the key CARES Residential Module VICs. These represent characteristics that will be associated with each individual in the CARES "Reference Population" for which residential exposures are being estimated. The preferred source for each characteristic and comments are also provided in Table 7. Residential characteristics and their underlying data sources must be statistically matched to the primary CARES reference population (which is based on U.S. Census and CSFII participants). For purposes of "matching" (see CARES Reference Population documentation) residential characteristics with the Primary VICs associated with the "Reference Population," it is necessary to explicitly address the level of stratification available and the "representativeness" of each of the underlying data sources. For example, NHAPS and the ORETF and REJV surveys have more robust demographic information to facilitate more detailed stratification and matching to individuals in the CARES Reference Population. However, it is not possible to stratify other data sets beyond a limited set of age/gender strata or subgroups.

Residential-specific VICs can contain characteristics that are static or dynamic. Static characteristics are those that do not change during the calendar year period in which potential exposures are estimated; examples include presence of a lawn, pet ownership, and presence of a garden. Other residential characteristics can be classified as dynamic; examples include assignment of macro-locations and durations spent in each location (time-macro location patterns). Dynamic characteristics can change from day to day throughout the calendar year. It is also important to note that each individual in the CARES reference population will also be

assigned exposure factors, some of which can also be considered residential characteristics; these include activity-level-specific inhalation rates and hand-to-mouth event frequencies (for children, i.e., toddlers).

Table 7 CARES Residential Module VICs.

CARES Residential Module VIC	PREFERRED SOURCE of DATA FOR CHARACTERISTIC	COMMENTS
RESIDENTIAL FACTORS		
Housing Type (single family, apt., condo, rental, mobile homes)	U.S. Census	CARES reference population characteristic
- foundation type		
- house volume	PFT database	Alpha CARES will not include indoor air model, but will accommodate module output as input for inhalation exposure estimation; further key indoor air model inputs such as house volume and air exchange rate will be provided as characteristics for each individual in the Reference Population
- fraction of indoor surface areas covered by surface types (floor coverings – tile, carpet, wood (hard vs. soft))	User specified	Appropriate transferable residue data are matched to surface type specified by user
Presence of a Lawn, if yes, size	REJV and ORETF surveys	Size assignment based on National Gardening Association data in the ORETF survey database and published literature (Vinlove and Torla, 1995)
Presence of an Ornamental Garden, if yes, size?	REJV and ORETF surveys	Size assignment based on National Gardening Association data in the ORETF survey database
Presence of Vegetable Garden , if yes, size?	REJV and ORETF surveys	Size assignment based on National Gardening Association data in the ORETF survey database
Presence of Fruit and/or Nut Trees, If yes, specify number and sizes	REJV and ORETF surveys	Size assignment based on National Gardening Association data in the ORETF survey database
Presence of Swimming Pool? Presence of Spa? If yes, specify	User specified	Survey data not yet identified
- pet ownership status & types (dogs and cats, etc.); pet size assignment (user specified)	REJV	Species-specific pet size assignment (random) based on domesticated dog and cat veterinary literature

CARES Residential Module VIC	PREFERRED SOURCE of DATA FOR CHARACTERISTIC	COMMENTS
Clothing configuration – related to season duration, climate, temp	User specified	ORETF survey data provide guidance; categories: Naked (no clothing – worst case) Short pants, sleeveless shirt, no shoes or gloves Short pants, sleeveless shirt, shoes and socks, no gloves Long pants, short-sleeve shirt, shoes and socks Long pants, long-sleeve shirt, shoes and socks
- residence time (length of time in current residence)	Not applicable to alpha CARES	Assumed to remain in same residence entire calendar year
Macro-level time-activity profiles (durations of time spent in various environments)	Dynamic residential VIC derived from NHAPS	e.g., age/gender-specific percentiles for duration of time spent outdoors
Respiration Rate	EPA EFH and C-EFH (data tables extracted and made available in CARES)	Random assignment of activity level for each scenario; random sample and assign respiration rate percentile for each level, I.e., sedentary, light, moderate, heavy levels, to each person in the Reference Population; age intervals by gender
- Occupation category and length of time at current job	Not applicable	Potential para-occupational exposures may be addressed in future CARES versions
PRODUCT USE-RELATED (must be specified for each product/scenario addressed in a given CARES simulation)		
- probability for being a product user vs. non-user	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- probability of professional vs. consumer applicator	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- application method(s)	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- application site(s)	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- application rate(s)	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- frequency of application (monthly)	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- probability of application (weekday vs. weekend)	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- treatment intervals	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- number of applications per year	User specified or REJV survey	Input for calendar-based product use event allocation algorithms

CARES Residential Module VIC	PREFERRED SOURCE of DATA FOR CHARACTERISTIC	COMMENTS
- reentry interval	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- probability of co-occurrence among identified product/scenarios	User specified or REJV survey	Input for calendar-based product use event allocation algorithms
- market share for each identified product/scenario	User specified or REJV survey	Input for calendar-based product use event allocation algorithms

6. Residential Scenario-Specific Algorithms

This section presents general and exemplary scenario-specific input variables used in the CARES residential module.

6.1 Input Variables - General

Input variables included in the CARES residential model that can be considered "general" are those that are used across exposure scenarios. The general input variables are listed in Table 8. Each of the general input variables can be specified as point values (e.g., central tendency). Further, some of the input variables (when adequate data sets exist) can be represented as parametric or non-parametric distributions, as appropriate. As noted previously, distributional specification should include credible minimum and maximum values.

Table 8 INPUT VARIABLES - GENERAL

Exposure		
	Clothing Penetration Fraction (Uncovered)	*unitless*
	Clothing Penetration Fraction (Covered)	*unitless*
	Ingestion Rate (Granules/Pellets) (Child)	*g/day*
	Ingestion Rate (Grass/Plants) (Child)	*cm^2/day*
	Ingestion Rate (Soil) (Child)	*mg/day*
	Ingestion Rate (Paint Chips) (Child)	*mg/day*
	Ingestion Rate (Water) (Adult)	*L/hr*
	Ingestion Rate (Water) (Child)	*L/hr*
	Transfer Efficiency (HtoM) (per Contact) (Child)	*unitless*
	Removal Efficiency (HtoM) (per Contact) (Child)	*unitless*
	Fraction Transferred (HtoM) (Total) (Child)	*unitless*
	Reference Duration	*Day*
Dose	Fraction Absorbed (Dermal + Inh) (Dur App)	*unitless*
	Fraction Absorbed (Dermal)	*unitless*
	Fraction Absorbed (Ingestion)	*unitless*
	Fraction Absorbed (Inhalation)	*unitless*
	NOEL (Dermal) (Applied Dose)	*mg/kg/day*
	NOEL (Ingestion) (Applied Dose)	*mg/kg/day*
	NOEL (Inhalation) (Applied Dose)	*mg/kg/day*
	NOEL (Absorbed Dose) (Systemic)	*mg/kg/day*
Human Factors	Area (Hands) (Uncovered) (Adult)	*cm^2*
	Area (Hands) (Covered) (Adult)	*cm^2*
	Area (Upper Body) (Uncovered) (Adult)	*cm^2*
	Area (Upper Body) (Covered) (Adult)	*cm^2*
	Area (Lower Body) (Uncovered) (Adult)	*cm^2*
	Area (Lower Body) (Covered) (Adult)	*cm^2*
	Area (Feet) (Uncovered) (Adult)	*cm^2*
	Area (Feet) (Covered) (Adult)	*cm^2*
	Area (Hands) (Uncovered) (Child)	*cm^2*
	Area (Hands) (Covered) (Child)	*cm^2*
	Area (Upper Body) (Uncovered) (Child)	*cm^2*
	Area (Upper Body) (Covered) (Child)	*cm^2*
	Area (Lower Body) (Uncovered) (Child)	*cm^2*
	Area (Lower Body) (Covered) (Child)	*cm^2*
	Area (Feet) (Uncovered) (Child)	*cm^2*
	Area (Feet) (Covered) (Child)	*cm^2*
	Area (Total) (Adult)	*cm^2*
	Area (Total) (Child)	*cm^2*
	Area (Hands) (HtoM) (Child)	*cm^2*
	Contact Frequency (HtoM) (Child)	*events/hr*
	Inhalation Rate (Adult)	*m^3/hr*
	Inhalation Rate (Child)	*m^3/hr*
	Body Weight (Adult)	*kg*
	Body Weight (Child)	*kg*

6.2 Input Variables - Scenario-Specific

In contrast to general exposure variables, scenario-specific variables have also been organized for the CARES residential exposure module. An example set of scenario-specific input variables is presented in Table 9 for a lawn care scenario (applicator and post-application; adults and children). It is important to note that the CARES residential module is being structured to allow for multiple, alternative scenario-specific algorithms and their respective input variables to be selected by users. This reflects the ongoing need to refine and update algorithms for a given exposure scenario and compare the alternatives to existing equations. In this particular example, the lawn care scenario can be based on the use of dermal exposure algorithms that include body-part-specific "Transfer Factors" (unitless factors); alternatively, the lawn care scenario can be evaluated using algorithms based on whole-body surface contract rate metrics referred to as Transfer Coefficients (cm^2/hr).

Table 9 LAWN CARE SCENARIO-SPECIFIC INPUTS (INCLUDES DERMAL TRANSFER FACTOR-BASED APPROACH)

Source	Application (AI per Area Treated)	*lb ai/acre*
	Application (AI per Amount of Form Used)	*lb ai/gal*
	Area Treated	*acre*
	Amount of Formulation as Used (By Volume)	*gal*
	Amount of Formulation as Used (By Weight)	*mg*
	Fraction AI in Formulation as Used	*unitless*
	Density of Formulation	*g/cm^3*
Environment	Air concentration (Indoor) of AI	*microg/m^3*
	Dilution factor (Outdoor air)	*unitless*
	Volume of air (Outdoor, imaginary)	*m^3*
	Concentration of AI in Water	*mg/m^3*
	Permeability Coefficient	*cm/hr*
	Flux Rate of AI through Impregnated Material	*mg/m^2/day*
	Fraction Transferred to Whole Body (Dermal)	*unitless*
	Fraction AI available (Ingestion)	*unitless*
	Transferable Residue (Surface) (Env/Pet)	*mg/cm^2*
	Soil Density (Outdoor)	*g/cm^3*
	Thickness of Effective Soil Layer	*cm*
	Ground Cover (Grass/Plants)	*g/cm^2*
	Fraction AI Dislodgeable from Surface (Env/Pet)	*unitless*
	Fraction AI Dislodgeable from Grass/Plants	*unitless*
	Fraction AI Dislodgeable from Soil	*unitless*
	Fraction AI in Paint Chips	*unitless*
	Fraction AI Dissipated Daily	*unitless*

Exposure	Unit Exposure (Der + Inh) (During App)	*mg/lb ai*
	Unit Exposure (Dermal) (During Application)	*mg/lb ai*
	Unit Exposure (Inhalation) (During App)	*mg/lb ai*
	Film Thickness of Formulation on Dermal Area	*cm*
	Transfer Coefficient (Dermal) (Adult)	*cm^2/hr*
	Transfer Coefficient (Dermal) (Child: age > 6)	*cm^2/hr*
	Transfer Coefficient (Dermal) (Child: 1<age<6)	*cm^2/hr*
	Transfer Coefficient (Dermal) (Child: age < 1)	*cm^2/hr*
	Fraction Transferred to Hand (Dermal)	*unitless*
	Transfer Factor - Hands (Uncovered)	*unitless*
	Transfer Factor - Hands (Covered)	*unitless*
	Transfer Factor - Upper Body (Uncovered)	*unitless*
	Transfer Factor - Upper Body (Covered)	*unitless*
	Transfer Factor - Lower Body (Uncovered)	*unitless*
	Transfer Factor - Lower Body (Covered)	*unitless*
	Transfer Factor - Feet (Uncovered)	*unitless*
	Transfer Factor - Feet (Covered)	*unitless*
	Area Exposed (Film Thickness) (Adult)	*cm^2*
	Area Exposed (Film Thickness) (Ch: age > 6)	*cm^2*
	Area Exposed (Film Thickness) (Ch: 1 < age < 6)	*cm^2*
	Area Exposed (Film Thickness) (Ch: age < 1)	*cm^2*
	Area Contacted with Imp Material (Adult)	*cm^2*
	Area Contacted with Imp Material (Ch: age>6)	*cm^2*
	Area Contacted with Imp Material (Ch: 1<age<6)	*cm^2*
	Area Contacted with Imp Material (Ch: age<1)	*cm^2*
	Area Mouthed with Imp Mat (Child: age>6)	*cm^2*
	Area Mouthed with Imp Mat (Child: 1<age<6)	*cm^2*
	Area Mouthed with Imp Mat (Child: age<1)	*cm^2*
	Exposure Duration (Adult)	*hr/day*
	Exposure Duration (Child: age > 6)	*hr/day*
	Exposure Duration (Child: 1 < age < 6)	*hr/day*
	Exposure Duration (Child: age < 1)	*hr/day*
	Exposure Duration (HtoM) (Child: age > 6)	*hr*
	Exposure Duration (HtoM) (Child: 1 < age < 6)	*hr*
	Exposure Duration (HtoM) (Child: age < 1)	*hr*
	Exposure Duration (Impreg Mat) (Adult)	*hr*
	Exposure Duration (Impreg Mat) (Ch: age>6)	*hr*
	Exposure Duration (Impreg Mat) (Ch: 1<age<6)	*hr*
	Exposure Duration (Impreg Mat) (Ch: age<1)	*hr*
	Exposure Duration (Water) (Adult)	*hr*
	Exposure Duration (Water) (Child: age > 6)	*hr*
	Exposure Duration (Water) (Child: 1 < age < 6)	*hr*
	Exposure Duration (Water) (Child: age < 1)	*hr*

	t (= Post Application Day)	*day*
	Area Exposed (Film Thickness) (Child)	cm^2
	Area Contacted with Imp Material (Child)	cm^2
	Area Mouthed with Imp Material (Child)	cm^2
	Exposure Duration (HtoM) (Child)	*hr*
	Exposure Duration (Imp Material) (Child)	*hr*
	Exposure Duration (Water) (Child)	*hr*

6.3 Exposure Scenario Algorithms

Appendix C presents the exposure and absorbed dose algorithms (equations) and associated input variables organized by scenario. As noted previously, for some scenario-specific pathways and routes, multiple, alternative algorithms are provided to the user.

7. Calendar Based Residential Exposure Modeling

7.1 Conceptual Approach

The temporal use of pesticide products in residential environments is important to determine associated exposure events for a given sub-population. Use patterns are dependent on such characteristics as demographics (gender, age, economic status, etc.) geographical location, product application methods and post-application activities. Further, the time domain must be understood at both the micro-level, e.g., during the course of a given day, as well as at the macro-level, e.g., throughout the calendar year. Some residential exposure events are highly regular. For example, people usually eat every day, and each episode of food consumption carries with it a potential exposure event. On the other hand, treatment for termites may occur only every two to four years, while other events such as treating a lawn with a weed control product may occur a few times per year. One key issue in modeling such exposures is developing a scheme for utilizing information on pesticide use patterns to develop random allocations of events across an entire year.

Multiple tables of product use data are required to allocate events across an entire year. The following is a listing of required tables:

1. Product-related
   - Ingredients & Products
   - Products & Efficacy Periods
2. Household-related
   - Products & Scenarios
   - Scenarios & Doers vs. Non-Doers
   - Products & Professional vs. Consumer Use
3. Use-related
   - Scenarios & Seasonal Use
   - Scenarios & Day of Week Use
   - Products & Re-Entry Periods
   - Scenarios & Co-occurrences of Use
   - Scenarios & Annual Numbers of Use
4. Market Share

Making cumulative exposure assessments dictates the need for product use information on multiple active ingredients. Table 10 is a sample table for N number of ingredients. The first column lists the ingredients and the second lists the associated products. It must be noted that it is possible for the same ingredient to be represented in more than one product.

Table 10 A sample table for "Ingredients & Products"

ACTIVE INGREDIENT	PRODUCT
Ingredient 1	Product 1
Ingredient 2	Product 2
Ingredient 2	Product 3
Ingredient 3	Product 4
…….	…….
Ingredient N	…….

The probability of using a product again after a previous use is assumed to depend upon the efficacy period (in days) of the active ingredient in the product. Values for the efficacy periods

can be deduced from product label information or from efficacy studies conducted by product manufacturers. Each product is assumed to have its own value for efficacy period. Table 11 shows this dependency of efficacy period on product.

Table 11 A sample table for "Products & Efficacy Periods"

PRODUCT	EFFICACY PERIOD (Days)
Product 1	Period 1
Product 2	Period 2
…….	…….

Products are used for specific scenarios. Scenarios include "Lawn Care", "Ornamental Plant Care", "Indoor Fogger Use", etc. Table 12 shows the relationships between products and scenarios. It is possible for the same product to be used in multiple scenarios and also possible for more than one product specified for use in the same scenario.

Table 12 A sample table for "Products & Scenarios"

PRODUCT	SCENARIO
Product 1	Scenario 1
Product 1	Scenario 2
Product 2	Scenario 3
Product 3	Scenario 3
…….	…….

Given a sub-population, there are finite probabilities whether the individuals live in residences where any of the product use scenarios occur. These probabilities are tabulated in Table 13. Doers are designated as those who will perform a certain scenario activity in their residence. Each row in this table must add to 1.0.

Table 13 A sample table for "Scenarios & Doers vs. Non-Doers"

SCENARIO	DOER Probability	NON-DOER Probability
Scenario 1	0.3	0.7
Scenario 2	0.45	0.55
…….	…….	…….

Given a product, it must be specified whether a professional applicator or a household consumer applies the product. This specification dictates the estimation of "During Application" exposures (usually based on PHED-type analyses). Table 14 lists the products and applicators types.

Table 14 A sample table for "Products & Professional vs. Consumer Use"

PRODUCT	SCENARIO
Product 1	Professional
Product 2	Consumer
…….	…….

There is a probability distribution of product use scenarios as a function of season (summer, fall, etc.). If seasons are represented by the twelve months, for a given scenario, each month can be assigned a finite probability for the occurrence of that scenario. Table 15 shows the distributions of product use scenarios as a function of month. Each row in this table must add to 1.0.

Table 15 A sample table for "Scenarios & Seasonal Use"

PRODUCT	Jan	Feb	……..	Dec
Scenario 1	0.05	0.1	……..	0.05
Scenario 2	0.01	0.01	……..	0.01
…….	……..	……..	……..	……

Similar to the previous table, there is a probability distribution of product use scenarios as a function of day of week (Sunday, Monday, etc.). For a given scenario, each day of the week can be assigned a finite probability for the occurrence of that scenario. Table 16 shows the distributions of product use scenarios as a function of day of the week. Each row in this table must add to 1.0.

Table 16 A sample table for "Scenarios & Day of Week Use"

PRODUCT	Sun	Mon	……..	Sat
Scenario 1	0.2	0.1	……..	0.2
Scenario 2	0.15	0.15	……..	0.15
…….	……..	……..	……..	……

Given a product, the re-entry period (in days), after product application, must be specified. This specification dictates the residue levels in the different exposure media based on decay characteristics. Table 17 lists the products and re-entry periods.

Table 17 A sample table for "Products/Scenario & Re-Entry Periods"

PRODUCT/SCENARIO	RE-ENTRY PERIOD (Days)
Product 1/Scenario	0.5
Product 2/Scenario	0.33
…….	…….

When a certain product is used for a certain scenario during a certain time period (e.g., a day), it is possible that a different product is used the same day for a different scenario. Such possibilities are classified as co-occurrences or correlations of scenarios for the given time period. Table 18 shows the co-occurrences of scenarios for any given day. In the above table the cells along the diagonal starting from the top left will equal 0.0. The other cells will range between 0.0 and 1.0.

Table 18 A sample table for "Scenarios & Co-Occurrences of Use"

	Scenario 1	Scenario 2	……..
Scenario 1	0.0	0.2	……..
Scenario 2	0.1	0.0	……..
…….	……..	……..	……

A critical table for estimating exposures for periods up to a year is the numbers of annual use as a function of scenario. This relationship is shown in Table 19.

Table 19 A sample table for "Scenarios & Numbers of Annual Use"

PRODUCT	NUMBER of ANNUAL USE
Scenario 1	12
Scenario 2	8
…….	…….

Information on market share for the different products is required to estimate probability distributions for using a specific product given a scenario. These distributions will also be dependent on the active ingredients considered. In Table 20, below, all the cells should add to 1.0.

Table 20 A sample table for "Market Share"

	Ingredient 1	Ingredient 2	……..
Product 1	0.1	0.0	……..
Product 2	0.0	0.05	……..
…….	……..	……..	……

7.2 Stochastic, Calendar-Based Product Use Event Allocation Algorithms - Case Study Illustration: Indoor Total Release Foggers

A case study is presented below for a single product use category, i.e., indoor total release foggers to illustrate the CARES Residential Module's stochastic, calendar-based product use event allocation algorithms. Based on the limited availability of factual data, most of the input parameters for event allocation will be single values. However, for those data sets that have distributional information, provision will be made to accommodate them. The example shown below is a hypothetical single product use distribution. It is important to recognize that the implementation of the event allocation methods in CARES will necessarily be generalized to accommodate multiple product event allocation across the calendar year as described above in the conceptual approach.

7.2.1 The Distribution of the Number of Fogger Events

The scenario described in this example is the use of indoor total release foggers. However, the general algorithms are applicable to any irregularly used pesticide product. There are several important sources of information regarding fogger use. First, the frequency of fogger use in terms of number of episodes of fogger use across the year is known. Table 21 displays a hypothetical use distribution. Note that this is only for persons using foggers. The National Home and Garden Pesticide Use Survey shows that only 34.7 % of the population actually use any pesticide in the home in a given year. So it follows that all fogger users cannot comprise more than 34.7% of the population.

Table 21 Fogger use frequency for persons using foggers

Number of Uses	Percentage
1 Time	28
2 Times	34
3 Times	18
4 Times	8
5-9 Times	7
10-25 Times	4
26-50 Times	0.5
51-100 Times	0.3
Over 100 Times	0.2

For categories where a range of values is reported (e.g. 10-25 times) it is assumed that all values are equally likely. This is quite conservative in that the percentages tend to decline with use frequency. For the over 100 category, it is assumed that the frequencies between 101 and 122 are equally likely. This defacto assigns zero probability to use frequencies in excess of 122 times a year [more than every third day use]. This last probability assignment is reasonable because higher use frequencies are indicative of misuse.

