



**Cumulative and Aggregate Risk Evaluation System**

# Technical Manual



March 20, 2002  
CARES 1.0

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## **Name Change**

CropLife America was formerly known as the American Crop Protection Association



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- C – Residential White Paper**
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# 1. Introduction and Overview

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# Chapter 1 – Introduction and Overview

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## 1.1 Executive Summary

The Food Quality Protection Act mandates that the US Environmental Protection Agency evaluate both the aggregate and cumulative risks associated with pesticide use. Aggregate risk assessment takes into account multiple sources and routes of exposure for a single chemical while cumulative risk assessment combines exposures to two or more chemicals that share a common mechanism of toxicity. **CARES** (Cumulative and Aggregate Risk Evaluation System), a computer program developed by CropLife America (formerly the American Crop Protection Association) is designed to perform such analyses.

CARES utilizes relevant databases to evaluate potential risk from dietary, drinking water, and residential sources and from oral, dermal, and inhalation routes of exposure. Risks can be calculated deterministically for Tier 1 screening, and probabilistically using Monte Carlo simulation of individuals for higher tier analyses. CARES allows the user to estimate doses and risks from acute, short term, intermediate term, and chronic exposures. CARES allow users to interactively query the program and identify the factors contributing to the highest percentiles of risk.

CARES is an object-oriented program created using a standard windows interface. The program is user-friendly, intuitive, easy to use, and capable of providing accurate and reliable tabular and graphical reports. Documentation, manuals and tutorials accompanying CARES will be of high caliber and easy to use. Version control will be accomplished by official release of approved versions.



## 1.2 What is CARES?

CARES (Cumulative and Aggregate Risk Evaluation System) is an object-oriented, windows-based PC program. CARES is comprised of modules (objects) that can be selected, linked and executed using a programming canvas provided by an interface program called Notitia. The Notitia interface allows the user to choose from a menu of exposure sources (dietary, water, and residential) and exposure durations. The user inputs toxicity and chemical specific exposure data and conducts either an aggregate or cumulative risk evaluation for populations of interest. CARES has report writing and data querying subroutines that allows the user to view the results of the risk assessment, determine source contribution and print summary reports. CARES stores the detailed determinants and assumptions of each risk assessment so that the analysis can be reproduced.

### 1.3 What Does CARES Do?

CARES permits the user to produce transparent and reproducible risk assessments. In these assessments exposure from dietary, drinking water, and residential sources (18 scenarios) are aggregated or are accumulated for chemicals that share a common mechanism of action. Acute (1-day), short term (2-30 days), intermediate-term (1 to 3 months), and chronic (1 year) exposures and risks can be evaluated using CARES. CARES calculates doses deterministically for Tier 1 screening or probabilistically using Monte Carlo simulation for higher tier analyses.

### 1.4 Toxicity Endpoint Selection

In order to conduct an aggregate or cumulative risk assessment, the user must decide what duration of exposure will be simulated and the toxicity endpoints that will be used for each route of exposure. Table 1.1 provides a list of some of the alternative toxicity endpoints that may be available from standard studies. Ideally, the uncertainty factors assigned to a chemical will be the same for each pathway and a group uncertainty factor can be assigned to chemicals that share a common mechanism. Risk is expressed as percentile distributions of toxicologically equivalent doses, or margins of exposures, or hazard indices.

**Table 1.1 - Toxicity Endpoint Selections**

User Required Input	User Choices
Exposure Duration	<ul style="list-style-type: none"><li>• Acute (1-Day),</li><li>• Short-Term (1-Week)</li><li>• Intermediate Term (13 Weeks)</li><li>• Chronic (1 Year)</li></ul>
Route	<ul style="list-style-type: none"><li>• Oral</li><li>• Dermal</li><li>• Inhalation</li></ul>
Pathway	<ul style="list-style-type: none"><li>• Dietary</li><li>• Water</li><li>• Residential Exposure</li></ul>
Toxicity Endpoint	<ul style="list-style-type: none"><li>• NOEL</li><li>• LOEL</li><li>• ED10, ED50</li><li>• Relative Potency Estimate</li></ul>
Uncertainty Factor	<ul style="list-style-type: none"><li>• Inter-subject</li><li>• Inter-species</li><li>• Other: Data Quality Factor(s)</li><li>• FQPA Factor (Increased Susceptibility)</li></ul>
Risk Metrics	<ul style="list-style-type: none"><li>• Toxicity Equivalent Quotient</li><li>• Margin of Exposure</li><li>• Hazard Index</li></ul>

## 1.5 How to Aggregate

Aggregate assessments account for multiple sources and routes of exposure for a single chemical. CARES calculates source and route-specific doses for an individual on the same day and combines them to obtain the aggregate dose. For higher tier assessments, distributional analyses using Monte Carlo simulation provide a scientifically defensible methodology for combining doses from multiple sources. The technique involves constructing a probability distribution for the aggregate dose in a specified population by examining the aggregate doses for different individuals.