If these assumptions are accepted, then a probability distribution that can be used to randomly assign the number of fogger use events per year has been determined. That is, the probability of zero events is 0.653; the probability of 1 event is 0.097 (the product of 0.347 [the probability of one or more event] and 0.28 [the probability of 1 event given that at least one event occurred]). In a like manner probabilities are assigned for the occurrence of 2 through 122 fogger events. Once these probabilities have been assigned, it is possible to randomly generate annual numbers of events.

7.3 Distributing Fogger Events over the Year

The temporal structure of application events over the year must also be determined. Table 22 gives a hypothetical use pattern for the "North Central U.S."

Table 22 Hypothetical percentage of fogger use by month of year: North Central U.S.

Month	Percentage of total usage
January	3.4
February	3.0
March	4.4
April	5.8
May	8.4
June	18.5
July	17.3
August	14.7
September	12.3
October	8.6
November	1.8
December	1.8

If a single fogger event is under consideration, the data in Table 22 can be directly used to assign this event to a particular month. Once the event has been assig ned to a month, it is assumed that all days within a month are equally likely. In practice, the particular day of application is selected via a single random number, using the inverse method. For example, the probability of a pesticide being applied on J anuary 1 is 0.034 ÷ 31 or 0.0010968. If the generated random number is less than or equal to 0.0010968, the application is assigned to January 1; if the random number is greater than 0.0010968 but less than or equal to 0.0021935, the application is assigned to January second and so on. This process is illustrated graphically in Figure 6.

Assigning subsequent events requires some thought. That is, if a fogger application is made on June 5, it is quite unlikely that a subsequent application will be made on June 6, but after some time has elapsed, the probability of a fogger application would be essentially unaffected. Assume the data suggests that, on average, a fogger treatment provides control for 30 days. Assume that efficacy declines in a linear fashion such that there is zero probability of a fogger application on the day immediately following an application, and that the probability rises to the baseline probability 31 days after application. Consider the January 1 example. The probability of a subsequent application is zero on January 2, $0.0010968 \times 1/30 = 3.7 \times 10^{-5}$ on January 3, and $0.001742 \times 29/30 = 1.060 \times 10^{-3}$ on January 31. In assigning events it is also important to

realize that this relationship is symmetric. That is, if an event is assigned on day 233 of the year, there cannot be a second event on day 234, but there also cannot be an event on day 232, because this would also result in events on two adjoining days. Similarly, consideration of the probability of an event 10 days earlier is reduced because of the assumed temporal dependence. In practice, if the period 30 days prior the event is treated in exactly the same manner as the period 30 days after the event, a correct distribution of days across the year is obtained. This adjustment results in a set of probabilities for the entire year that no longer sum to one. This is handled by a simple procedure called renormalization wherein all of the probabilities, including those that have been adjusted, are summed, and each probability is divided by this sum. The result of this is that the daily application probabilities again sum to one. This adjustment and renormalization procedure is provided for a second fogger event, but the approach is entirely general. That is, one could use the same procedure to randomly distribute 122 fogger events across the year.

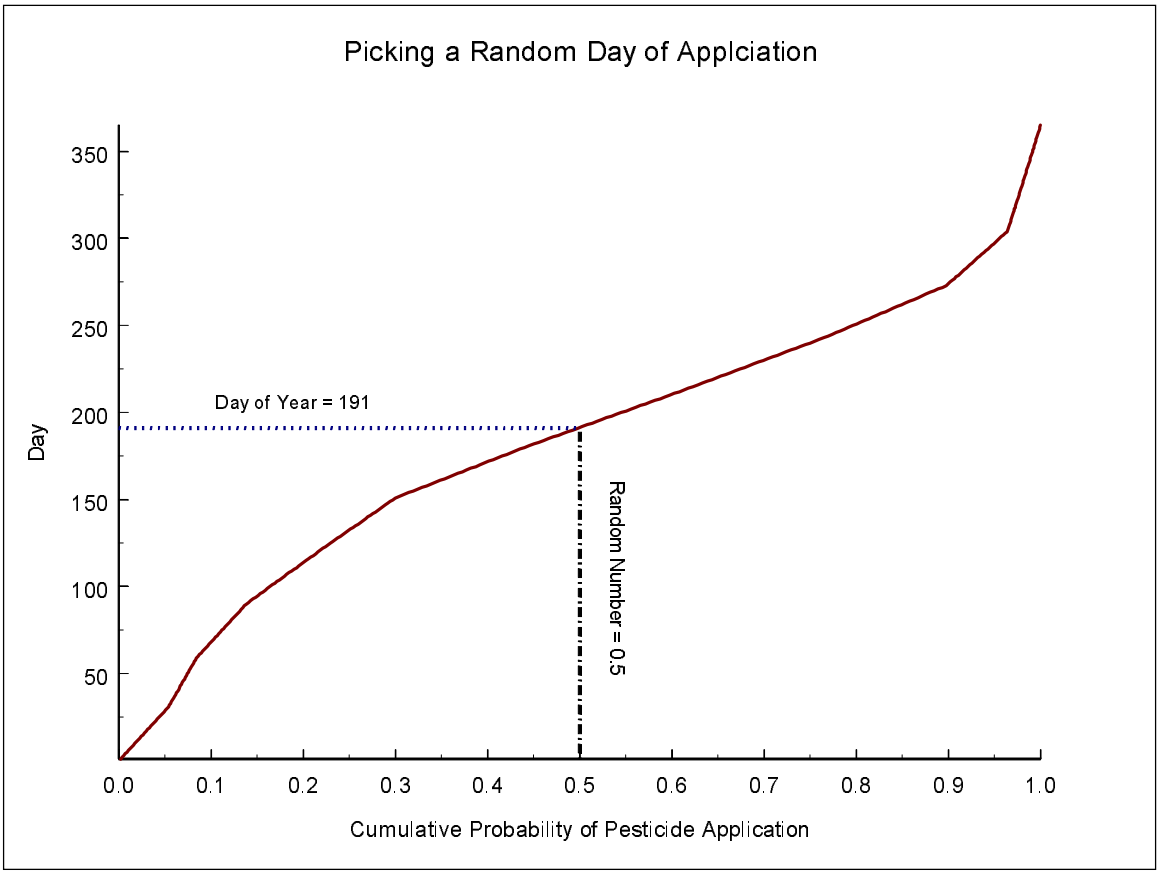


Figure 6 Picking a random application day. If a random number equal to 0.05 is generated, the day assigned is 191.

7.4 Assigning the Number of Fogger Products Used Per Event

Once the distribution of fogger events across the year have been assigned, the question arises of how many actual foggers are used per event. Again, it is possible to obtain the data that can address this issue.

Table 23 Number of products used per event.

Number of Products	Percentage
1	16
2	19
3	26
4+	39

Table 23 shows that 16% (0.16) of fogger events involve only a single product, while 39% (0.39) involve 4 or more fogger products. Unlike the other sources of use information this is not very easily translated to a useful distribution. That is, say it is assumed that in the 4+ category, 13% each was for 4, 5, and 6 products. This might be defensible, but does not address the important issue of area treated. That is, 5 foggers released in a 3600 square foot house might actually have less exposure consequence than a single fogger released in a 600 square foot apartment. Moreover, other data from industry show that in over 90% of fogger events, a single fogger per room is used, and that almost all fogger events (99%+) involve no more than 2 foggers per room. As an interim measure, one could assign numbers of foggers per event using the information from Table 23 and the convention that a maximum of six products per event be considered. However, if this is done, one must adopt the convention that while some exposures, such as those associated with disposal of the units, would scale essentially linearly with numbers of products, other exposures such as inhalation or dermal contact might be affected little, if at all, by the use of more products per event.

7.5 Assigning Fogger Products to an Event

Also of interest is the product to which the user is exposed. It is suggested that market share data, or preferably, product use diary data available from the REJV, be used to assign events to products. That is, if Product X has 33% market share, 1/3 of all fogger events will be assigned to this product. Note that this assumes that all foggers used in a given event are the same formulation which is a reasonable assumption. However, products are assigned randomly according to market share for each fogger event. That is, it is not assumed that a given individual might preferentially use good old Product X.

7.6 Integrating the Temporal Model**

To recapitulate, four modeling strategies have been presented for defining exposure in a temporal framework:

1. Randomly generating the number of fogger events per year.
2. Randomly distributing these events over the year.
3. Randomly generating the number of fogger products used per event.
4. Randomly picking the fogger product used per event.

These four components are integrated by picking an individual from the population of interest. Note that there is no random generation of personal characteristics such as age, gender, or body weight; these are characteristics of the individuals and will be used in all modeling. This use of a standard population permits the integration of modeling results across such diverse sources as foggers and food, and thus provides a defensible aggregate risk assessment. Once an individual is selected, the four steps presented above are performed to generate an annual fogger exposure profile, which incorporates the temporal distribution of events, the foggers used per event and the type of foggers used in each event. A flow chart of this process is shown in Figure 7.

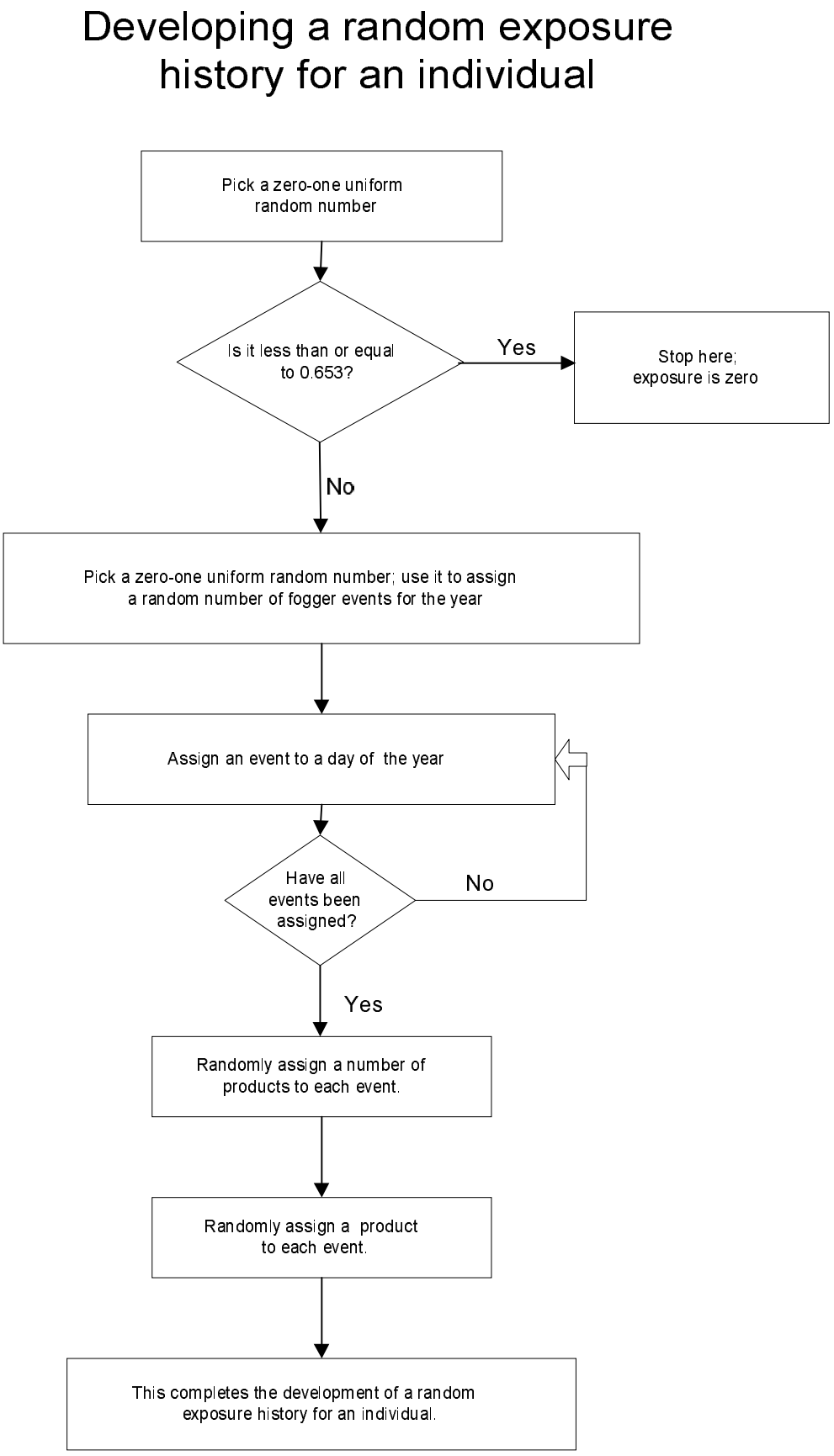


Figure 7Flow chart of stochastic modeling sequence

8. CARES Residential Module Quality Assurance Features

Quality assurance is a central theme for data and model management systems. CARES will be addressing quality assurance procedures for data entry, exposure assessment algorithms, software performance, and exposure/risk assessment reporting and review.

For example, the CARES residential module will include several features to facilitate quality assurance reviews of CARES-based exposure/risk assessments by the primary assessor, as well as external (secondary) reviewers. These features will include, for example, a function to allow printing (as hard copy or file) of all inputs selected for the residential assessment (deterministic or stochastic modes). This feature will allow reviewers to easily re-construct an assessment developed by another individual.

Additional quality assurance documentation will be developed and published as part of the ongoing CARES effort, including documentation specific to the CARES residential module.

9. CARES Residential Module Verification, Evaluation and Validation

The CARES residential module will undergo procedures related to verification, evaluation and validation. Definition of the specific procedures and the resulting analyses are ongoing. The results of this process will be published in future CARES-related documentation associated with the residential module.

10. Updates & Future Enhancements

As existing data sources are updated or added, and as new or revised exposure assessment methods are developed, the CARES residential module can be revised to accommodate them. For example, Appendix I presents recent revisions to the EPA' residential exposure assessment SOPs which will be reflected in the alpha version of CARES. In addition, a variety of future enhancements are being considered with respect to the CARES residential module. At present, these include the integration of indoor air modeling tools, micro-event modeling algorithms and associated data sources, updated EPA SOP algorithms and advanced statistical methods for utilizing survey data (e.g., REJV) for stochastic modeling. The CARES documentation will be updated to present discussions of potential enhancements or to detail the data sources, methods and software implementation for each specific enhancement that is adopted.

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Appendix D – Residential Algorithms

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Appendix D – Residential Algorithms

CARES Residential Algorithms

January 12, 2002

1.0 Residential Product Use Scenarios

The following scenarios are currently represented in the CARES model:

- 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
- Custom

2.0 Exposure Pathways and Assessment Methods

During Application		
Dermal		
Unit Exposure, Area Treated	(Dermal 101)	Adult
Unit Exposure, Amount of Formulation Used	(Dermal 102)	Adult
Inhalation		
Unit Exposure, Area Treated	(Inhalation 101)	Adult
Unit Exposure, Amount of Formulation Used	(Inhalation 102)	Adult
Post Application (Adults & Children)		
Dermal		
Transfer Coefficient (Residue)	(Dermal 103)	Adult/Child
Transfer Coefficient (Area Treated)	(Dermal 104)	Adult/Child
Transfer Factor (Residue)	(Dermal 105)	Adult/Child
Transfer Factor (Area Treated)	(Dermal 106)	Adult/Child
Fraction Transferred	(Dermal 107)	Adult/Child
Flux Rate	(Dermal 108)	Adult/Child
Water Concentration	(Dermal 109)	Adult/Child
Film Thickness (DERMAL Model)	(Dermal 110)	Adult/Child
Ingestion		
Granules/Pellets (Formulation)	(Ingestion 101)	Child
Grass/Plants	(Ingestion 102)	Child
Soil	(Ingestion 103)	Child
Paint Chips	(Ingestion 104)	Child
Flux Rate	(Ingestion 105)	Child
Water Concentration	(Ingestion 106)	Adult/Child
Hand-To-Mouth Transfer		
Mass Balance	(Ingestion 107)	Child
Fraction Transferred	(Ingestion 108)	Child
EPA SOPs Method	(Ingestion 109)	Child
Inhalation		
Air Concentration, Specified	(Inhalation 103)	Adult/Child
Air Concentration, Calculated	(Inhalation 104)	Adult/Child

3.0 Algorithms

Variables requiring user input for an exposure assessment method are marked in the accompanying tables. User inputs for some exposure assessment methods are generated as outputs from other methods. For example, the Ingestion 107 Hand-To-Mouth Transfer (Mass Balance) method requires input from Dermal 106 Transfer Factor (Area Treated) method.

Dermal 101

Method: Unit exposure, Area treated

Application: **During**
Receptor: **Adult**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (AI per Area Treated)	*kg ai/m^2*	*x*
	Area Treated	*m^2*	*x*
Environment			
Exposure	Unit Exposure (Dermal) (During application)	*mg/kg ai*	*x*
	Reference Duration	*day*	*x*
Human Factors	Body Weight (Adult)	*kg*	*x*
	Fraction Absorbed (Dermal)	*unitless*	*x*
Exposure	Exposure (Adult)	*mg/kg/day*	

Outputs:

$$Exposure_{Adult} = \frac{(Unit\ Exposure)_{Dermal} \times (Application)_{Area\ Treated} \times (Area\ Treated)}{(Reference\ Duration) \times (Body\ Weight)_{Adult}}$$

Dermal 102

Method: Unit exposure, Amount of Formulation Used

Application: **During**
Receptor: **Adult**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (Amount of AI Used)	*kg ai/m^3*	*x*
	Amount of Formulation Used	*m^3*	*x*
Environment			
Exposure	Unit Exposure (Dermal) (During Application)	*mg/kg ai*	*x*
	Reference Duration	*day*	*x*
Human Factors	Body Weight (Adult)	*kg*	*x*
	Fraction Absorbed (Dermal)	*unitless*	*x*
Calculations			
Outputs			
Exposure	Exposure (Adult)	*mg/kg/day*	

Outputs:

$$Exposure_{Adult} = \frac{(Unit\ Exposure)_{Dermal} \times (Application)_{Amt\ Form\ Used} \times (Amount\ of\ Form\ Used)}{(Reference\ Duration) \times (Body\ Weight)_{Adult}}$$

Dermal 103

Method: Transfer Coefficient (Residue)

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment	Transferable Residue (Surface) (Environment/Pet)	*mg/cm^2*	*x*
Exposure	Transfer Coefficient (Adult/Child)	*cm^2/hr*	*x*
	Fraction Transferred to Hand (Dermal) (Child)	*unitless*	*x*
	Exposure Duration (Adult/Child)	*hr/day*	*x*
Human Factors	Body Weight (Adult/Child)	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	
	Exposure (Hand, Child)	*mg*	

Outputs:

$$Exposure_{Adult/Child} = \frac{(Trans\ Residue) \times (Transfer\ Coefficient)_{Adult/Child} \times (Exposure\ Duration)_{Adult/Child}}{(Body\ Weight)_{Adult/Child}}$$

$$Exposure_{Hand,Child} = (Trans\ Residue) \times (Trans\ Coeff)_{Child} \times (Frac\ Trans)_{Hand,Child} \times (Exposure\ Duration)_{Chil}$$

Dermal 104

Method: Transfer Coefficient (Area Treated)

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (AI per Area Treated)	*kg ai/m^2*	
Environment	Fraction AI Dislodgeable in Surface	*unitless*	
Exposure	Transfer Coefficient (Adult/Child)	*cm^2/hr*	*x*
	Fraction Transferred to Hand (Dermal) (Child)	*unitless*	*x*
	Exposure Duration (Adult/Child)	*hr/day*	*x*
Human Factors	Body Weight (Adult/Child)	*kg*	*x*
	Fraction Absorbed (Dermal)	*unitless*	*x*
Correction Factors			
CF_1	Correction Factor (milligrams/kilogram)	*10^6*	
CF_2	Correction Factor (m^2/cm^2)	*$1x10^{-4}$*	
Calculations			
Trans Residue	Transferable Residue	*mg/cm^2*	*x*
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	
	Exposure (Hand, Child)	*mg/day*	

Calculations:

$$Trans\ Residue = (Application)_{Area\ Treated} \times CF_1 \times CF_2 \times (Frac\ AI\ Dislodge)$$

Outputs:

$$Exposure_{Adult/Child} = \frac{(Trans\ Residue) \times (Transfer\ Coefficient)_{Adult/Child} \times (Exposure\ Duration)_{Adult/Child}}{(Body\ Weight)_{Adult/Child}}$$

$$Exposure_{Hand,Child} = (Trans\ Residue) \times (Trans\ Coeff)_{Child} \times (Frac\ Trans)_{Hand,Child} \times (Exposure\ Duration)_{Chil}$$

Dermal 105

Method: Transfer Factor (Residue)

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment	Transferable Residue (Surface) (Environment/Pet)	*mg/cm^2*	*x*
Exposure	Transfer Factor – Hands (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Hands (Covered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Upper Body (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Upper Body (Covered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Lower Body (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Lower Body (Covered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Feet (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Feet (Covered) (Adult/Child)	*unitless*	*x*
	Clothing Penetration Fraction (Uncovered) (Adult/Child)	*unitless*	*x*
	Clothing Penetration Fraction (Covered) (Adult/Child)	*unitless*	*x*
	Reference Duration	*day*	*x*
Human Factors	Surface Area (Hands) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Hands) (Covered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Upper Body) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Upper Body) (Covered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Lower Body) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Lower Body) (Covered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Feet) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Feet) (Covered) (Adult/Child)	*cm^2*	*x*
	Body Weight (Adult/Child)	*kg*	*x*
	Fraction Absorbed (Dermal)	*unitless*	*x*
Calculations			
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	
	Exposure (Hand, Child)	*mg/day*	

Outputs:

[next page]

Outputs:

$$Exposure_{Adult/Child} = \frac{\sum\left\{\left(Trans\ Factor\right)\times\left(Surf\ \ Area\right)_{Adult/Child}\times\left(Cloth\ Pen\ Factor\right)\right\}\times\left(Trans\ \ Res\right)}{\left(Reference\ \ Duration\right)\times\left(Body\ Weight\right)_{Adult/Child}}$$

- summation across all body parts (uncovered and covered)

$$Exposure_{Hand,Child} = \frac{\sum\left\{\left(Trans\ Fact\right)\times\left(Surf\ \ Area\right)_{Child}\times\left(Cloth\ Pen\ Factor\right)\right\}\times\left(Trans\ \ Res\right)}{\left(Reference\ \ Duration\right)}$$

- summation across hands (uncovered and covered)

Dermal 106

Method: Transfer Factor (Area Treated)

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (AI per Area Treated)	*kg ai/m^2*	*x*
Environment	Fraction AI Dislodgeable in Surface	*unitless*	*x*
Exposure	Transfer Factor – Hands (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Hands (Covered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Upper Body (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Upper Body (Covered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Lower Body (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Lower Body (Covered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Feet (Uncovered) (Adult/Child)	*unitless*	*x*
	Transfer Factor – Feet (Covered) (Adult/Child)	*unitless*	*x*
	Clothing Penetration Fraction (Uncovered)	*unitless*	*x*
	Clothing Penetration Fraction (Covered)	*unitless*	*x*
	Reference Duration	*day*	*x*
Human Factors	Surface Area (Hands) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Hands) (Covered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Upper Body) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Upper Body) (Covered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Lower Body) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Lower Body) (Covered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Feet) (Uncovered) (Adult/Child)	*cm^2*	*x*
	Surface Area (Feet) (Covered) (Adult/Child)	*cm^2*	*x*
	Body Weight (Adult/Child)	*kg*	*x*
Correction Factors			
CF_1	Correction Factor (milligrams/kilogram)	*10^6*	
CF_2	Correction Factor (m^2/cm^2)	*$1x10^{-4}$*	
Calculations			
Trans Residue	Transferable Residue	*mg/cm^2*	
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	
	Exposure (Hand, Child)	*mg/day*	

Calculations:

$$Trans\ Residue = (Application)_{Area\ Treated} \times CF_1 \times CF_2 \times (Frac\ AI\ Dislodge)$$

Outputs:

$$Exposure_{Adult/Child} = \frac{\sum \{(Trans\ Factor) \times (Surf\ Area)_{Adult/Child} \times (Cloth\ Pen\ Factor)\} \times (Trans\ Residue)}{(Reference\ Duration) \times (Body\ Weight)_{Adult/Child}}$$

- summation across all body parts (uncovered and covered)

$$Exposure_{Hand,Child} = \frac{\sum \{(Trans\ Fact) \times (Surf\ Area)_{Child} \times (Cloth\ Pen\ Factor)\} \times (Trans\ Residue)}{(Reference\ Duration)}$$

- summation across hands (uncovered and covered)

Dermal 107

Method: Fraction Transferred

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Amount of Formulation as Used (By Weight)	*mg*	*x*
	Fraction AI in Formulation	*unitless*	*x*
Environment	Fraction AI Dislodgeable on Surface (Environment/Pet)	*unitless*	*x*
Exposure	Fraction Transferred to Whole Body (Dermal)	*unitless*	*x*
	Fraction Transferred to Hand (Dermal) (Child)	*unitless*	*x*
	Reference Duration	*day*	*x*
Human Factors	Body Weight (Adult/Child)	*kg*	*x*
Calculations			
Trans Residue	Transferable Residue	*mg*	
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	
	Exposure (Hand, Child)	*mg/day*	

Calculations:

$$Trans\ Residue = (Amt\ Form\ Used) \times (Frac\ \ AI\ Form) \times (Frac\ AI\ \ Dislodge)$$

Outputs:

$$Exposure_{Adult/Child} = \frac{(Trans\ Residue) \times (Fraction\ Transferred)_{Whole\ Body, Adult/Child}}{(Reference\ Duration) \times (Body\ Weight)_{Adult/Child}}$$

$$Exposure_{Hand, Child} = \frac{(Trans\ Residue) \times (Fraction\ Transferred)_{Hand, Child}}{(Reference\ Duration)}$$

Dermal 108

Method: Flux Rate

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment	Flux Rate of AI through Impregnated Material	*mg/m^2/day*	*x*
Exposure	Exposure Duration (To Impregnated Material) (Adult/Child)	*hr*	*x*
	Fraction Transferred to Hand (Dermal)	*unitless*	*x*
	Reference Duration	*day*	*x*
Human Factors	Surface Area Contact with Impregnated Material (Ad/Ch)	*cm^2*	*x*
	Body Weight (Adult/Child)	*kg*	*x*
Correction Factors			
CF_2	Correction Factor (m^2/cm^2)	*1x10^{-4}*	
CF_3	Correction Factor (hr/day)	*24*	
Calculations			
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	
	Exposure (Hand, Child)	*mg/day*	

Outputs:

$$Exposure_{Adult/Child} = (Flux\ Rate\ AI) \times \frac{(Surface\ Area)_{Contact,Adult/Child} \times (Exposure\ Duration)_{Adult/Child} \times CF_2}{(Reference\ Duration) \times (Body\ Weight)_{Adult/Child} \times CF_3}$$

$$Exposure_{Hand,Child} = (Flux\ Rate\ AI) \times \frac{(Surface\ Area)_{Contact,Child} \times (Fraction\ Transferred)_{Hand,Child} \times (Exposure\ Duration)_{Child} \times CF_2}{(Reference\ Duration) \times CF_3}$$

Dermal 109

Method: Water Concentration

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment	Concentration of AI Pool Water	*mg/m^3*	*x*
	Permeability Coefficient	*cm/hr*	*x*
Exposure	Exposure Duration (Adult/Child)	*hr*	*x*
	Reference Duration	*day*	*x*
Human Factors	Surface Area (Whole Body) (Adult/Child)	*cm^2*	*x*
	Body Weight (Adult/Child)	*kg*	*x*
Correction Factors			
CF_4	Correction Factor (m3/cm3)	*1x10^{-6}*	
Calculations			
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	

Outputs:

$$Exposure_{Adult/Child} = (Conc\ AI\ Water) \times (Permeability\ Coeff)$$

$$\times \frac{(Surface\ Area)_{Contact,Adult/Child} \times (Exposure\ Duration)_{Adult/Child} \times CF_4}{(Reference\ Duration) \times (Body\ Weight)_{Adult/Child}}$$

Dermal 110

Method: Film Thickness (DERMAL Model)

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment	Density of Formulation	*mg/cm^3*	*x*
	Fraction of AI in Formulation	*unitless*	*x*
Exposure	Film thickness of Formulation on Dermal Area	*cm*	*x*
	Fraction Transferred to Hand (Dermal) (Child)	*unitless*	*x*
	Reference Duration	*day*	*x*
Human Factors	Surface Area (Exposed to Formulation) (Adult/Child)	*cm^2*	*x*
	Body Weight (Adult/Child)	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	
	Exposure (Hand, Child)	*mg/day*	

Outputs:

$$Exposure_{Adult/Child} = \frac{(Density\ Form)\times(Frac\ AI\ Form)\times(Film\ Thick)\times(Surf\ Area)_{Exposed,Adult/Child}}{(Reference\ Duration)\times(Body\ Weight)_{Adult/Child}}$$

$$Exposure_{Hand,Child} = (Density\ Formulation)\times(Fraction\ AI\ Formulation)\times(Film\ Thickness)$$
$$\times\frac{(Surface\ Area)_{Exposed,Child}\times(Fraction\ Transferred)_{Hand,Child}}{(Reference\ Duration)}$$

Ingestion 101

Method: Granules/Pellets (Formulation)

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Fraction AI in Formulation as Used	*unitless*	*x*
Environment			
Exposure	Ingestion Rate (Granules/Pellets) (Child)	*mg/day*	*x*
Human Factors	Body Weight (Child)	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Outputs:

$$Exposure_{Child} = \frac{(Ingestion\ Rate)_{Granules/Pellets,Child} \times (Fraction\ AI\ in\ Granules/Pellets)}{(Body\ Weight)_{Child}}$$

Ingestion 102

Method: Grass/Plants

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (AI per Area treated)	*kg ai/m^2*	*x*
Environment	Ground Cover (Grass/Plants)	*g/cm^2*	*x*
	Fraction AI Dislodgeable from Grass/Plants	*unitless*	*x*
Exposure	Ingestion Rate (Grass/Plants) (Child)	*mg/day*	*x*
Human Factors	Body Weight (Child)	*Kg*	*x*
Correction Factors			
CF_1	Correction Factor (milligrams/kilogram)	*10^6*	
CF_2	Correction Factor (m^2/cm^2)	*$1x10^{-4}$*	
CF_6	Correction Factor (mg/g)	*$1x10^3$*	
Calculations			
Residue	Residue (Grass/Plants)	*mg ai/mg soil*	
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Calculations:

$$Residue_{Grass/Plants} = \frac{(Application)_{Area\ Treated} \times (Frac\ AI\ Grass/Plants) \times CF_1 \times CF_2}{(Ground\ Cover) \times CF_6}$$

Outputs:

$$Exposure_{Child} = \frac{(Residue)_{Grass/Plants} \times (Ingestion\ Rate)_{Grass/Plants,Child}}{(Body\ Weight)_{Child}}$$

Ingestion 103

Method: Direct: Soil

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (Area Treated)	*kg ai/m^2*	*x*
Environment	Soil Density (Outdoor)	*g/cm^3*	*x*
	Thickness of Effective Soil Layer	*cm*	*x*
	Fraction AI Dislodgeable from Soil	*unitless*	*x*
Exposure	Ingestion Rate (Soil) (Child)	*mg/day*	*x*
Human Factors	Body Weight (Child)	*kg*	*x*
Correction Factor			
CF_1	Correction Factor (milligrams/kilogram)	*$1x10^6$*	
CF_2	Correction Factor (m^2/cm^2)	*$1x10^{-4}$*	
CF_6	Correction Factor (mg/g)	*$1x10^3$*	
Calculations			
Residue	Residue (Soil)	*mg ai/mg soil*	
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Calculations:

$$Residue_{Soil} = \frac{(Application)_{Area\ Treated} \times (Fraction\ AI\ Soil) \times CF_1 \times CF_2}{(Soil\ Density) \times (Thickness\ Soil\ Layer) \times CF_6}$$

Outputs:

$$Exposure_{Child} = \frac{(Residue)_{Soil} \times (Ingestion\ Rate)_{Soil,Child}}{(Body\ Weight)_{Child}}$$

Ingestion 104

Method: Paint Chips

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Fraction AI in Paint Chips	*unitless*	*x*
	Fraction AI (in Paint Chips) available for ingestion	*unitless*	*x*
Environment			
Exposure	Ingestion Rate (Paint Chips) (Child)	*mg/day*	*x*
Human Factors	Body Weight (Child)	*Kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Outputs:

$$Exposure_{Child} = \frac{(Ingestion\ Rate)_{Paint\ Chips,Child} \times (Frac\ AI\ in\ Paint\ Chips) \times (Frac\ AI\ Available)}{(Body\ Weight)_{Child}}$$

Ingestion 105

Method: Water Concentration (Swimming Pool)

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Water Concentration (Swimming Pool)	*mg ai/m^3*	*x*
Environment			
Exposure	Ingestion Rate (Pool Water) (Adult/Child)	*m^3/hr*	*x*
	Exposure Duration (in Pool) (Adult/Child)	*hr*	*x*
	Reference Duration	*day*	*x*
Human Factors	Body Weight (Adult/Child)	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Outputs:

$$Exposure_{Adult/Child} = \frac{(Water\ Conc)_{Swimming\ Pool} \times (Ing\ Rate)_{Pool\ Water,Adult/Child} \times (Exp\ Dur)_{Adult/Child}}{(Reference\ Duration) \times (Body\ Weight)_{Adult/Child}}$$

Ingestion 106

Method: Flux Rate

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Flux rate of AI	*mg/cm^2/day*	*x*
Environment			
Exposure	Surface area (impregnated material) mouthed (child)	*cm^2*	*x*
Human Factors	Body weight (child)	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (child)	*mg/kg/day*	

Outputs:

$$Exposure_{Child} = \frac{(Flux\ \ Rate\ AI) \times (Surface\ \ Area\ \ Impregnated\ \ Material)_{Mouthed}}{(Body\ \ Weight)_{Child}}$$

Ingestion 107

Method: Hand-To-Mouth Transfer (Mass Balance)

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment			
Exposure	Exposure (Hand (Dermal),Child)	*mg/day*	*Dermal 106*
	Contact Frequency (Hand-To-Mouth) (Child)	*events/hr*	*x*
	Transfer Efficiency (Hand-To-Mouth) (per Contact) (Child)	*unitless*	*x*
	Exposure Duration (Hand-To-Mouth) (Child)	*hr*	*x*
Human Factors	Area (Hands) (Uncovered) (Child)	*cm²*	*x*
	Area (Hands) (Hand-To-Mouth) (Child)	*cm²*	*x*
	Body Weight (Child)	*kg*	*x*
Calculations			
Transfer Factor	Transfer Factor (Hand-To-Mouth)	*unitless*	
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Calculations:

$$Transfer\ Factor_{Hand-To-Mouth} = (Transfer\ Eff) \times \sum_{n=1}^{[(Contact\ Freq)\times(Exp\ Duration)]} [1-(Transfer\ Eff)]^{n-1}$$

Outputs:

$$Exposure_{Child} = \frac{(Exposure)_{Hand(\ Dermal\ ),Child} \times (Transfer\ Factor)_{Hand-To-Mouth}}{(Body\ Weight)_{Child}} \times \frac{(Area)_{Hands,Uncovered}}{(Area)_{Hands,HtoM}}$$

Ingestion 108

Method: Hand-To-Mouth Transfer (Fraction Transferred)

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment			
Exposure	Exposure (Hand)(Dermal) (Child)	*mg/day*	*Dermal 106*
	Fraction Transferred (Hand-To-Mouth) (Child) *(Based on Total Contacts Per Day)*	*unitless*	*x*
Human Factors	Area (Hands) (Uncovered) (Child)	*cm^2*	*x*
	Area (Hands) (Hand-To-Mouth) (Child)	*cm^2*	*x*
	Body Weight (Child)	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Outputs:

$$Exposure_{Child} = \frac{(Exposure)_{Hand(Dermal),Child} \times (Fraction\ Transferred)_{Hand-To-Mouth}}{(Body\ Weight)_{Child}} \times \frac{(Area)_{Hands,Uncovered}}{(Area)_{Hands,HtoM}}$$

Ingestion 109

Method: Hand-To-Mouth Transfer (EPA SOP)

Application: **Post**
Receptor: **Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (Area Treated)	*kg ai/m^2*	*x*
Environment	Fraction AI Dislodgeable in Surface	*unitless*	*x*
Exposure	Contact Frequency (Hand-To-Mouth) (Child)	*events/hr*	*x*
	Transfer Efficiency (Hand-To-Mouth) (per Contact)	*unitless*	*x*
	Exposure Duration (Child)	*hr*	*x*
	Surface Area of Hands Mouthed (Child)	*cm^2*	*x*
Human Factors	Body Weight (Child)	*Kg*	*x*
Correction Factors			
CF_1	Correction Factor (milligrams/kilogram)	*10^6*	
CF_2	Correction Factor (m^2/cm^2)	*$1x10^{-4}$*	
Calculations			
	Transferable Residue	*mg/cm^2*	
Outputs			
Exposure	Exposure (Child)	*mg/kg/day*	

Calculations:

$$Trans\ Residue = (Application)_{Area\ Treated} \times (Frac\ AI\ Dislodge) \times CF_1 \times CF_2$$

Outputs:

$$Exposure_{Child} = \frac{(Trans\ Residue) \times (Contact\ Freq)_{HtoM,Child} \times (Surf\ Area)_{HtoM,Child} \times (Trans\ Eff)_{HtoM} \times (Exposure\ Duration)_{Child}}{(Body\ Weight)_{Child}}$$

Inhalation 101

Method: Unit exposure, Area treated

Application: **During**
Receptor: **Adult**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (AI per Area Treated)	*kg ai/m^2*	*x*
	Area Treated	*m^2*	*x*
Environment			
Exposure	Unit Exposure (Inhalation) (During Application	*mg/kg ai*	*x*
	Reference Duration	*day*	*x*
Human Factors	Body Weight (Adult)	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Adult)	*mg/kg/day*	

Outputs:

$$Exposure_{Adult} = \frac{(Unit\ Exposure)_{Inhalation} \times (Application)_{Area\ Treated} \times (Area\ Treated)}{(Reference\ Duration) \times (Body\ Weight)_{Adult}}$$

Inhalation 102

Method: Unit exposure, Amount of Formulation Used

Application: **During**
Receptor: **Adult**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Application (Amount of AI in Formulation)	*kg ai/m^3*	*x*
	Amount of Formulation Used	*m^3*	*x*
Environment			
Exposure	Unit Exposure (Inhalation) (During Application)	*mg/kg ai*	*x*
	Reference Duration	*day*	*x*
Human Factors	Body Weight	*kg*	*x*
Calculations			
Outputs			
Exposure	Exposure (Adult)	*mg/kg/day*	

Outputs:

$$Exposure_{Adult} = \frac{(Unit\ Exposure)_{Inhalation} \times (Application)_{Amt\ Form\ Used} \times (Amount\ of\ Form\ Used)}{(Reference\ Duration) \times (Body\ Weight)_{Adult}}$$

Inhalation 103

Method: Air Concentration (Specified)

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source			
Environment	Air concentration of AI (Indoor or Outdoor)	*µg/m^3*	*x*
Exposure	Exposure Duration (Adult/Child)	*hr/day*	*x*
Human Factors	Inhalation Rate (Adult/Child)	*m^3/hr*	*x*
	Body Weight (Adult/Child)	*kg*	*x*
Correction Factor			
CF_5	Correction Factor (mg/µg)	*1x10^{-3}*	
Calculations			
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	

Outputs:

$$Exposure_{Adult/Child} = \frac{(Air\ Conc\ AI) \times (Inhalation\ Rate)_{Adult/Child} \times (Exposure\ Duration)_{Adult/Child} \times CF_5}{(Body\ Weight)_{Adult/Child}}$$

Inhalation 104

Method: Air Concentration, Calculated

Application: **Post**
Receptor: **Adult / Child**

Category	Variable Description	Units of measure	User Input Required
Inputs			
Source	Amount of Formulation (As Used) (By Volume)	m^3	*x*
	Fraction of AI in Formulation (As Used)	*unitless*	*x*
	Density of Formulation	mg/m^3	*x*
Environment	Dilution Factor (Indoor or Outdoor Air)	*unitless*	*x*
	Volume (Indoor or Outdoor, Imaginary)	m^3	*x*
Exposure	Exposure Duration (Adult/Child)	*hr/day*	*x*
Human Factors	Inhalation Rate (Adult/Child)	m^3/hr	*x*
	Body Weight (Adult/Child)	*kg*	*x*
Calculations			
	Air Concentration	mg/m^3	
Outputs			
Exposure	Exposure (Adult/Child)	*mg/kg/day*	

Calculations:

$$Air\ Concentration = \frac{(Amt\ Form) \times (Frac\ AI\ Form) \times (Density\ Form) \times (Dilution\ Factor)}{(Volume)}$$

Outputs:

$$Exposure_{Adult/Child} = \frac{(Air\ Concentration) \times (Inhalation\ Rate)_{Adult/Child} \times (Exposure\ Duration)_{Adult/Child}}{(Body\ Weight)_{Adult/Child}}$$

4.0 Correction Factors

Correction Factor	Description	Value
CF_1	Correction Factor (mg/kg, milligram/kilogram)	$1x10^{6}$
CF_2	Correction Factor (m^2/cm^2, square meter/square centimeter)	$1x10^{-4}$
CF_3	Correction Factor (hr/day, hour/day)	24
CF_4	Correction Factor (m^3/cm^3, cubic meter/cubic centimeter)	$1x10^{-6}$
CF_5	Correction Factor (mg/µg, milligram/microgram)	$1x10^{-3}$
CF_6	Correction Factor (mg/g, milligram/gram)	$1x10^{3}$

Appendix E – Water Module White Paper

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CARES

Water Module Specifications

CARES White Paper

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Water Module Specifications

Executive Summary

The CARES Water Module will not contain any new predictive models nor will it set policy on the proper incorporation of water residue data into exposure assessments. Instead, the CARES Water Module will reflect current policy and hopefully be able to accommodate future development. The CARES Water Module will accept any regional, seasonal water residue data that the user can provide as input, whether they are of a monitoring or modeling origin. The CARES Water Module will take these data and match them to the 100,000 individuals in the Reference Population in a statistically valid manner, and thereby derive probabilistic estimates of dose from residues in water.

This white paper will support the development of the CARES Water Module as follows:

- List the technical hurdles associated with matching water concentration data to all 100,000 members of the CARES Reference Population
- Propose alternative solutions to each of these technical challenges, and review the strengths and weaknesses of each of the various possible solutions
- Explicitly describe the solution methods chosen for the CARES Water Module
- Discuss possible enhancements for subsequent versions of this module

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Table of Contents

[Editor's Note: Page numbers have been adjusted to correspond to this document.

List of Tables

List of Figures

1. Introduction

The Cumulative and Aggregate Risk Evaluation System (CARES) is designed to estimate pesticide exposure to individuals by single chemicals by multiple pathways (aggregate assessment) as well as exposure to multiple compounds that share a common mechanism of toxicity (cumulative assessment). Although the Food Quality Protection Act[1] requires that such assessments be performed, there are currently no freely available models for this purpose. The CARES program is intended to fill this void and need.

1.1 Background and Purpose

Several modules are planned for the CARES program, each with a distinct purpose. The CARES Water Module will not contain any new predictive models nor will it set policy on the proper incorporation of water residue data into exposure assessments. Instead, the CARES Water Module will reflect current policy and hopefully be able to accommodate future development. The CARES Water Module will accept any regional, seasonal water residue data that the user can provide as input, whether they are of a monitoring or modeling origin. The CARES Water Module will take these data and match them to the 100,000 individuals in the Reference Population in a statistically valid manner, and thereby derive probabilistic estimates of dose from residues in water.

This paper discuss the development of concentration or residue profiles only and does not address the issue of daily consumption amounts for the various forms of water. This latter issue is discussed elsewhere in another CARES White Paper (Dietary).

1.2 Organization of the Paper

This white paper will support the development of the CARES Water Module as follows:

- Explicitly state the objectives and underlying assumptions of the CARES Water Module
- Define the technical hurdles associated with matching water concentration data to all 100,000 members of the CARES Reference Population
- Propose alternative solutions to each of these technical problems, and review the strengths and weaknesses of each of the various possible solutions
- Explicitly describe the solution methods chosen for the CARES Water Module
- Discuss possible enhancements for subsequent versions of this module

2. Objective and Assumptions

2.1 Objective of the Water Module

Based on information provided by the user, the CARES Water Module will fill a 365-day array of drinking water concentrations for each of the 100,000 individuals in the CARES Reference Population. The daily array of residues for each individual begins on that person's birthday and continues until his/her next birthday.