Aggregate risk can be characterized by a distribution of a risk metric such as margin of exposure (Figure 1.1). The entire distribution of aggregate dose and its risk metric is then compared to a safety standard in order to reach a risk management decision.

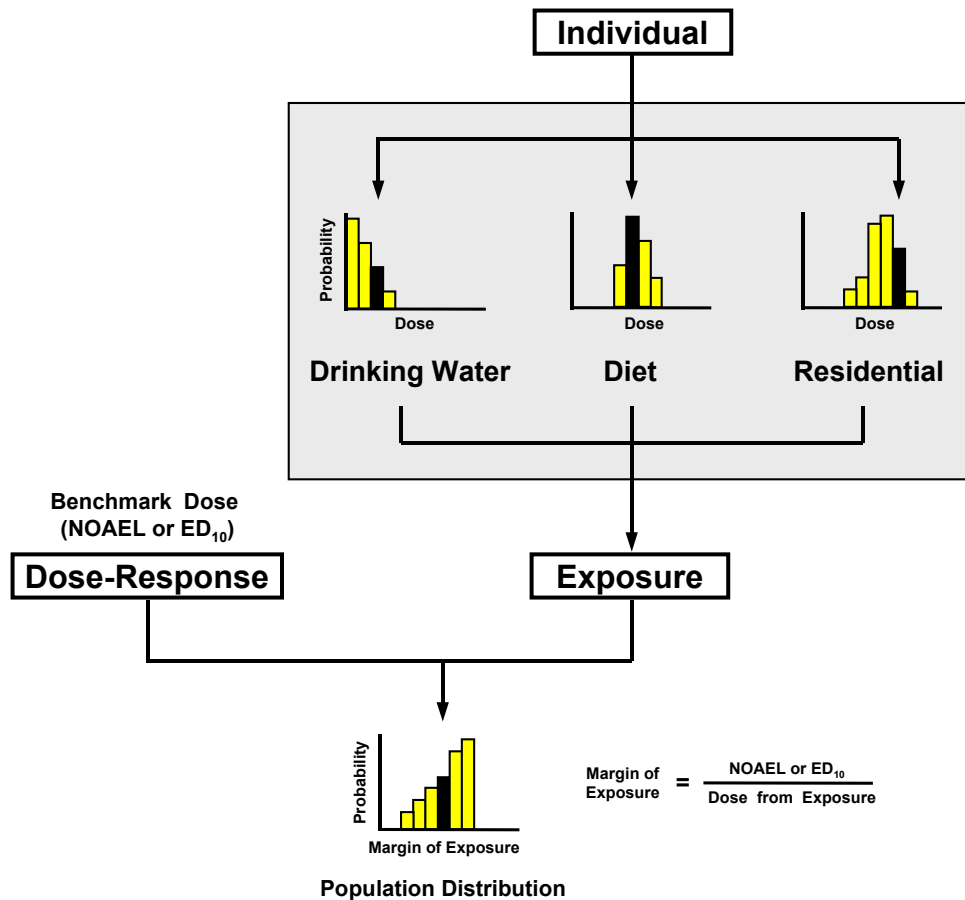
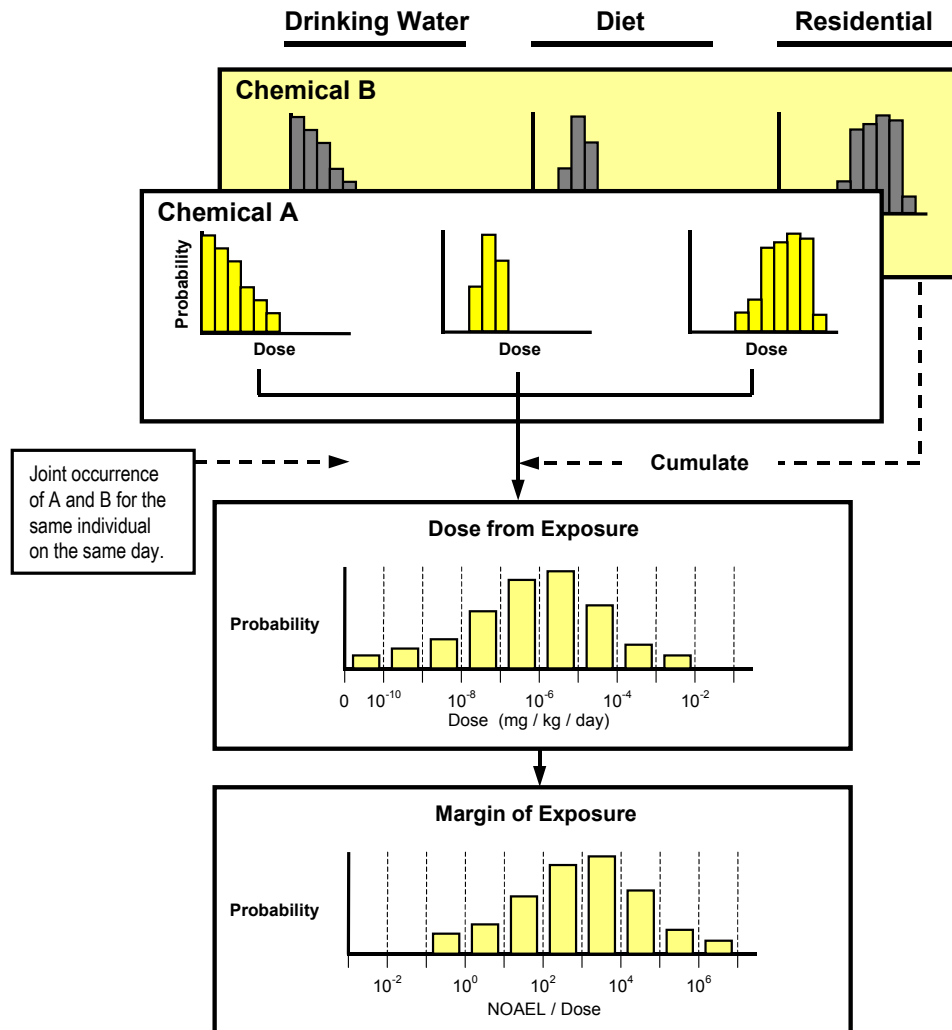