As with all other dietary routes of exposure in CARES, the daily dose attributable to water is defined as the simple product of the concentration in the water multiplied by the quantity of water consumed on that day. The daily consumption profiles for various types of water are being developed elsewhere in the CARES program, and are not discussed here. This document addresses only the issue of properly matching provided residue data to each individual in the CARES Reference Population.

2.2 Assumptions

The CARES Reference Population characterizes the individual by multiple characteristics available from the U.S. Census Bureau, including gender, age, geographic location (state and Public Use Microdata Area or PUMA), and the source of tap water at the home. The information available from the Census on the nature of the water source is extremely limited: indicating only whether it is a private dug well, a private drilled well, a community water supply, or "other" (springs, cisterns, etc.). The Census data does not contain other potentially helpful data, such as the private well depth, the identity of the specific Community Water System supplying water to the person's home, or whether the Community Water System uses surface or ground water.

Current regulatory policy provides for various "tiers" of exposure assessment in which various simplifying assumptions are successively relaxed. Exposure profiles will be more or less robust depending on the level of refinement (analysis tier). For lowest tier assessments, a single FIRST (surface water) or SCI-GROW (ground water) concentration may be available. For higher tier assessments of exposure via surface water, PRZM/EXAMS computer simulations based on the Index Reservoir scenarios are currently used. For ground water, no higher-tier computer models are now available, although this is an area of current interest for US EPA. For both ground and surface water, the highest level of assessment would generally rely upon extensive monitoring data from actual drinking water sources, possibly enhanced by some form of additional computer modeling for regions or climatic conditions not monitored.

As monitoring and modeling technologies advance, and the amount of available data increases, it is anticipated that the level of "reality" included in regulatory exposure assessments significantly increase. Until then, the CARES Water Module needs to address the current "state-of-the-art" and make the best possible use of the available tools to estimate residues, which generally have very limited geographic granularity and make severe simplifying assumptions.

2.3 Monitoring vs. Modeling

The CARES Water Module will accept residue data derived from either computer modeling or monitoring studies. It is assumed that both monitoring and modeling residue estimates may be available, and both will be used to estimate exposure for different geographic regions or different types of water sources in the same region, if that is what the user desires. Various groups have discussed the strengths and weaknesses of monitoring versus modeling approaches to

understanding probable ground and surface water residues; two significant contributions[2,3] include a recent (1998) ILSI RSI report "A Framework for Estimating Pesticide Concentrations in Drinking Water for Aggregate Exposure Assessments," and the ECOFRAM report, which is geared more towards ecological assessments. This discussion is not intended to be a thorough review of the complex subject, but highlights relevant to the development of the CARES Water Module will be summarized.

2.3.1 Background Comment on Monitoring Data

A consensus is that Water Monitoring programs can provide very valuable data but that their design is nowhere near as straightforward as it may first appear. The key step that is often given insufficient attention is the problem formulation step where the objectives, desired endpoints and statistical constraints are defined and agreed. Once this has been rigorously done, the many conflicting factors must be balanced and a clear protocol established. A very attractive option for reducing costs and avoiding duplication is to dovetail new studies with existing (often government run) monitoring programs. It would be ideal to see the various government stake holders with an interest in monitoring data combine their resources to produce a single comprehensive monitoring program to meet multiple objectives.

A key issue is the careful interpretation of water monitoring data. The interpretation must consider spatial and temporal "scaling" and underlying assumptions. When describing the study, it is essential to describe the above factors to provide the "context" which is essential to make sense of the measured numbers. It is therefore critical for monitoring study authors to provide full and specific descriptions of key factors such as: site selection, whether stratification was employed, the adequacy of the analytical methods, and the presence of QA/QC data. Only then can the study author convey a realistic view on the uncertainties associated with the measurements.

2.3.2 Applicability of Monitoring and Modeling to Human vs. Ecological Risk Assessments

While there has been much recent public and regulatory debate about the use of probabilistic modeling (and to a lesser extent monitoring) data for Ecological Risk Assessments, it is important to realize that the endpoints and concerns of ecological risk assessments are subtly different from those involved in human risk evaluations. For example, the spatial and temporal scales tend to be more local/ shorter and the local variability is higher in Ecological Risk Assessment. This variability has helped to drive the increased interest in probabilistic methodologies. Moreover, the high variability and extremely limited monitoring data available at an appropriate local scale has meant that modeling has become the generally accepted optimal approach for early tier risk assessments even despite the lack of accepted flowing water models and scenarios. The task facing regulatory ecological risk assessment experts now is to blend together the modeling predictions with the limited amount of valid and spatially relevant monitoring data to build confidence in model output such that there is more general confidence that the model output is suitably predictive in all of the aquatic settings of ecological interest.

On the other hand, Human Risk Assessment (i.e. drinking water exposure assessment) differs in some interesting ways. For example, the spatial and temporal scales are broader for most SW derived drinking water, and monitoring data are more frequently available on this scale. Hence measured monitoring data tend to be a more frequently used approach for HRA cumulative assessments relative to ecological assessments. However, models are still often necessary for dealing with both new chemistries and uses or regions where only limited drinking water monitoring data are available. For both ecological and human exposure assessments, the general trend is for use of more monitoring data as one progresses toward the higher-tiers.

2.3.3 Discussion of Pro's and Con's of Modeling and Monitoring

A series of strengths and weaknesses of monitoring in comparison with modeling have been identified; these are summarized in Table 1 below.

Table 24 – Relative Strengths and Weaknesses of Modeling and Monitoring

Modeling	Monitoring
PRO Cost Effective (generally less expensive than monitoring) Ability to predict concentrations over a continuum in space and time Comparative exposure assessments are possible Relatively quick - days to months Can evaluate "what-if" scenarios and sensitivities (e.g. climate, soil, application date) Can incorporate effectiveness of possible mitigation alternatives Not constrained by analytical LOD Can quantify relative to "benchmarks"	**CON** Costly Time involved is weeks to several years Difficult to design cost effective AND technically viable sampling programs May require many years of monitoring and/or paired studies to evaluate effectiveness Handling non-detects is difficulty Results blindly accepted as "true" values regardless of QA/QC and study design issues Sampling represents discrete points in space and time that can only be put into context with modeling Study only represents one unique combination of conditions Can be constrained by analytical precision and LOD Difficult to interpret results in a probabilistic fashion due to typically low N values Subject to distortion by "unusual" weather Cause & effect difficult to assign
CON Simplifications required in the representation of prototype systems There is general public reluctance to accept predicted data Calibration/validation is needed to assess how closely predicted values match reality Many of the input values have high uncertainties associated with them The selected input parameters may not be environmentally feasible Model algorithms may oversimplify or misrepresent compound behavior Tends to use conservative assumptions Levels of uncertainty in inputs not obvious Data on pesticide use unavailable Useful watershed and flowing water scenarios not currently available	**PRO** Provides an actual measurement of chemical residue concentration, hydrologic response etc Avoids conservatism resulting from compounding conservative assumptions When done well it is an excellent tool Accounts for the inherent heterogeneity of the system There is a greater acceptance of measured data There is public confidence in monitoring data Real world hydrology Accounts for actual pesticide usage Does not require algorithm/ model development & validation

As discussed in the ILSI report,[2] the most powerful use of monitoring studies is as a combination approach using thoroughly planned monitoring data across several years to calibrate models in which regulators have confidence. Modeling will provide probabilistic estimates of exposure across time and space to set the monitoring data into context by consideration of the actual rainfall experienced and the watershed(s) involved.

2.3.4 Aspects Of Different Monitoring Studies Used To Evaluate Pesticide Runoff into Surface Water

A critical factor in the interpretation and use of Surface Water monitoring data is that of scale. The available data may range in scale from very small test plots of less than 0.05 hectare to large basins spanning the entire continent (eg. the Mississippi River at New Orleans). As indicated in Table 2 (below), only watersheds of basin scale or larger can be used as sources of drinking water. Thus only monitoring data from such larger scale basins should be used in Human Risk Assessment. The conclusion reinforced the earlier statement that great care has to be taken to selecting monitoring programs to exactly match the problem formulation.

Table 25 – Effect of Scale on the Interpretation of Modeling and Monitoring Data

Factor	Too Small to Supply Drinking Water		May Supply Drinking Water
	Small-Scale Test Plots	Sub-basins	Basins
Drainage area size	<0.05 hectare	10 to 40 hectare	10 to >100 km^2
Flow regime	Overland (partial)	overland, ephemeral streams, ponds	perennial streams, rivers, lakes, reservoirs
Point of interest	runoff potential	worst-case exposure	large-scale exposure, dilution
Site characterization	high	moderate/high	low
Control over system	high	moderate	low
Simulate precipitation	yes	difficult	no
Study duration	days	season-years	years
Field heterogeneity	neglected	represented	represented
Field-scale influences on pesticide transport	neglected	represented	represented
Artificial Drainage	low	may be studied	include as realistic
Focus	research, idealized system	evaluate proposed labeled use of product	reality
Calibration w/ transport model	event based	continuous simulation	multiple segments, continuous simulation
Extrapolating model to field scale	questionable	inherent	difficult to verify w/out observations
Extrapolating model to other fields	questionable	questionable	questionable

2.3.5 Tiered Exposure Assessment Techniques

For simple reference, a brief description of proposed tiered exposure assessment techniques for evaluating drinking water exposure is given in Table 3. This information should be viewed only as one possible snapshot of a continuously evolving reg ulatory assessment process.

Table 26 – Proposed Exposure Assessment Tiers for Evaluating Drinking Water Exposure

Tier	Dug Wells	Drilled Wells	Community Water System		
			Ground Water	Reservoir	Flowing Water
1	SCIGROW	SCIGROW	SCIGROW	FIRST	FIRST
2	Calibrated PGW (Prospective Ground Water) dataset[1] with aquifer dilution component and 36-year weather	Statistical sampling of regional monitoring data (or regression-based predictions from regional monitoring data)	Statistical sampling of regional monitoring (or regress-ion-based predictions from regional monitoring data) of wells from appropriate aquifer(s)	Statistical sampling of regional monitoring (or regression-based predictions from regional monitoring data) from appropriate sized static water systems or Regional Index Reservoir w/ 36-year weather (for each region, produces 36 scenario-years).	Statistical sampling of regional monitoring (or regression-based predictions from regional monitoring data) from appropriate sized flowing water systems or Regional Index River model w/ 36-year weather
3	Population-weighted sampling of regionalized monitoring and/or modeling data specific to the pesticide(s) of interest, appropriately adjusted for variations in local hydrology and well vulnerabilities.		Population-weighted sampling of regionalized monitoring and/or modeling data specific to the pesticide(s) of interest, appropriately adjusted for variations in local watershed and drinking water intake characteristics.		
4	Probabilistic (possibly Monte-Carol based) assessments taking the Tier 3 analyses to a higher level of accuracy by incorporating temporal variation in land use, weather, and other factors known to influence concentrations in ground and surface water				

[1] Although PGW wells are drilled, not dug, they are shallow wells (< 30 ft) that monitor the top of the aquifer and are therefore expected to be a better predictor of concentrations in dug, potable wells, which are generally shallower and more otherwise more vulnerable than drilled, potable wells.

2.3.6 Use of Existing Monitoring Data

Notwithstanding the earlier comments about the need to carefully tailor monitoring data to the specific issue, there is potential value to making use of results from ongoing monitoring programs from government, academia, and industry. Some of the more significant programs include NAWQA, the Heidelberg Water Quality Laboratory monitoring work in Ohio, MSEA studies, the USGS mid-continent monitoring program, and various registrant-sponsored studies from the Crop Protection Industry.[4-8] Although some of these studies include water samples not collected at drinking water intakes, the data certainly can be used to estimate potential exposures via drinking water. These data can also be used to help refine runoff and leaching modeling approaches.

2.3.7 Exchanging Time and Space

An important and often over-looked theme in the interpretation of monitoring data is the extent to which time and space are "exchangeable." The question is whether a monitoring study with a large number of sites across a large geographic extent for a relatively short period of time is able to adequately characterize potential residue levels for a long period of time at a single site. There is a complex balance between time and space as we attempt to weigh the relative benefits of sampling many sites in a short period of time (1 year) or fewer sites over a long period of time (multi-year). It seems clear that it should not be necessary or practical to sample myriads of sites over many years to understand the distribution or "see the true peaks," but this is an area where additional scientific effort may be needed.

2.4 Environmental Degradates

In general, environmental degradates (often imprecisely referred to as "metabolites") will simply be treated as another analyte in the cumulative assessment. It is important to note that such degradates should be included in the parent assessment only if they share a common mechanism of toxicity. A special case that must be considered by the CARES Water Module is the possibility of degradate-formation in water treatment facilities. This is a unique, separate issue that is discussed in section 3.2.2.

3. Technical Hurdles

As should be obvious from the brief discussion already presented, there are several basis technical questions that must be addressed in order to convert user-provided residue data into a sensible set of 365-daily concentration arrays for all 100,000 members of the CARES Reference Population. These questions include:

1. How should we deal with the **varying sources of dietary water** that an individual may consume during the year?
2. How should we model the effect of **water treatment** on the residues?
3. What should be the smallest possible geographic units of analysis in the assessment (denoted here as **geographic granularity**)?
4. How should **temporally sparse data be interpolated** to fill out the required array of daily residue levels?
5. How should **"zeroes" or undetected** pesticide residue levels in water be modeled?
6. Are there special technical concerns as we sample from conventionally **calendarized data** (January 1 through December 31) to create a daily-array of residue levels from birthday to birthday for each member of the CARES Reference Population?
7. What are the special concerns with the development of residue time series for multiple pesticides when a **cumulative assessment** is performed, such that co-occurrence is properly characterized?
8. How may residue profiles for **highly vulnerable water sources** be adjusted for systems with lower pesticide use and/or lower intrinsic vulnerability?
9. What level of flexibility should be provided to the user to use residue data from one geographic region and apply it to a different geographic region for which no data are otherwise available (denoted here as **geographic surrogation**)?

3.1 Varying Sources of Dietary Water

3.1.1 Sources of Tap Water

All real individuals consume tap water from a variety of sources. For example, a person might regularly drink tap water from home as well as at work, school, stores, airports, houses of friends and neighbors or other locations outside the home. Whether residues of crop protection products and their degradates will be higher at the home or away from home depends on the characteristics of the specific sources and the chemicals under consideration.

If the source of a person's tap water at home is a Community Water System, then likely the source for most places outside the home will also be a Community Water System. Most likely the quality of the tap water will be similar (often the source will be the same Community Water System).

If the source of a person's tap water at home is a well, then the source of tap water outside the home will not be the same source. In the majority of cases, the source will be a Community Water System. In almost no cases will the source outside the home be a dug well. The only exception would be when visiting or working at a private home with a dug well. In general, for people drinking from well water at both home and away from home, the person's source of tap water outside the home is likely to be of higher quality. This is because wells at commercial facilities are likely to be screened deeper into the water table and of better quality construction to prevent leakage around the well casing.

Because a recently completed survey provides information on consumption of tap water in and outside the home for people of all ages, CARES should be coded to allow for two sources of tap water, in and outside the home. There are various reasonable default assumptions for determining the source of tap water outside the home:

- If the home source is a Community Water System, then the source of tap water outside the home could also be considered to be the same Community Water System.
- If the person's source of water is a drilled well, then the source of water outside the home could also be considered to be a drilled well unless the person is located near an area served by a Community Water System (it is not immediately clear how this determination could reasonably be made for all 100,000 members of the CARES Reference Population).
- If the person's source of water is a dug well, then the source of water outside the home should be considered to be a drilled well unless the person is located near an area served by a Community Water System (as above, it is not clear how this determination could be made).

A special concern for those individuals using a Community Water System as their source of tap water is that the source utilized by the facility may be changed during the year as a general practice or in response to unusual circumstances such as drought. It is unclear whether this can or needs to be modeled in order to get a realistic overall impression of exposure to pesticides for the sub-populations of interest.

3.1.2 Other Dietary Water

All individuals consume types of water other than that which comes directly from a tap. The obvious examples include bottled water, water used in cooking, and various commercial sources of water. Little to no data exists on the actual residue levels in such sources of dietary water, but there are various "bracketing" assumptions that could be made concerning such residues. They could be:

- Set to "zero" (see Section 3.7).
- Set equal to tap water concentrations.
- Set to a constant or distributional multiplier of the residues present in tap water.

In unusual cases, it is possible that actual residue data may be available for these other dietary sources of water. For instance, bottled water may be monitored in future years as part of the USDA Pesticide Data Program (PDP). However, it seems likely that comprehensive monitoring data are not likely to be available in the short-term and need not be considered by the CARES Water Module at this time.

3.2 Effect of Water Treatment

3.2.1 Reduction of Residues via Treatment

A significant portion of the consumed water in the United States has received some level of treatment. Some form of treatment (at least disinfection) is required for all surface water and for all water used in commercially processed foods. Ground water may also be treated before consumption. Treatments include both physical and chemical methods. Physical treatment options include simple filtration to remove sticks, leaves, and sediment, sand filters, highly efficient membrane filters, etc. Chemical methods of treatment include flocculation to remove suspended solids, use of activated carbon to remove various compounds, and treatment with various halogens including chlorine to reduce bacterial levels in potable water. In addition, in certain areas UV radiation or other techniques may be used to treat consumed water. Of course, there is also treatment of water within the home before it is consumed. For example, water added to condensed soup is then raised to a relatively high temperature before being consumed.

The effects of water treatment on chemical residue levels are dependent on the type of treatment, the intensity of treatment, and the characteristics of the chemical compound. For example, residue levels of highly sorptive compounds would be significantly decreased by simple filtration techniques. Some compounds are greatly affected by chlorination or bromination, others by heating. Completely ignoring the potential for treatment effects would result in less accurate estimates of the pesticide exposure properly ascribed to dietary water.

Within the CARES Water Module, one could allow the user to specify the effects of treatment for various types of water for all of the compounds being analyzed. For example, a person may consume water from a Community Water System with simple filtration as a part of prepared foods at home, bottled water, and commercially processed water in soda. It may be sensible to permit the CARES user to specify that residues in the local Community Water System are reduced by a set factor (eg., 50%), that bottle water contains no residues, and that the filtration systems used typically in commercial plants remove the compound completely. Although it is not practical at this time, future versions of CARES may be able to take into account the effects of food preparation (heating, boiling, etc.) on residues in consumed drinking water.

3.2.2 Treatment-Related Degradate Creation

The CARES user should take into consideration the possible formation of degradates (sometimes imprecisely referred to as "metabolites") of interest during the water treatment process. In other words, if there is substantial evidence that a specific treatment process could result in conversion to a relevant degradate, then appropriate adjustment to the treatment factor should be made. As noted above, such degradates should be included in the parent assessment only if they share a common mechanism of toxicity.

It is important for the user to base all decisions concerning the use of a treatment factor on actual data. Of course, assumptions can be made based on laboratory testing. However, the CARES user should be attentive to the conditions under which any such data were derived. The user should consider whether or not the test conditions and therefore any results are relevant to the treatment of drinking water.

Case 1: Degradate which is as toxic as parent (or assumed as such).

Adjust treatment factor for known conversion from parent to degradate and represent degradate as parent. Assumes there is not full conversion and some mass of parent may be lost to another degradation process.

Case 2: Degradate which is more/less toxic than the parent.

Adjust treatment factor for parent based on a ratio of toxicity while considering conversion from parent to degradate.

Otherwise, the degradate in this case would have to be addressed individually based on its conversion rate by adjusting observed or modeled parent residues.

Of course the simplest case is one where there is a known direct conversion (by a particular treatment method) to a degradate of equal toxicity. In this case the adjustment factor in CARES should not be used. For example, 30% degradation of parent to equal part degradate.

Representing a degradate as parent equivalents is the simplest and most efficient way to handle this issue. Single-valued or distributional values for the "degradate factor" could be implemented within CARES, and it is possible that different values should be permitted for different types of water treatment facilities (eg. surface water vs. ground water, cooking at home, etc.).

3.3 Geographic Granularity

Geographic granularity refers to the spatial resolution or smallest "geographic unit of analysis" to be used by the CARES water module for integrating drinking water concentrations into the aggregate residue risk assessment. Granularity encompasses two aspects within the CARES program: 1) the smallest geographic region that may be applied in data aggregation and interpretation (i.e., the desire to subdivide the risk assessment down to the state, regional, or possibly the water supply level); and 2) the smallest geographic units used during the assignment of residues to specific members of the CARES Reference Population.

Spatial resolution is important in developing accurate estimates of exposure for the Reference Population. Individuals have potential exposure from numerous sources, including tap water at their residence and work place and imported commodities (e.g., bottled water or soft drinks) originating from water sources in other counties or states. The occurrence of agricultural chemicals in a specific drinking water supply is dependent on regional and local factors that determine the susceptibility to, and retention of, chemical residue in that supply. These factors include the spatial variability in climate, geomorphology, crop production and pest pressures (and consequently chemical use), and agronomic practices in the contributing watershed or aquifer system and the hydrodynamic response of the water body.

Assimilating this information into a risk assessment can be a monumental task because of limitations in readily available spatial information. In practice, much of the relevant spatial information presently available has not been compiled into national databases. Often data resides only at county level or higher resolution. Therefore, spatial information can only be addressed in a crude and cursory manner in the early stages of the risk assessment process. Information refinement often occurs when there is a need to focus on specific issues or areas or concern. What will really drive the accuracy of the CARES assessment is the ability to provide data at progressively smaller units of analysis, and/or our ability to model the same. For example, assuming appropriately refined monitoring or modeling data are available, it should be more accurate to build exposure profiles on a site-specific basis for each individual, rather than to lump huge regions together (e.g., assume a single concentration profile for the entire southeast).

Our knowledge of exposure therefore currently varies, depending on the progression of the risk assessment and the availability of data. In some cases, drinking water exposure concentrations may be limited to a few data sets (exposure profiles) that by necessity or default must represent broad geographical regions of the country. In other cases, it may be possible to generate multiple exposure profiles that are either keyed to specific point locations across the country or are representative of conditions that may exist within or across some larger regional area. As a result, aggregation of smaller units to larger geographic regions must be possible within CARES in order to maintain flexibility and accommodate different levels of refinement in the risk assessment.

In addition, the geographic unit of analysis needs to be compatible with methods that may be employed to assign exposure profiles to the Reference Population. Associating an exposure profile to an individual in the Reference Population can occur using several methods, including 1) assignment based on the proximity of the individual to an available exposure profile, 2) the random assignment to one of several exposure profiles within a regional boundary based on population weighting (proportion), and 3) data surrogation by assigning an exposure profile to an individual according to similar characteristics. Examples of each of these methods are discussed below.

- Proximity: An individual from the Reference Population is known to consume water from a given community water supply. At the current level of refinement, exposure profiles that are representative of community water supplies are available for a number of point

locations. The individual is assigned to an annual exposure series based on their proximity to a particular point location.

- Proportion: An individual from the Reference Population is known to consume water from a given community water supply. There are three community water supplies within the geographic unit of analysis (A, B, and C). The individual is assigned an annual exposure series from water supplies A, B, or C according to the relative probability of being served by that supply. A, B, and C serve 33, 47, and 20 percent of the total population served by community water supplies in the region, respectively. Therefore, in this example, it is most likely that the individual will be assigned an annual exposure series from water supply B.

- Surrogation: An individual from the Reference Population is known to consume water from a domestic well. The individual is assigned an annual exposure profile from a data set that has similar soils, climate, ground-water depth, and crop density to the geographic area in which the individual resides.

A number of geographic units of analysis were considered and evaluated for implementation into the CARES water module. Consideration was given to commonly available geographic units that already have a history of use in risk assessment and data surrogation. Delineations considered include state and county boundaries, US Farm Resource Regions, crop trial growing regions, Land Resource Regions (LRR's), Major Land Resource Areas (MLRA's), Land Resource Units (LRU's), Crop Reporting Districts, State Climatic Zones, Census PUMA's, and Hydrologic Units of various resolutions. Other desirable geographic units, although not readily available in a national database at the current time, would be the watershed boundaries (surface water), well -capture zones (ground water) and service areas of individual water sup plies. Descriptions of these geographic units are provided in Table 3 along with a qualitative assessment of their applicability with respect to data aggregation and exposure profile assignment to the Reference Population.

The boundaries of six of these possible classification systems are depicted in Figures 1-6. The intakes, service areas, and watershed boundaries of individual water supplies are not depicted because these boundaries have not yet been compiled into a single national database.

Four possible geographic units of analysis are recommended for possible use within CARES: states, US Farm Resource Regions, 8-digit Hydrologic Unit Codes, and watershed boundaries for individual water supplies. Justification is provided below.

- State boundaries. Political boundaries provide convenient units for regulatory decisions and enforcement. Also, information that may exist only at the state level can be utilized for exposure profile assignment. However, political boundaries have little correlation with watershed delineations and prohibit the ability to address the heterogeneity of land use, water resources, and population density across the state. Perhaps most importantly, states are one of the few geographic units for which definitive pesticide use data are available.

- US Farm Resource Regions. Regional classification developed by USDA based on cropping, agronomic, and farm-economics factors. Used by USEPA to develop scenarios for the OP Cumulative Exposure Assessment.

- 8-digit Hydrologic Unit Codes. HUC-8 boundaries are based on watershed delineations and therefore the classification system by design can be used to identify all contributing drainage areas to the basin outlet. The resolution is sufficiently course for integrating county-level information and is generally compatible for the analysis of NAWQA sampling points. HUC-8 watersheds can be selected from a region as representative watersheds for detailed evaluation and data surrogation. Although the watersheds of individual Community Water Systems rarely coincide precisely with HUC-8 boundaries, HUC's are

a convenient and widely used geographic unit of analysis in surface water assessments.

- Individual water supplies. USEPA is currently involved in a nationwide study to characterize watershed properties for community water supplies throughout the country, and this has already been for smaller geographic regions, such as the 12 state monitored by the Acetochlor Registration Partnership (ARP). This information has the potential to be used to develop water-supply specific exposure estimates by either data surrogation or individual model predictions.

In summary, four potential units of geographic analysis are potentially useful in the CARES water module: states, US Farm Resource regions, 8-digit Hydrologic Unit Codes, and the drainage area delineations of individual water supplies. The appropriateness of using a particular geographic unit of analysis is dependent on the availability of all required input data at the appropriate level of spatial resolution. Note that it is critical that these data layers be publicly available in order to be used by CARES, which is free software based entirely on public data.

Table 27 - Geographic Units Considered for the CARES Water Module

Geographic Unit	Description	Pros	Con
State	Political boundaries	Appropriate for cursory evaluations at the state level or for integrating state and county-resolution data. May permit exposure profile assignment to Reference Population individuals based on broad proximity or surrogation if exposure profiles are not prolific.	Does not address spatial variability in land use, population density, and other factors at the watershed or water supply scale.
County	Political boundaries	Accurate county-level cropping data are generally available from the USDA	Pesticide use data generally not publicly available to this level of spatial resolution
US Farm Resource Regions	USDA regional classification based on relatively broad economic and agronomic characteristics of farms within a region	Used with some modification in recently proposed EPA Cumulative Risk Assessment methodology for the OP insecticides.	Pesticide use data are not publicly available for these regions.
Crop trial growing regions	Regional classification based largely on state boundaries. Used to define cropping areas for design of residue crop studies under FIFRA	Provides general regional characterization of agricultural production areas for major crops. Applicability for utilizing existing modeling scenarios with Index Reservoir configuration based on surrogation.	Does not address spatial variability in land use, population density, and other factor at the watershed or water supply scale. Model scenarios only address variability in climate and soil properties.
Common Ecological Regions	Spatial framework for defining ecological units of the U,S. based on naturally occurring and recognizable features such as soil, geomorphology, climate, water, and vegetation. Cooperating agencies include: U.S. Department of Agriculture (Natural Resources Conservation Service, Forest Service, Agricultural Research Service), U.S. Department of the Interior (Bureau of Land Management, U.S. Geological Survey, Fish and Wildlife Service, National Biological Service, National Park Service), and the U.S. Environmental Protection Agency.	Provides better differentiation for smaller acreage crops than Land Resource Regions, state, and US Farm Resource regions.	May contain excessive number of regions for major crops. Does not address spatial variability in land use, population density, and other factor at the watershed or water supply scale. Does not reflect hydrology issues directly

Table 4 – Geographic Units Considered for the CARES Water Module (continued)

Geographic Unit	Description	Pros	Con
Land Resource Regions (LRR)	Geographically associated major land resource areas (MLRAs) , which approximate broad agricultural market regions.	Provides broad regional boundaries for major crops.	Does not depict high intensity agricultural areas for smaller acreage crops. Does not address spatial variability in land use, population density, and other factor at the watershed or water supply scale.
Major Land Resource Regions (MLRA)	Geographically associated land resource units (see below) with dominant physical characteristics of land use, elevation and topography, climate, water, soils, and potential natural vegetation.	Historical uses in FIFRA for model scenario development.	Impractical unit for risk assessment. Does not address spatial variability in land use, population density, and other factor at the watershed or water supply scale.
Land Resource Units (LRU) / Common Resource Areas (CRA)	Geographical areas, usually several thousand acres, characterized by a particular pattern of soils climate, water resources, and land uses. LRU's are the basic units from which MLRA's are determined.		Impractical unit for risk assessment. Unlikely unit for nationwide exposure distributions. Does not address spatial variability in land use, population density, and other factor at the watershed or water supply scale.
8-Digit Hydrologic Unit Codes (HUC-8)	Hierarchical classification of hydrologic drainage basins in the U.S. HUC-8 contains 2150 cataloging units.	Sufficiently course resolution for integrating county-level information and interpretation of NAWQA program. Representative HUC-8 can be selected for regional characterization.	Does not address spatial variability in land use, population density, and other factor at the water supply scale.
PUMA	Geographical cataloging unit of Census. One PUMA represents 250,0000 people.	Spatial resolution of Reference Population.	Boundaries do not coincide with watershed delineations or spatial factor details.
CWS service district	Population service boundaries of individual community water supplies.	Most precise possible assessment endpoint.	Not currently available in a national database.

CWS = community water supply

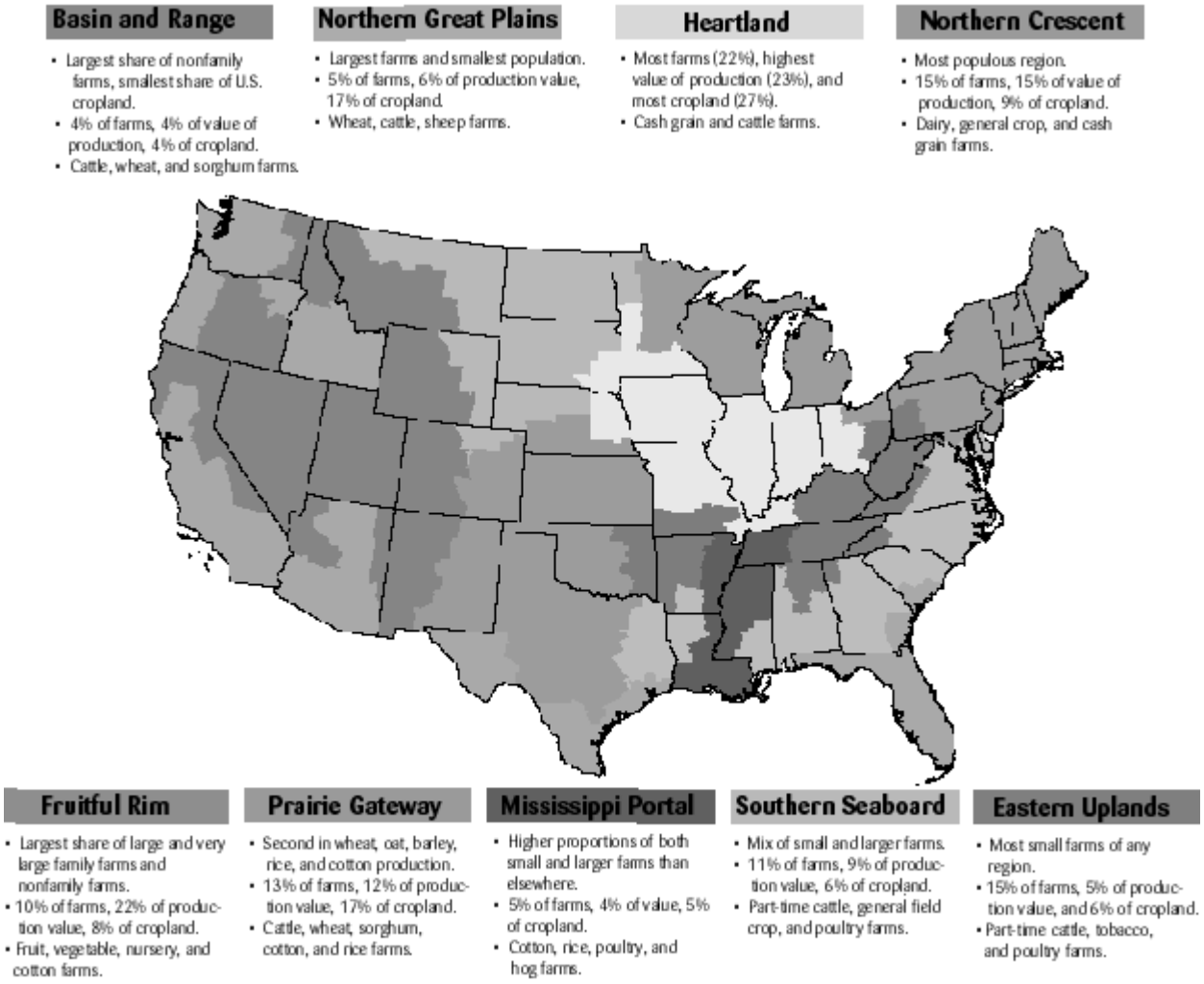

Figure 8 – US Farm Resource Regions

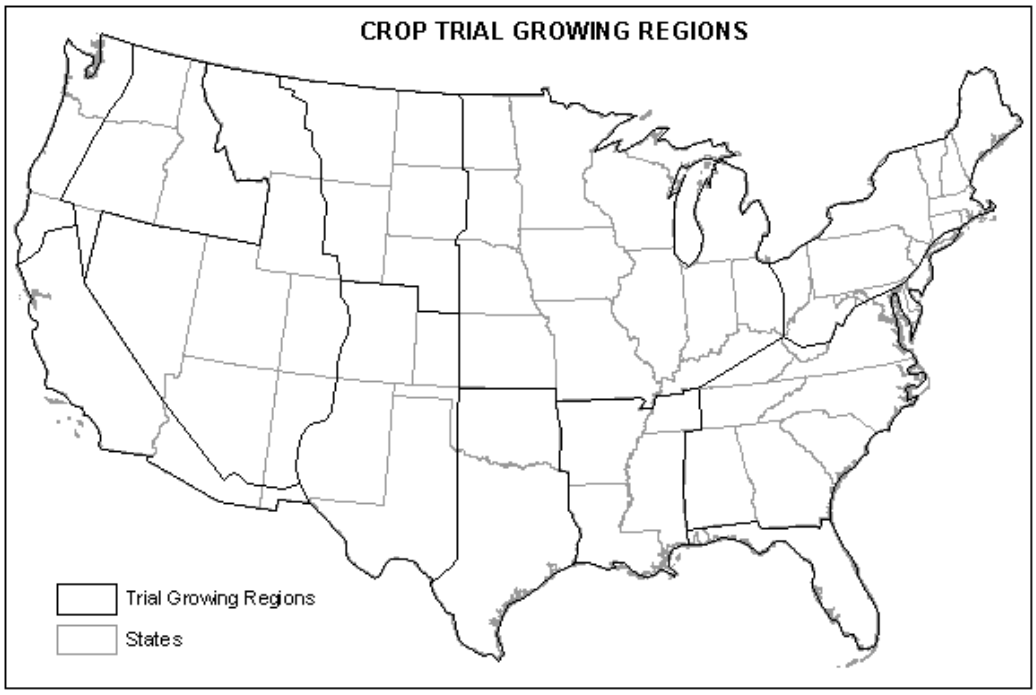

Figure 9 – Crop Trial Growing Regions

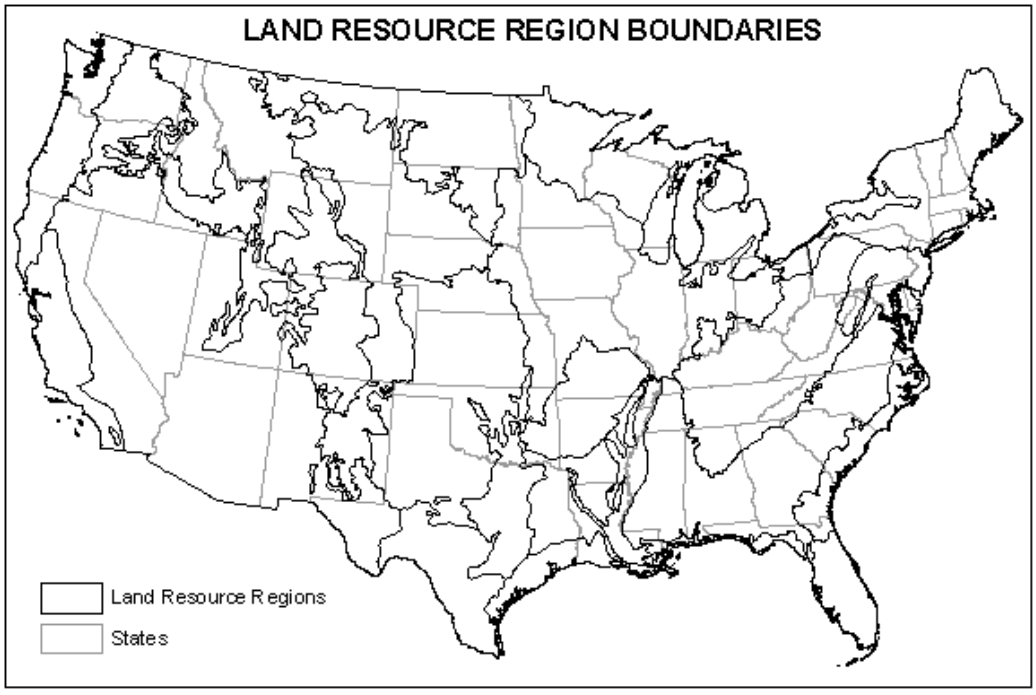

Figure 10 – Land Resource Regions

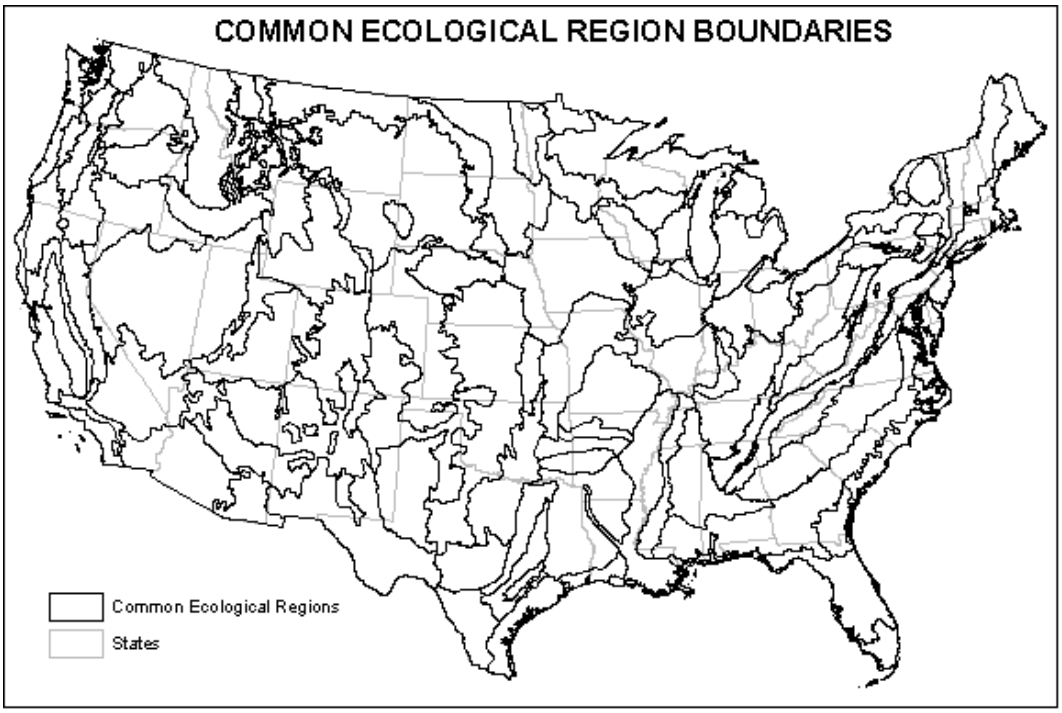

Figure 11 – Common Ecological Regions

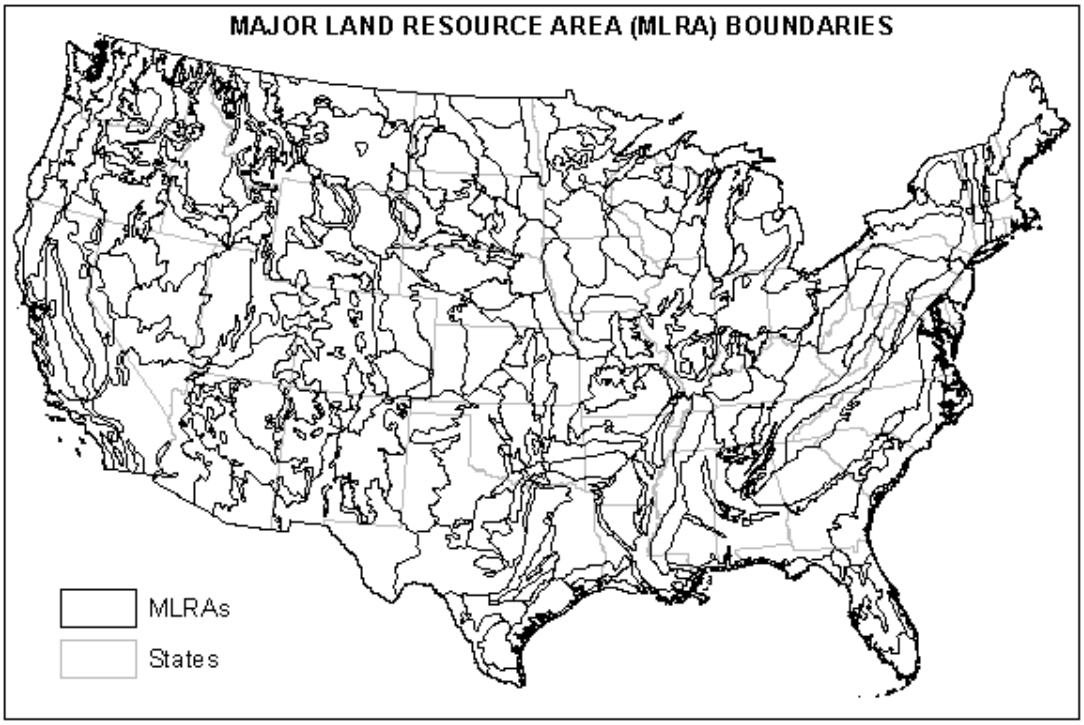

Figure 12 – Major Land Resource Areas (MLRA's)

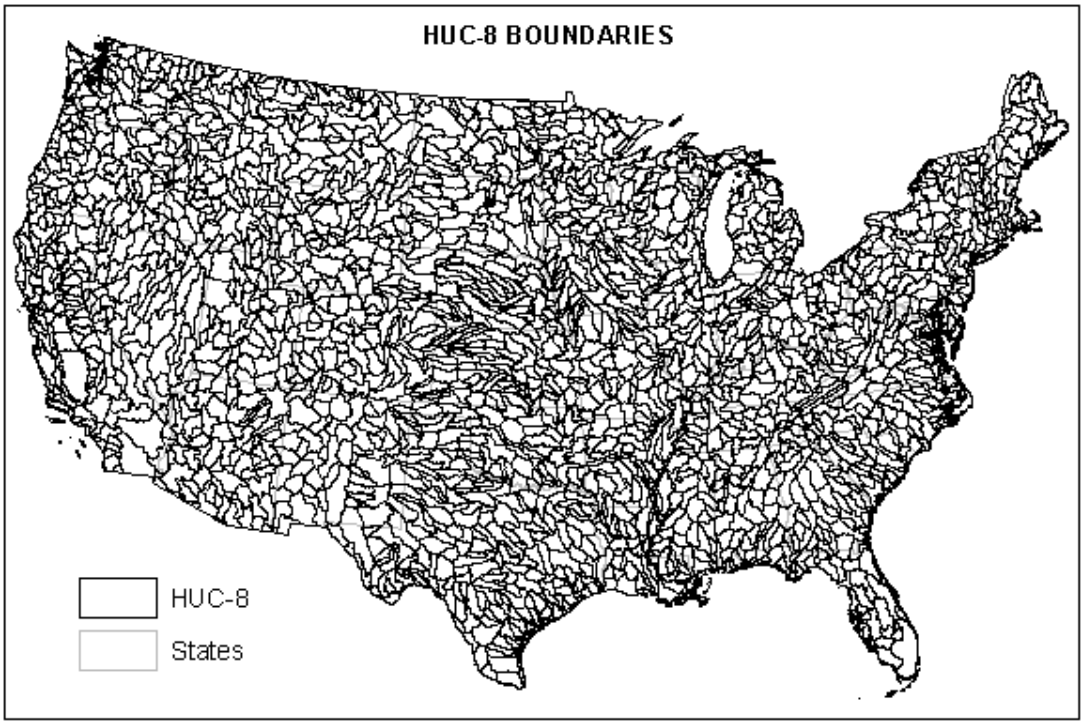

Figure 13 – 8-Digit Hydrologic Units (HUC's)

3.4 Temporal Interpolation of Sparse Data

Temporal patterns of chemical concentrations in drinking water supplies reflect the seasonal period of chemical use; meteorological conditions that drive chemical movement by spray drift, runoff, and leaching; the physicochemical properties of the chemical; the duration of the entry event; and the hydrodynamic response of the receiving water system. For a given entry event, river systems will typically exhibit relatively short duration pulses, on the order of days, compared to reservoir and aquifer systems that may have hydraulic residences times on the order weeks to months (Figure 7). If the use of a chemical is limited to a specific time of year, such as at pre-emergence or at planting, entry into drinking water sources are most likely to occur just after that same period of time. Spray drift to water bodies can only occur at the time of application, but other forms of drift (vapor, rain-borne, etc.) are possible for some period after application. Runoff loads are largely driven by the first significant storm events following application. Chemicals applied over a longer-duration season are likely to exhibit an extended period of entries and detections. Chemical runoff will not occur during periods of drought and will not be at detectable levels after the chemical has undergone sufficient degradation in the field.

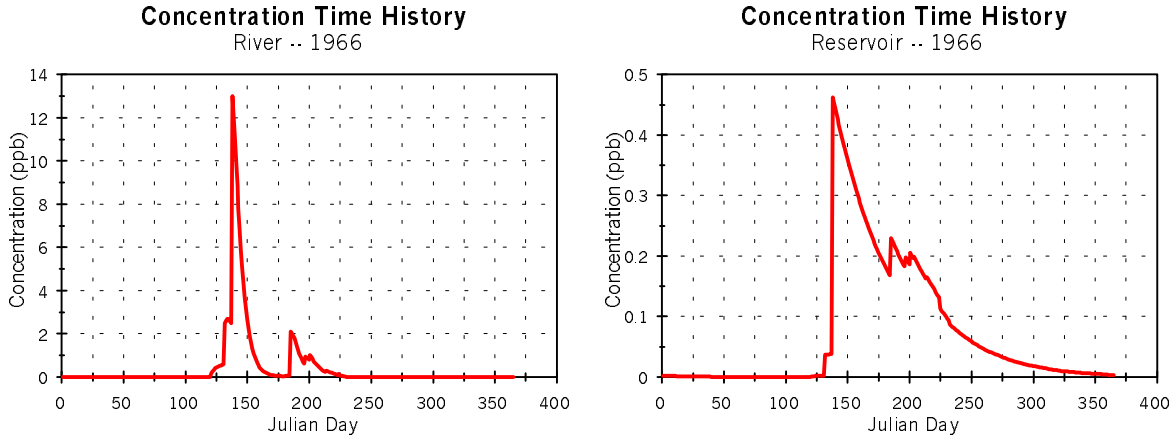

Figure 14 – Example Chemo-Graphs Showing Effect of Hydrologic Residence Times

Missing data are an inevitable consequence of monitoring studies because of economic and logistical constraints. In the CARES water module, methods for interpolating between measured data points will vary depending on the amount and timing of missing data as well as the temporal spacing of the sampling relative to the hydrodynamic response of the water system. Moreover, the existence of missing data adds another dimension to the general problem of how to deal with "non-detects" in monitoring data (see Section 3.5 "Dealing with Zeroes").

While it may be technically possible (in principal) to use available rainfall and/or flow data from nearby sources to help fill-in sparse data, such an approach is not tenable for a generalized exposure assessment tool such as CARES. Instead, this discussion will be confined to general mathematical approaches where no site-specific data are available.

3.4.1 Simple Linear/Nonlinear Interpolation

Certain comprehensive monitoring studies are designed to collect and analyze water samples at a frequency sufficient to directly construct daily chemo-graphs of chemical concentration over time. For a simple case of one to two consecutive days of missing data when sampling was taken on such a daily basis, a direct linear interpolation between the nearest previous observation and the following observation should be adequate to estimate the missing data.

For water bodies with slow response times, such as larger rivers and lakes, it is often seen that pesticide concentrations in the water column degrade according to linear, first-order kinetics. For missing data in these types of systems, linear interpolation on a log-scale would be the more appropriate method for filling-in missing portions of the data.

3.4.2 Use of Simulation Modeling for Interpolation

Cases with more than a 1-2 days of missing data and/or missing data in studies with sampling schedules at a frequency lower than daily present a need for a more complex approach to estimating missing data, particularly for rapidly flushing systems that have a hydraulic residence time on the order of days. In such flowing systems, there is some opportunity to miss important peak concentrations from pulse dose loads that may have occurred during this period.

An important practical consideration here is the overall size of the monitoring database being sampled. For large datasets with multiple years and multiple sites, it is likely that exposure profiles will be adequately represented across all sub-populations of interest, regardless of the method of interpolation chosen. However, if the monitoring data are very sparse (such as quarterly samples from just a few sites) it will generally be necessary to rely upon modeling to estimate exposure, and the sparse monitoring data could be optionally used to help “scale” the monitoring data. An example of this idea is shown in Figure 8.

It is assumed here that a user would provide both sparse monitoring and continuous modeling data to CARES. A year of the modeling data is selected (at random, as elsewhere) and a year of modeling is selected. Annualized time-weighted mean concentrations (AMC’s) of the monitoring and modeling data are calculated and the ratio is used as a constant multiplier of the modeling data, which is then used to fill the daily time series array.

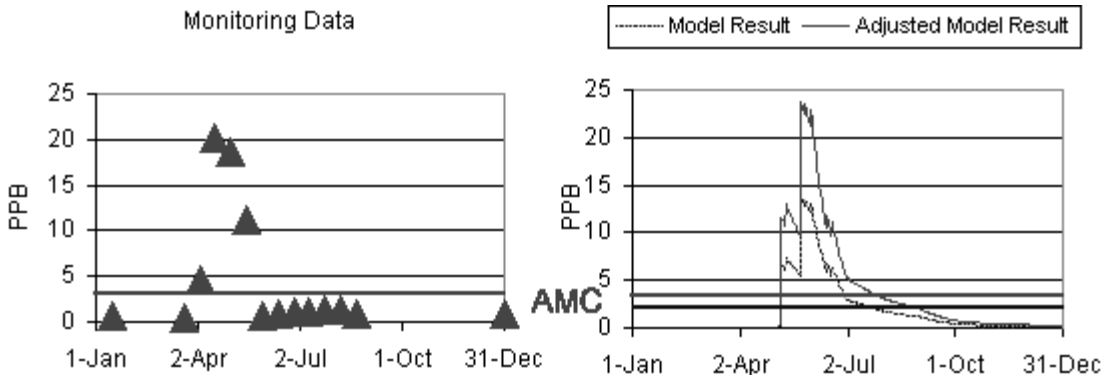

Figure 15 – Example Showing Use of Monitoring Data to “Scale” Model Predictions

In this example, the AMC's for the monitoring and modeling data are forced to be equivalent. Another option would be match other points on the distribution, such as 90th or 95th percentile levels of exposure. Of course, if very sparse modeling data that one is attempting to interpolate, this would generally require the assumption or fitting of a particular form of distribution to the modeling data.

3.4.3 Surrogation of Monitoring Data from an Adjacent System

Monitoring data from a system of similar geomorphology, land use, and climate can be used to supplement a missing period of data (if runoff or GW/ SW interactions are the drivers for chemical entry. Results can be adjusted to account for differences between sensitive variables including cropping (and/or chemical use) density. Some corrections in concentration timing and attenuation may be necessary to account for basin size and shape.

3.5 Dealing with Zeroes

At several points within the CARES Water Module, there will be instances where extremely low (near-zero) residues are appropriate. Examples of this would include:

- For surface water, low-vulnerability systems such as the Great Lakes, or specially-protected watersheds
- For ground water, extremely deep, properly-installed water supply wells
- Water sources in states without any use of the pesticide, either in -state or upstream (in the case of surface water supplies drawing from multi-state basins
- "Non-detects" in uncensored, raw analytical data from monitoring studies

It would seem reasonable to provide the CARES user with options for dealing with such "zero" residue cases. Among the possible options for setting such undetected residue include the following:

- Set such residues to zero
- Set them to a fixed, non-zero value, such as the LOQ, LOD, MRL, or a fraction of any of these values
- A statistically based function with desirable distributional characteristics, i.e. truncated log-normal, Gamma distribution, etc.

It is possible that the overall CARES exposure assessment will be sensitive to the assumptions that are made here for such "zero" residues. Thus it would be useful to provide the CARES user with several options in order to investigate whether this is the case for the assessment of interest.

It may be preferable to use the same method for dealing with zero residues across all modules within a particular run, in order to avoid introducing yet another source of uncertainty.

3.6 Calendarization Issues

As noted above, the residue profile for each individual will run from a person's birthday to his/her next birthday. It is the general philosophy within the CARES Water Module to preserve as much "realism" as possible when constructing the daily time series for each individual. This presents some unique technical questions when using finite monitoring or modeling data to construct a birthday-to-birthday profile for a particular person.

As an example, consider a person with a May 15 birthday and only three calendar years (January 1 to December 31) of available monitoring data from a number of monitoring sites. In keeping with

the philosophy of preserving a realistic time series, the three years of actual monitoring data has only two years of continuous data available from May 15 to May 14 (of the following year). An alternative is to allow the program to select May 15 through December 31 from Year 3 and fill in the period from January 1 through May 14 from Year 1 of the dataset or some other year. For many pesticides, the end of the calendar year represents a period of very low residue levels and would not invalidate such an approach. However, this is not always true, and there is a need for general guidance to deal with such circumstances.

Another related issue is to ensure that no bias introduced by the manner in which years of residue data are "sampled" as the daily profiles are constructed. This should be done randomly in order to assure no bias is possible, rather than (for instance) systematic use of Years 1, 2, 3, etc. Notice that resolution of the calendarization issue in the previous paragraph has the potential to introduce bias by undersampling both the very beginning and end of a time series. The problem would be particularly acute for very short time series of only a few years and a small number of sites. The solution chosen for implementation of CARES must address this.

Finally, it must be remembered that CARES is a cumulative assessment tool. The implications of this are discussed more completely in the following section, but it is critical to preserve the correct temporal dependencies when constructing residue profiles for multiple chemicals. If two chemicals could be used in a watershed during the same year, the modeling or monitoring for an individual using a water source in that watershed should also come from the same year. This implies that the sources of modeling or monitoring data for cumulative assessments must be properly matched for all the chemicals of interest, both spatially and temporally.

3.7 Cumulative Assessment Issues

In addition to single pathway or single compound exposure assessments, FQPA requires the EPA to conduct both aggregate (multiple pathway) and cumulative (multiple compounds sharing the same mechanism of toxicity) risk assessments. When using water modeling or monitoring values with either aggregate or cumulative exposure assessments, there are several things that must be considered.

3.7.1 Spatial Considerations

The location of the modeling scenario or monitoring results should be similar to that being used for the other pathways in the assessment. For example, when doing aggregate assessments, it would be inappropriate to utilize drinking water exposure values from the Midwestern part of the United States in combination with a residential scenario from the North Eastern part of the United States. Likewise, when doing a cumulative assessment, it would be inappropriate to combine residue values from monitoring studies conducted for one compound conducted in one area of the country with residue values for another compound from another area of the country. Residue values should always come from similar environmental and product use areas.

3.7.2 Short-Term Temporal Considerations

Pesticide concentration profiles in surface waters are not random but typically follow seasonal patterns. Even within seasons, increased concentrations are often the result of storm events. When doing aggregate assessments, it is important to keep track of the sequence of concentrations throughout the year. For example, concentrations resulting from spring runoff should never be combined with a residential use pattern that occurs late in the summer. When doing cumulative assessments, concentrations should always be taken from the same period of time (within a few days or weeks) for all compounds whether they be obtained from modeled scenarios or from monitoring data. Summer concentrations for one compound should not be

combined with spring concentrations for another compound. Modeled or monitoring scenarios from different temporal regimes should not be combined into a single assessment.

3.7.3 Coincident Exposure Considerations

If possible, aggregate assessments should reflect the actual probability of usage in each of the various pathways being considered. For example, if high amounts of rainfall increase the runoff of a pesticide but decrease the probability of a residential turf usage, then this joint probability should be taken into account as part of the aggregate assessment.

Cumulative assessments should only be done when the probability of coincident exposure is high. For example, if compound A is only used on corn and soybeans and compound B is only used on citrus, it is highly unlikely that there is an area or time when both might be used. In addition, because use of some compounds may exclude or lessen the use of other compounds, use of maximum values for all compounds across a watershed may be highly unlikely. Currently models such as PRZM cannot simulate the heterogeneity of multiple compound applications and runoff from multiple fields within a watershed. Single compounds are then modeled and then the data are combined. However, as mentioned in the previous section on "calenderization," care must be taken to use the same year and similar scenarios each of the compounds being modeled rather than using an unlikely combination of the worst case year and runoff scenario for each compound.

3.8 Tap Water Source Categories (Vulnerability)

Not all tap water sources are created equal. There are obvious major differences, such as ground water vs. surface water, and flowing water vs. man-made impoundments (reservoirs) or lakes. Some water sources are more likely to contain pesticide residues, for instance:

- Shallow, vulnerable private wells near mix/load areas
- Small reservoirs in areas of intense agricultural production, such as the Shipman IL Index Reservoir

Similarly, other drinking water sources are very unlikely to contain pesticide residues:

- Water sources far removed from any past or current use of the pesticide in question
- Deep, properly constructed and properly protected drinking water wells
- One of the Great Lakes

Unfortunately, no generally accepted methodology is available yet for more precisely placing all of the nation's water sources into vulnerability categories. However, there are various governmental initiatives that have the potential to make such a categorization system possible in the future. For instance, the EPA, USDA, and USGS have recently launched at Interagency Governmental Workgroup, which has tackled the issue of developing a new exposure assessment modeling tool for describing pesticide residue profiles at the water intake level of spatial specificity. Regression modeling approaches could be used to place all of the nation's supplies into broad vulnerability classes. To the extent that cropping practices heavily influence vulnerability, much of this is already possibly using a GIS overlay of county-level cropping data with the recently digitized watershed boundaries of all of the nation's surface water supplies.

A special consideration is how to deal with blended sources, Community Water Systems which use mixtures of ground and surface water, or switch from surface to ground water at certain times of the year, such as during drought. As a "bracketing assumption," one simple way of handling this would be to permit the user to assume residues in such sources are either entirely surface water or entirely ground water, depending on the nature of the pesticide(s) under study.

3.9 Surrogation of Residue Data

It will nearly always be the case in CARES that the user will need to estimate residues for geographic regions in which the pesticide is used but no water monitoring or modeling data are available for that specific region. In such cases, it will be necessary to use "surrogate" data from a nearby region. This issue was already briefly mentioned in Section 3.3, Geographic Granularity.

Considerable care should be taken when using surrogate data. Pesticide use practices, soils, climate, hydrology, and other critically-important factors can vary dramatically even over short distances, making geographic surrogation a "risky business." The user should attempt to match as many of these factors as possible when practicing data surrogation. A potentially useful rule here would be to use surrogate data only within defined larger geographic regions, such as the US Farm Resource Regions.

It should be obvious, but surrogation should only be done among similar types of water sources. In the extreme case, this would most certainly mean that ground water data from one state should not be used to estimate concentrations in surface water of another state, but there may be other more subtle cases, such as whether data from reservoirs can be used to estimate residues in flowing water.

4. Solution Chosen for CARES Water Module

In Section 3, we presented the major technical questions and possible answers to each. In this portion of the paper, we select the particular solution chosen for the initial version of the CARES Water Module. The intent of this section is to provide specific, clear guidance to the programmers -- uncluttered with caveats, explanations, plans for the future, etc. The more complicated approaches presented as possibilities in Section 3 are not being abandoned forever -- they are simply not being included in the initial version of the CARES Water Module. Subsequent versions will likely incorporate many of these ideas as experience is gained with the use and utility of CARES in the regulatory environment for which it is intended In Section 5, we suggest the most likely areas for future refinement of the CARES Water Module.

4.1 Varying Sources of Dietary Water

Residues in all dietary tap water will be set equal (home tap water assumed equal to tap water away from home). Residues in all other dietary sources of water will be set as follows:

- Set to "zero."
- Set equal to tap water concentrations.
- Set to a constant or distributional multiplier of the residues present in tap water.

4.2 Effect of Water Treatment

The user may provide a pair of pesticide-specific treatment factors: one for surface water and one for ground water sites. Blended CWS sites can be set to either the surface water or ground water treatment factor. Private wells will have no treatment factor. The treatment factors can be either constants or distributional multipliers, and are intended to include the combined net effects of removal of the parent pesticide and possible formation of relevant degradates. As noted above, such degradates should be included in the parent assessment only if they share a common mechanism of toxicity. Values greater than 1.0 should be permitted for the lumped adjustment factors to account for a possible net increase in toxicity.

4.3 Geographic Granularity

The smallest geographic unit of analysis will be the State.

4.4 Temporal Interpolation of Sparse Data

The user will be allowed to choose three methods for interpolating sparse monitoring data:

- Linear
- Linear on a logarithmic scale
- Scaling of modeling data (as shown in Figure 8)

4.5 Dealing with Zeroes

The user will be allowed to specify extremely low ("zero") concentrations in one of two ways:

- Set them equal to true zero
- Set them to a small, specifiable non-zero value

The method chosen by the user in the Water Module should be consistent with the method chosen in the other CARES Modules within a particular run.

4.6 Calendarization Issues

When sampling from multiple years of residue to fill a daily residue profile from birthday to birthday, all years in the sampled data will have equal probability of selection. If the last year of the monitoring data is selected, the daily profile will be completed by taking data from the beginning of the first year of the dataset.

If there is only one year of residue data available, the data will be "wrapped around" to the beginning of the single year as in the above case of sampling the last year of a multiple-year dataset.

4.7 Cumulative Assessment Issues

In cumulative assessments where co-incident exposure to two or more modeled pesticides is possible, the same year of data should be taken when constructing the daily time series for an affected individual in the CARES Reference Population.

4.8 Tap Water Source Categories (Vulnerability)

For all 50 states, the total population served by the following types of Community Water Systems will be determined:

- Ground water
- One of the Great Lakes
- Surface water sources other than the Great Lakes
- Blended (ground/surface) sources

Individual members of the CARES Reference Population will be randomly assigned to one of the above four categories, such that their overall sampling weights sum as closely as possible to the actual population served by that source type in that state. For each CARES assessment, the user will be permitted to set the residues for blended systems either to those provided for ground or to those provided for surface water sources other than the Great Lakes.

An example of the type of data required for this purpose is shown in Figure 9.

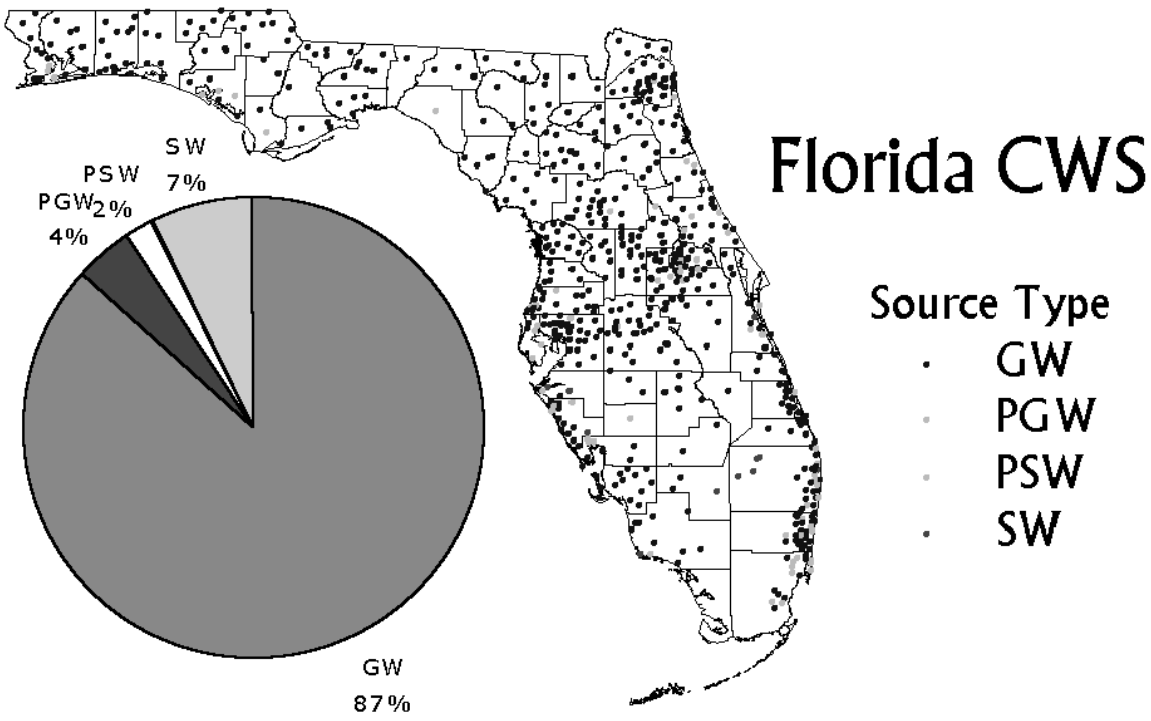

Figure 16 - Community Water Systems (CWS) source-types for the state of Florida, with a pie chart showing the distribution of total population served by different CWS source-types in Florida.

4.9 Surrogation of Residue Data

Data for the same tap water source category may be surrogated from one state to another. Surrogation from one state to another will be permitted, though this will prompt a warning. No scaling factors will be permitted to adjust residue levels when surrogating data.

4.10 Standard File Formats

Residue data provided to CARES will have the following data structure as tab-delimited text files. Missing data will simply be ignored and will not prompt an error. During selection of residue data, population weighting will be permitted.

Monitoring Data File Format (if for N analytes, all concentrations are kept in the same record)

- Source Type (Great Lakes, ground water, other surface water)
- State
- City
- Lat/Long
- HUC
- River vs. reservoir (for SW) Dug vs. drilled (for GW)
- Population Served

- Raw vs. Finished Water (do not apply treatment factors to finished water residues)
- Date
- Concentration of Analyte 1
- Concentration of Analyte 2
  . . .
- Concentration of Analyte N

Surface Water Modeling Data File Format for Raw Source Water Residues (treatment factors always applied when provided)

- State
- Weather Station Name
- Index Reservoir Scenario Identifier
- Population Weighting Factor
- Analyte
- Date
- Concentration

No Tier 2 ground water modeling data are currently accepted

An entry screen will also be provided for the user to enter either constant (Tier 1) or distributional residue concentrations for each of the three distinct water source types (Great Lakes, ground water, other surface water sources) in each of the 50 states.

5. Future Enhancements

A possible vision of an enhanced future version of the CARES Water Module is shown in Figure 10. The key difference between this and the currently recommended version is a better representation of variation in source vulnerability. This is deemed important because the current modeling tools represent only very high-end exposure sites and are not intended to characterize exposures in more typical locations. This is illustrated in Figures 11 and 12 for ground and surface water, respectively.

Another likely change in future versions of the CARES Water Module is the geographic granularity. For instance, use data and other factors may be available at a geographic resolution of the 8-digit HUC's in the near future, which would be a more attractive geographic unit of analysis, particularly for surface water assessments. Another option is to use the PUMA's themselves as the geographic unit of analysis. This is illustrated in Figures 13 and 14.

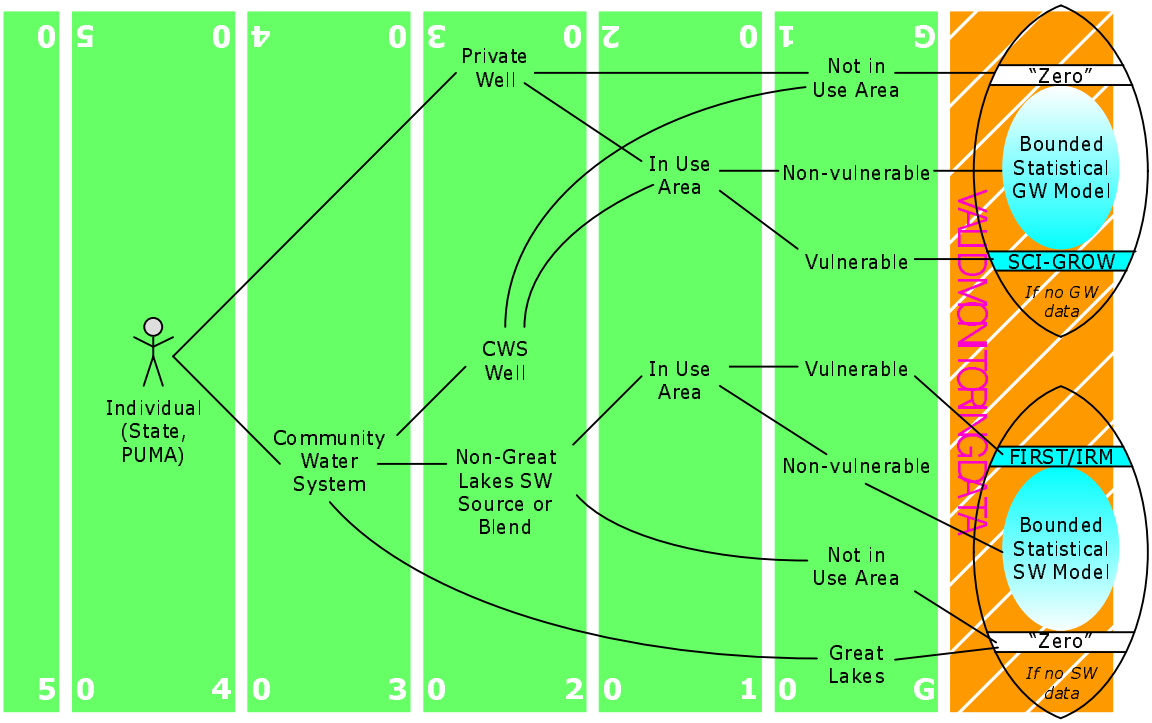

Figure 17 - Schematic of procedures to be used within the CARES Water Module

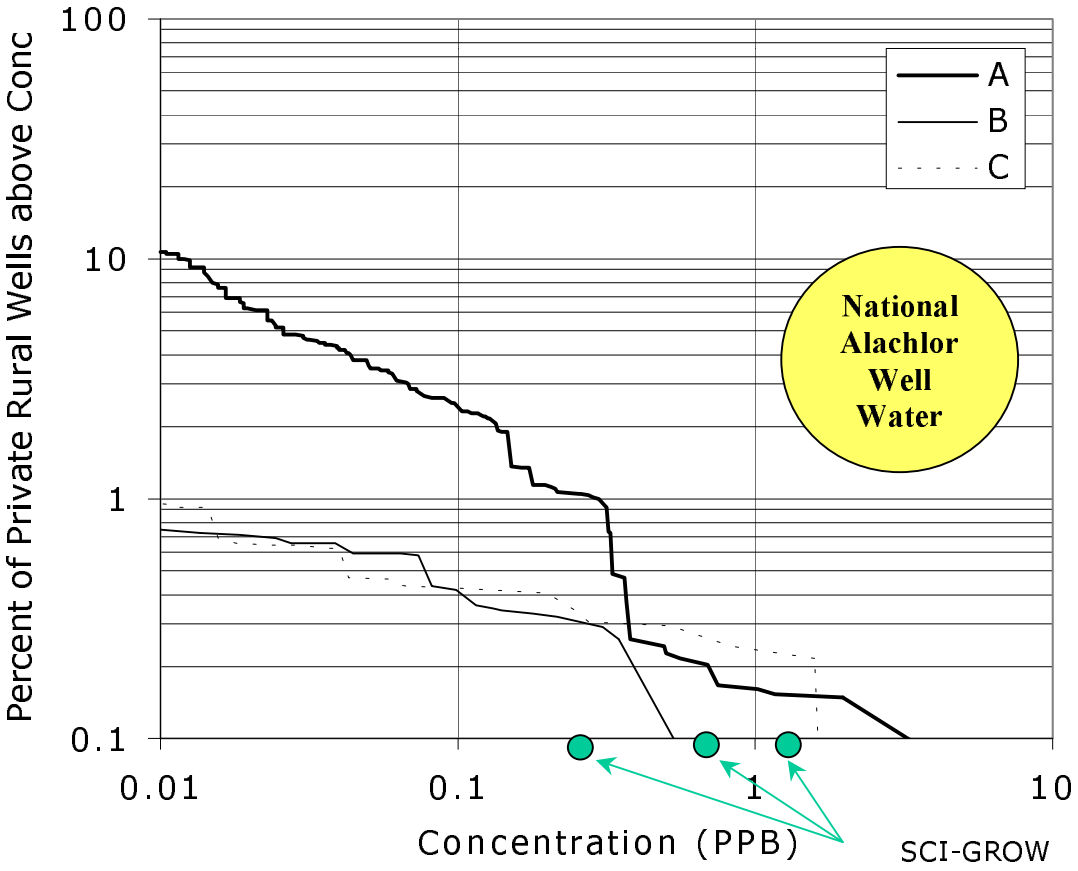

Figure 18 - Comparison of SCI-GROW model predictions for three pesticides with a use-area-wide monitoring survey

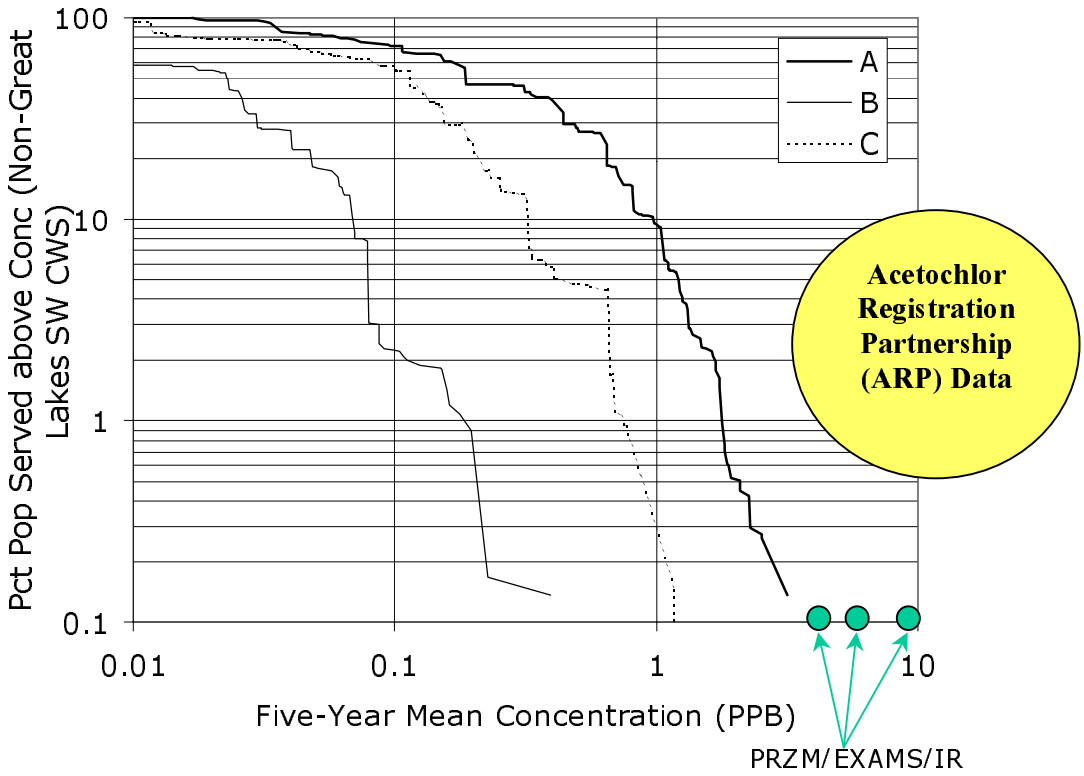

Figure 19 - Comparison of PRZM/EXAMS/IR model predictions of long-term mean concentrations for three pesticides with a use-area-wide monitoring survey

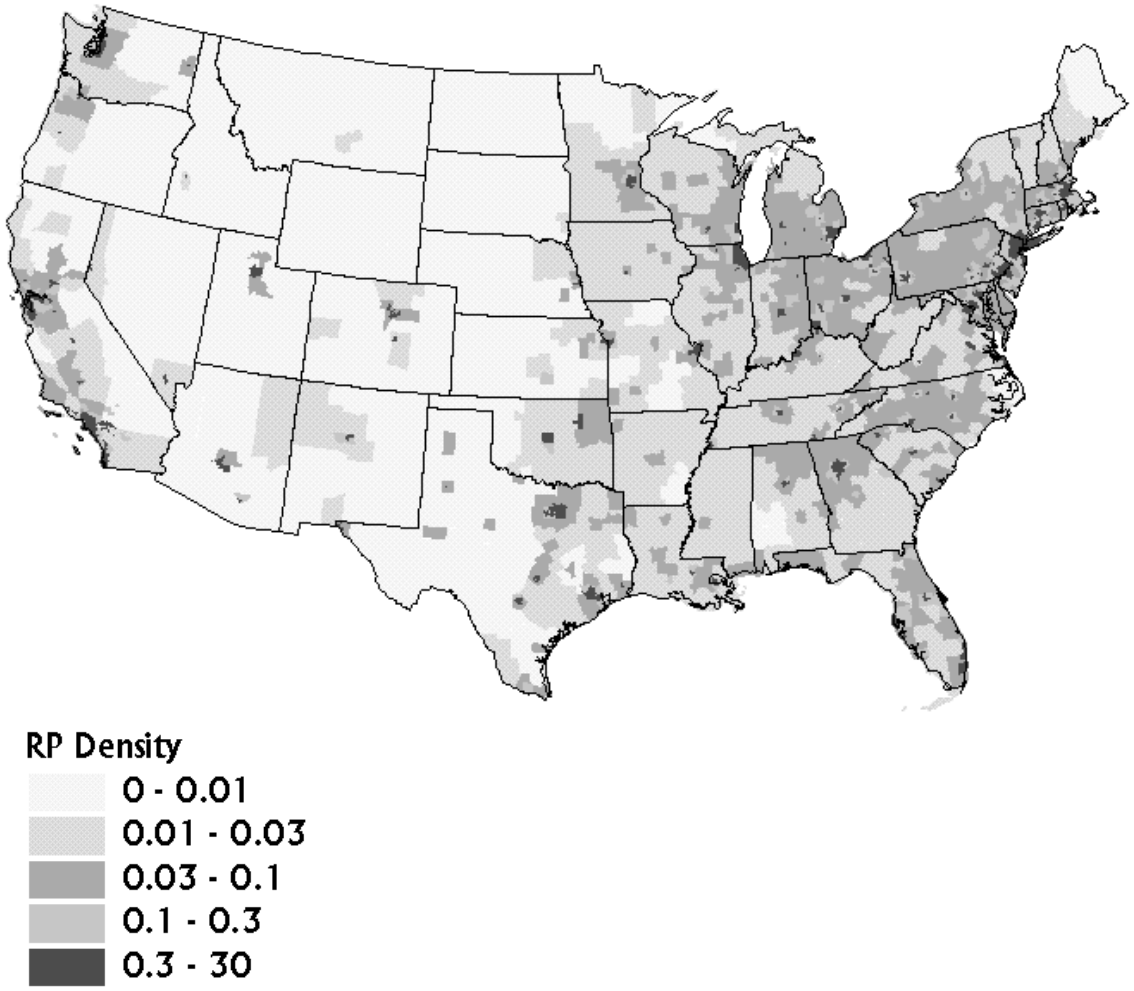

Figure 20 – Reference Population Density
(Alaska and Hawaii not shown but are in the ref. pop.)

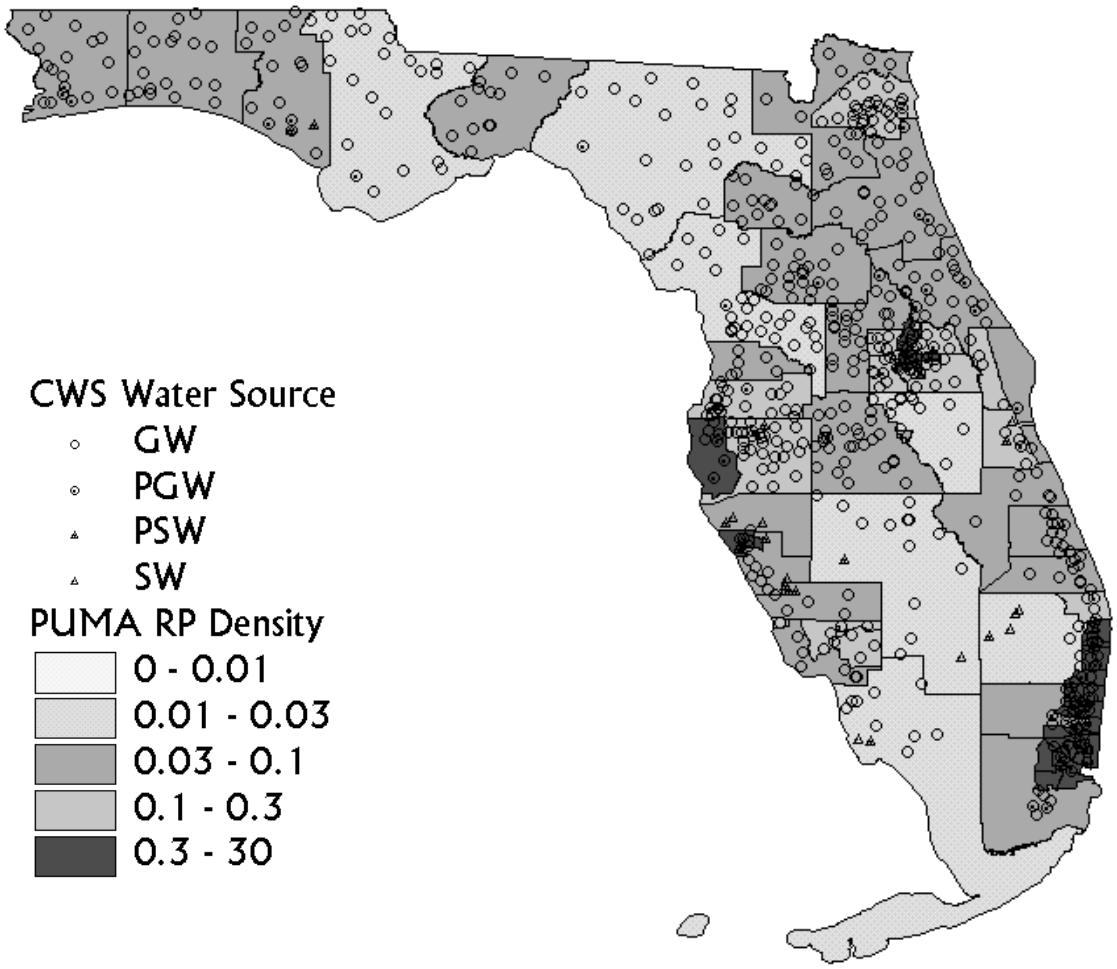

Figure 21 – Reference Population Density in the State of Florida, showing CWS intakes

6. References

1. *Food Quality Protection Act of 1996*. Public Law 104-170, August 3, 1996.

2. "A Framework for Estimating Pesticide Concentrations in Drinking Water for Aggregate Exposure Assessments," ILSI Risk Science Institute, Washington, DC, 1999.

3. ECOFRAM. ECOFRAM Aquatic Report. Ecological Committee on FIFRA Risk Assessment Methods. Joint USEPA, industry, and academia workgroup on probabilistic risk assessment for pesticides, 1999. Available for download at: http://www.epa.gov/oppefed1/ecorisk/.

4. Aventis CropScience drinking water monitoring studies for bromoxynil, carbaryl, and fipronil.

5. Monsanto drinking water monitoring studies for alachlor and triallate (14 other analytes monitored).

6. OP Task Force drinking water monitoring study for 6 OP insecticides.

7. Syngenta drinking water monitoring studies for atrazine and simazine.

8. Acetochlor Registration Partnership drinking water monitoring studies for acetochlor (10 other analytes monitored).

Appendix 1. Reference Data Tables

Table 28 - CWS in State of Florida Serving More Than 100,000 Peo ple

PWS_ID	System Name	City	State	ZIP	Pop. Served	Source Type	County	HUC
4130871	MDWASA - Main System	Miami	FL	33233	1705156	GW	Dade	????????
6290327	City Of Tampa-Water Dept	Tampa	FL	33619	475000	SW	Hillsborough	????????
2161327	JEA: North Grid	Jacksonville	FL	32206	413212	GW	Duval	????????
2161328	JEA: South Grid	Jacksonville	FL	32206	396461	GW	Duval	????????
6521405	Pinellas County Utilities	Largo	FL	33778	374078	GW	Pinellas	????????
4504393	Palm Beach County #8 WTP	West Palm Beach	FL	33417	370878	GW	Palm Beach	????????
3480962	Orlando Utilities Commission	Orlando	FL	32802	356041	GW	Orange	????????
6521715	St Petersburg, City Of	Odessa	FL	33556	293726	GW	Hillsborough	????????
1170525	Escambia Co. Utility Authority	Pensacola	FL	32514	269545	GW	Escambia	????????
3050223	Cocoa, City Of	Cocoa	FL	32923	187526	GW	Brevard	????????
6411132	Manatee Cnty Public Works	Bradenton	FL	34202	186000	SW	Manatee	????????
3051447	Melbourne, City Of	Melbourne	FL	32935	174489	SW	Brevard	????????
4060486	Fort Lauderdale, City Of	Ft Lauderdale	FL	33312	172680	GW	Broward	????????
1370655	Tallahassee, City Of	Tallahassee	FL	32304	162750	GW	Leon	????????
4131618	North Miami Beach	N. Miami Beach	FL	33162	160000	GW	Dade	????????
6531014	Lakeland, City Of	Lakeland	FL	33801	154570	GW	Polk	????????
2010946	Gainesville (Murphree WTP)	Gainesville	FL	32614	150000	GW	Alachua	????????
4060642	Hollywood, City Of	Hollywood	FL	33021	142705	GW	Broward	????????
4130604	Hialeah, City Of	Hialeah	FL	33012	142000	PGW	Dade	????????
3484093	RCID Central	Lake Buena Vista	FL	32830	136500	GW	Orange	????????
6290787	HCPUD/South Central	Tampa	FL	33601	134741	GW	Hillsborough	????????
6290388	HCPUD/Northwest Utilities	Tampa	FL	33602	130000	GW	Hillsborough	????????
6581591	Sarasota Co Special Util Dist	Sarasota	FL	34232	123446	GW	Sarasota	????????
5364048	Lee County Utilities	Fort Myers	FL	33902	123200	GW	Lee	????????
6520336	Clearwater Water System	Clearwater	FL	33758	109350	GW	Pinellas	????????
4500130	Boca Raton Wtp	Boca Raton	FL	33431	109000	GW	Palm Beach	????????

Table 29 - Breakdown of Reference Population by State (# in Ref. Pop. = 100,000)

Region	Division	State	N	% of Total N	Weight	% of Total Weights
MW	ENC	IL	4,477	4.477	11,128,928.79	4.6112
		IN	2,104	2.104	5,346,791.79	2.2154
		MI	3,627	3.627	9,119,092.44	3.7785
		OH	4,110	4.110	10,627,707.94	4.4036
		WI	1,938	1.938	4,742,965.92	1.9652
	WNC	IA	1,031	1.031	2,629,850.22	1.0897
		KS	990	0.990	2,354,311.02	0.9755
		MN	1,825	1.825	4,246,796.55	1.7596
		MO	1,951	1.951	4,992,682.18	2.0687
		ND	287	0.287	594,476.43	0.2463
		NE	622	0.622	1,517,431.87	0.6287
		SD	343	0.343	635,322.97	0.2632
NE	MA	NJ	3,101	3.101	7,525,422.57	3.1181
		NY	7,072	7.072	17,242,923.03	7.1446
		PA	4,416	4.416	11,537,538.41	4.7805
	NE	CT	1,190	1.190	3,169,010.66	1.3131
		MA	2,338	2.338	5,845,623.17	2.4221
		ME	475	0.475	1,150,066.71	0.4765
		NH	422	0.422	1,056,830.25	0.4379
		RI	371	0.371	957,329.53	0.3967
		VT	216	0.216	519,674.47	0.2153
S	ESC	AL	1,487	1.487	3,948,075.02	1.6359
		KY	1,327	1.327	3,513,633.91	1.4559
		MS	1,024	1.024	2,468,750.93	1.0229
		TN	1,827	1.827	4,745,574.24	1.9663
	SA	DC	225	0.225	557,175.01	0.2309
		DE	248	0.248	655,184.09	0.2715
		FL	4,926	4.926	12,613,118.86	5.2262
		GA	2,579	2.579	6,261,623.69	2.5945
		MD	1,904	1.904	4,667,234.59	1.9339
		NC	2,615	2.615	6,374,680.32	2.6413
		SC	1,262	1.262	3,376,445.82	1.3990
		VA	2,303	2.303	5,944,346.09	2.4630
		WV	635	0.635	1,724,997.43	0.7147
	WSC	AR	884	0.884	2,321,611.82	0.9620
		LA	1,632	1.632	4,154,997.12	1.7216
		OK	1,680	1.680	3,025,126.49	1.2535
		TX	7,025	7.025	16,657,843.74	6.9021
W	MTN	AZ	1,790	1.790	3,552,611.00	1.4720
		CO	1,349	1.349	3,263,525.06	1.3522
		ID	408	0.408	1,000,402.33	0.4145
		MT	409	0.409	758,914.14	0.3145
		NM	908	0.908	1,509,655.48	0.6255
		NV	544	0.544	1,178,662.23	0.4884
		UT	791	0.791	1,623,525.62	0.6727
		WY	196	0.196	437,610.99	0.1813
	PAC	AK	541	0.541	528,034.18	0.2188
		CA	12,622	12.622	28,865,589.99	11.9604
		HI	673	0.673	1,059,405.80	0.4390
		OR	1,172	1.172	2,899,667.18	1.2015
		WA	2,108	2.108	4,714,636.19	1.9535

Table 30 - Breakdown of Reference Population by Source of Water

Source	Frequency	Percent	Cumulative Frequency	Cumulative Percent
CWS or Pvt Co	81,989	81.99	81,989	81.99
Drilled Well	15,031	15.03	97,020	97.02
Dug Well	1,818	1.82	98,838	98.84
Spring, Creek, etc.	1,162	1.16	100,000	100.00

Table 31 - Breakdown of US Population by Source of Water

Source	Frequency	Percent	Cumulative Frequency	Cumulative Percent
CWS or Pvt Co	2.0275E8	84.01	2.0275E8	84.01
Drilled Well	32,586,781	13.50	2.3534E8	97.51
Dug Well	3,861,586	1.60	2.3920E8	99.11
Spring, Creek, etc.	2,143,278	0.89	2.4134E8	100.00

Appendix F – Validation Plan

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Cumulative and Aggregate Risk Evaluation System

CARES Validation Plan

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CARES Validation Plan

Part 1 – Plan Description

Purpose and Scope

This Validation Plan provides a management tool for organizing validation efforts and a report index describing the objectives, methods, and results of all formal validation, verification, and testing activities performed on or produced in conjunction with the Cumulative and Aggregate Risk Evaluation System (CARES) software program attendant with its public release in 2002.

The Validation Plan is designed to serve two functions. First, the plan is as an organizational tool for identifying, organizing, and tracking specific validation tasks, work activities, and projects from conception to completion. Rather than attempting to define all the needed tasks and approaches to CARES validation up front, the organization of this document, particularly it's hierarchical outline format, allows for addition, modification, or even reorganization of tasks as experience and need dictate during the testing phase. The second function of the Validation Plan is to document the results of the multiple validation activities, thereby serving as a composite summary report. Thus, the Validation Plan is dynamic and flexible in character during the course of performing validation studies, yet provides closure and a definitive report on the composite of individual tasks and products that constitute the overall validation objective.

Part 1 describes the procedural aspects of conducting validation activities using this plan. Part 2 is an outline of proposed and/or enacted validation activities.

Overview

Figure 1 illustrates the various components of this plan and the general workflow associated with their use. The Validation Plan consists of an outline of Validation Categories that covers the spread of required work. The outline format allows the scope of validation work to be arranged (and rearranged, as needed) into meaningful groups and sub-groups, serving in effect as a comprehensive table of contents of the various validation efforts. The lowest level of the outline is the point of departure for generating a Validation Project that describes a concrete work effort and the intended deliverable. The Validation Project Form describes the objectives of the specific project and is used to track and manage the effort. The Validation Project Report documents the objectives, methods used, and results of the validation task. The Feedback and Change Form is used to describe any changes to the program made during testing or any problem that needs to be addressed. The Validation Task Group reviews the changes made and determines whether their impact on the program requires any type of re-validation. The following sections discuss each component in more detail.

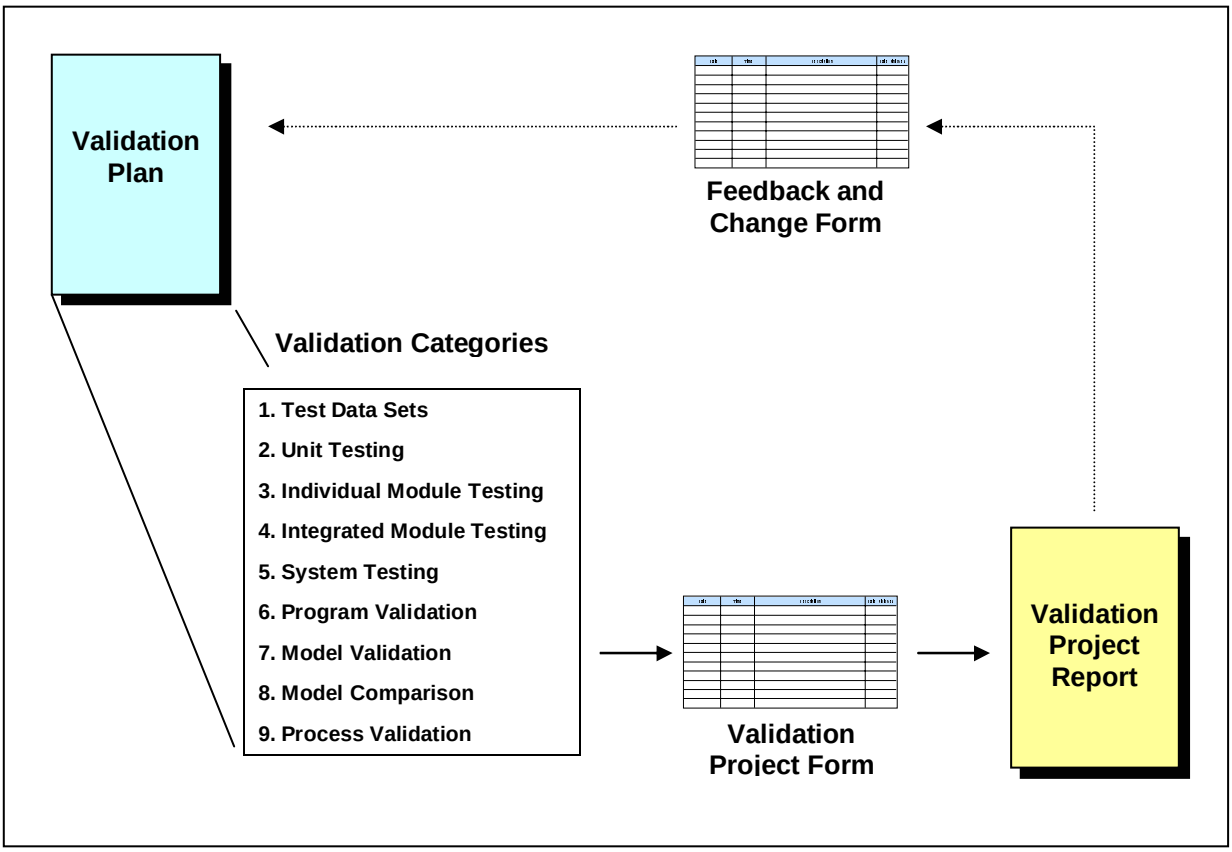

Figure 1. Validation Plan Components and Workflow

Validation Categories

The term "validation" yields a variety of meanings depending on whom you ask. To software engineers it may signify an exhaustive list of verification tests. To model designers it might mean comparison of predicted outcomes with empirical observations. To others it might mean evaluating the outcome of one model with that of similar models purported to address the same problem. In the wake of the Good Laboratory Practices Act, validation refers more to a set of software development documents than to any specific testing protocol.

All of these viewpoints are both relevant and necessary to the goal of pr oviding a comprehensive validation of the CARES program. Accordingly, the organization of this plan is based on an outline consisting of nine categories or types of efforts that collectively cover the range of required validation activities or products. The categories and the scope of work involved in each are summarized in Table 1.

Table 1. Definition of Validation Categories

Verification	**1. Test Data Sets**	Definition and development of standardized data sets.
	2. Unit Testing	Verifying the proper functioning of small distinct parts throughout the program (for example, screen objects, algorithms, calculations).
	3. Individual Module Testing	Verifying the proper functioning of individual modules with defined input and output parameters (for example, the exposure modules).
	4. Integrated Module Testing	Verifying the proper functioning of modules that integrate data streams (such as Aggregation and Cumulation and the CSU module).
	5. System Testing	Verifying and characterizing the performance of the system as a whole.
Other Validation	**6. Program Validation**	A non-testing category that documents general topics regarding the program (such as conformance to programming and interface standards, and usability testing).
	7. Model Validation	Comparison and evaluation of outputs to reasonable experience or empirical data.
	8. Model Comparison	Comparison and evaluation of outputs between other similar software.
	9. Process Validation	Establishing documentation that the system performs as intended (primarily following the System Development Life Cycle methodology).

Note that the first five categories follow a progressive approach to testing consistent with the modular nature of CARES. Since a standard test data set is a fundamental requirement for use in testing, it is the subject of the first validation category. Progressive testing begins with a detailed examination of the performance of the smallest units, such as every input/output option on every screen, and continues in an expanding manner through intra- and inter-module testing, finally culminating in tests appropriate to system-wide functions. The remaining four categories address the several types of validation activities. In all, these nine categories allow for a comprehensive coverage and overview of the various verifications and validation projects needed.

Validation Project (and Form)

This plan is also intended to serve as a management tool to help define and track the progress of validation activities and products. As the plan develops, new validation topics are added to the outline format under the appropriate validation category. Thus, the outline serves as a flexible working area to gather, arrange, and display the range of tasks and work products required to achieve the overall validation goal for CARES. Starting at the level of the validation categories, each succeeding branch of the outline progressively refines the description of a scope of work that needs be done. When the scope of work is refined to the level that it can be managed as a specific project, it is ready to be written up as a Validation Project.

A Validation Project is defined as a specific work effort with a work description, schedule, and deliverable. Examples of validation projects are: a discrete testing objective, a series of related testing tasks, production of a validation document, model comparison, etc. Validation Projects should be prioritized and carefully evaluated for proper timing.

A Validation Project Form is used to describe and manage the Validation Project. The form assigns a tracking number to the work based on the outline number in the Validation Plan. The form includes management information (who, where, when), a project description (objective, scope, deliverables). If the outline number changes due to rearrangement of the plan, a cross-reference list will be maintained.

A copy of the **Validation Project Form** is included in the Appendix

Validation Project Report

The Validation Project Report is the closure document that provides details covering the objectives, methods, and results of the Validation Project. In some cases, the report may refer to additional documents that are deliverables. Reports can be submitted in whatever format best suits the need. However, each report must include conduction details, where applicable, such as the CARES build number and the testing environment (CPU, RAM, etc.).

A list of the required **Report Details** is included in the Appendix

Scope of the Plan

This Validation Plan covers the period between the release of the alpha versions of CARES (2001) and its final public release. Future changes to CARES after the 2002 public release may require additional validation activities. The procedures for handling future validation requirements and changes are defined in the CARES Maintenance Plan.

Managing Changes – A Discussion of the Problem

How are validation requirements managed during construction? Since validation activities and system development or refinement will be running concurrently, consideration needs to be given to how new modifications impact the results of prior validation tasks. In other words, to what extent does validation need to be repeated after a programmatic change?

There are two factors that help determine the need for and the extent of repeating validation tasks following modifications to the software prior to its final release. Both work towards reducing the impact of change on the extent of re-validation. The first factor relates to the way CARES is constructed. The modular nature of the program, its extensive use of object oriented programming, and the broad standardization of procedures across the modules all contribute to isolating the impact of changes to defined areas. The extent and type of re-validation tasks can be better evaluated because the area of the change is well defined in relation to the system as a whole.

The second factor that helps guide the extent of re-validation following system modification is the progressive approach used to implement the validation plan. The conduction of validation activities should proceed in a progressive manner, addressing first the individual units and smallest system parts, followed by the functioning of modules, then inter-module interactions, and finally system-wide testing. This does not mean that there cannot be some overlap in the scope of the tests, but the more progressive the manner of conducting validation testing, the more control one has on defining the extent and need for re-validation resulting from changes.

As testing progresses to modular and system-wide levels, performance benchmarks are established. The confidence that modifications have been implemented properly and without unforeseen “side-effects” can be established through repeating higher-level tests. This is referred to as regression testing. Clearly, regression testing requires careful documentation of the approach and results of prior tests.

Another area of concern is how to determine the need for and the extent and type of re-validation required after the program is changed to correct problems uncovered during testing or to fix bugs and problems reported independently.

The method for managing changes due to construction, testing, and bug reports is based on the use of a Feedback and Change Form by the Validation Task Group.

Feedback and Change Form

This is a multi-purpose form designed to help accomplish the following:

- Provide a means for reporting bugs or suggesting modifications from any source so that these can be communicated to the development team.
- Provide for tracking and recording all changes to the program after a baseline build has been established (up to the point of the 2002 public release).
- Provide a mechanism to ensure that appropriate validation (or re-validation) accompanies all changes.

The form should be used to record any changes or fixes made to the program during the course of performing Validation Project activities. All changes and improvements to the program following the June 2001 release (established as the base build) should be briefly itemized using the form. Users or anyone else wishing to report a possible bug or problem, or even make a suggestion for improvement, should use the form to communicate their observation. Examples of using the form as a "bug" report include reporting of miscalculations, coding errors, interface glitches, performance problems, inconsistencies or gaps in validation documents.

A copy of the **Feedback and Change Form** is included in the Appendix

Validation Task Group

The Validation Task Group is responsible for ensuring that validation activities are conducted in accordance with this Validation Plan. The Group coordinates, prioritizes, issues, and manages all Validation Projects. The Group safeguards the integrity of prior validation results and evaluates the need for new validation or re-validation due to changes. Using the Feedback and Change Form, the Group monitors and maintains a record of all changes to the program and ensures that each receives appropriate validation as needed.

CARES Validation Plan

Part 2 – Validation Projects

1. Test Data Sets

1.1 Standard Data Set

A Standard Data Set should be prepared with the following specifications:

- Suitable for use at the individual module level and during aggregate and cumulative evaluation.
- Contains actual data drawn as subsets from the Reference Population.
- Small enough to run reasonably fast during use.
- Sample sizes are statistically adequate.
- Data is representative of the Reference Population.
- The set should illustrate actual and noticeable differences during contribution analysis to enhance illustration.
- The set should be designed and prepared so that it can serve the following:
    - Unit testing.
    - Modular testing.
    - System testing.
    - Illustration and testing of contribution and sensitivity analyses.
    - Screen shots for help aids and system documentation.
    - Actual data set used for training and illustrated in the User Guide.
    - The standard data set supplied to all pre-release testers and users.
    - A permanent data set for future uses (i.e., testing upgrades, validating performance, etc.).
    - Use as a standard for comparing CARES with other software.

Preparation of the Standard Data Set is a high priority item.

1.2 Additional Data Sets

Various additional data sets for specific purposes may be needed. The Reference Population is itself a standard data set.

2. Unit Verification Testing

2.1 Computational Algorithms

Compare computed results with those derived using external computational methods (e.g., from spreadsheets, statistical software, or other). Example calculations include descriptive statistics (e.g., mean, max, standard deviation, standard error, etc.) and other.

2.2 Monte Carlo Procedures

Simulate Monte Carlo results using alternate means (e.g., Crystal Ball, @Risk) and compare results.

2.3 Randomization Procedures

Verify that randomness is not affected by the computer used.

Verify repetition of results based on same random seed.

Define and perform additional appropriate tests.

2.4 Units Management

2.4.1 Unit Accuracy

Verify that all units are appropriate and that unit transformation formulas are accurate.

2.4.2 Unit Conversion

Verify that unit conversions perform accurately.

2.5 Interface Objects

Verify the proper functioning of each user-addressable object on every program screen

2.6 TBD

3. Individual Module Testing

3.1 Data Transfer (P, D, R, W, C)

3.1.1 Input Data Transfers

Compare source data with data contained in CARES data sheets.

3.1.2 Output Data Transfer

Compare CARES data sheet fields with data printed out.

3.1.3 Other Data Transfers

Define other data transfer areas and perform comparisons.

3.2 Modular Sensitivity Analysis

Perform appropriate tests for each module to determine how sensitive the outputs are to changes in the input variables.

3.3 Handling Non-Detects

Demonstrate proper handling of non-detects for individual exposure modules.

3.4 TBD

4. Integrated Module Testing

4.1 Sensitivity Analysis

At the level of the Contribution and Sensitivity module, evaluate the sensitivity of the output results to changes in assumptions and the magnitude of input variables.

4.2 TBD

5. System Testing

5.1 Stress Testing

Using the standard Reference Population, devise and conduct tests to determine effects of various stress indicators on system performance. Examples of stress indicators are:

- Subset sample size
- Multiplicity of subsets
- Monte Carlo Iterations
- Drill down level
- More

5.2 TBD

6. Program Validation

6.1 Programming Standards

Verify and report on the conformance of the program to the CARES Programming Standards White Paper (Sept. 13, 2000).

6.2 Interface Standards

Verify and report on the conformance of the CARES interface with the Microsoft Windows Interface Standards

6.3 TBD

7. Model Validation

7.1 Professional Evaluations

7.1.1 Exposure Modules (D, R, W)

For single exposure pathways, devise ad-hoc tests and evaluate the CARES output for reasonableness and consistency.

7.1.2 Aggregation and Cumulation

Devise ad-hoc tests and evaluate the CARES output for reasonableness and consistency.

7.2 Transparency

Review documentation (both digital and hard copy) pertaining to CARES to ensure that it meets the objectives of "open source" public software.

7.3 Assumptions

7.3.1 Verify Source and Accuracy

Verify that the assumptions built into algorithms or used by CARES conform to current guidelines or SOPs.

7.3.2 Record Keeping

Verify that the assumptions used by CARES are accurately recorded and maintained with any CARES run.

7.4 Real World Comparison

Where possible, devise and perform tests that would allow comparison of CARES outputs against other known observations of real world data.

7.5 TBD

8. Model Comparison

8.1 Inter-Model Comparisons

Using standardized data sets, compare the results obtained by CARES with that obtained using similar risk assessment software such as DEEM, Calendex, Lifeline, SHEDS.

Possible evaluations include:

- Similarities in predictions
- Consistency (or inconsistency) in any differences
- Sources of any differences (assumptions, data, procedures)

8.2 TBD

9. Process Validation

9.1 System Development Life Cycle Documentation

Verify the completeness and currency of the following System Development Life Cycle (SDLC) documents for CARES:

- Requirements Specification
- System Design
- Validation Plan
- Validation Project Reports
- User Guide
- Maintenance Plan

9.2 TBD

CARES Validation Plan

Appendix

- **CARES Validation Project Form**
- **CARES Validation Project Report Details Form**
- **CARES Feedback and Change Form**

CARES Validation Project Form

Validation Project Number	

Outline number from the Validation Plan – Part 2

Performing Organization / Individual

Organization
Address

Contact Name
Email
Phone
Fax

Project Description

Short Description
Scope and Methods
Constraints / Limitations

Project Initiation

Reviewed By / Date
Approved By / Date
Date Started
Comments

Project Completion

Reviewed By / Date
Approved By / Date
Date Completed
Comments

Use continuation pages, if needed.

Email form to DFarrier@alphaCARES.org or FAX to (970)-249-1360 *SRS-071201*

CARES Validation Project Report Details Form

A separate Validation Project Report must be submitted for each Validation Project. The report should include a description of the objects, the methods used, and the results obtained. Include complete description of data sets, setup options, and other details pertinent to the conditions of the validation. Reports may be prepared in any format deemed suitable. However, please provide the following information and ***include this form*** *with each Validation Project Report.*

Validation Project Number	

Performing Organization / Individual

Organization
Address

Contact Name
Email
Phone
Fax

Project Description

Short Description
Constraints, Problems Encountered, Comments

User Configuration *Internal Use*

PC Manufacturer (Indicate Desktop or Laptop)
Operating System and Version
Processor Type and Speed (MHz)
Working Drive Capacity (GB)
RAM Memory (MB)
Monitor Size and Screen Resolution

CARES System Used *Internal Use*

Version
Release Date
Build Number
Comments:

CARES Feedback and Change Form

Use this form for the following: (1) To suggest a change or enhancement to the CARES program or documentation, (2) To report a suspected problem or bug in the system, (3) To describe fixes needed to correct items found during testing, or (4) To document all changes made to the system beginning with the alpha version released in July 2001.

F/C Form Number *(Internal Use)*	

Date Submitted	

Submitting Organization / Individual

Organization
Address

Contact Name
Email
Phone
Fax

Problem Description *Use continuation sheets, if needed*

Report Type *1. Coding error, 2. Validation Fix, 3. Design Issue, 4. User Interface, 5. Documentation, 6.Suggestion, 7. Query, 8. Other*	

Severity *1. Fatal, 2. Serious, 3. Minor, 4. Unknown*	

Describe Problem and How to Reproduce It *Attach data files, output examples, screen shots, as needed.*
Suggested Fix

CARES Processing *Internal Use*

Affected Build Number and Release Date
User's Configuration Details
Reviewed By / Date
Resolved By / Date
Approved By / Date

CARES System Changes *Internal Use*

Changed Build Number and Release Date
Describe Changes *Attach continuation sheets.*
Re-Validation Review:

Include new Validation Project Number, if applicable

Email form to DFarrier@alphaCARES.org or FAX to (970)-249-1360 *SRS-071201*