Figure 1.1 – Illustration of Aggregate Risk Characterization

## 1.6 How To Cumulate

In cumulative risk assessments, the potential exposure to two or more chemicals is described as a joint probability distribution rather than as independent probability distributions for each chemical alone. For example, if residues of two chemicals are found on apples, then the cumulative dose resulting from apple consumption should reflect the joint occurrence of the two residue concentrations on the same apple. It is incorrect to combine the residue of one chemical present on one apple with the residue of the second chemical on a different apple unless the apples were consumed as a blended commodity.

Figure 1.2 illustrates a case where Chemicals A and B share a common mechanism of toxicity and a cumulative risk assessment is appropriate.



**Figure 1.2 - Illustration of Cumulative Risk for Multiple Chemical Exposures**

In this example, the probability of the joint occurrence of residues for Chemical A and B is determined and the concomitant exposure to both chemicals is cumulated. The composite distributions of doses for Chemicals A and B can then be expressed as a combined distribution of toxicologically equivalent doses. This is accomplished by multiplying the dose for each chemical by an appropriate toxicity equivalency factor (Table 1.2). Alternatively, the Hazard Index (HI) or Margin of Exposures (MOE) for each chemical can be combined using the equations in Table 1.2. It should be noted that these same equations could be used to combine exposures from different routes of exposure for a single chemical.

## 1.7 How to Combine Doses

The mathematical combination of doses across routes and across chemicals depends upon establishing a common ground for comparison. CARES will initially allow the user to select one of the three alternative combinatorial approaches identified in Table 1.2, and others as they become available.

**Table 1.2 - Alternate Methods for Calculating Cumulative Risk**

Method	Description	Cumulative Equation
Toxicity Equivalency Factor (TEF)	The hazard of each chemical in the class is expressed relative to a standard and then the dose is adjusted for relative potency.	$(Dose_a \cdot TEF_a) + (Dose_b \cdot TEF_b) + \dots$
Margin of Exposure (MOE)	The MOE is calculated for each chemical as a ratio of its benchmark dose to the dose from exposure. The MOEs are then combined.	$\frac{1}{(1/MOE_a) + (1/MOE_b) + \dots}$
Hazard Index (HI)	The HI is calculated as a ratio of the dose from exposure to the reference dose. The HIs are summed.	$Dose_a / RfD_a + Dose_b / RfD_b + \dots$

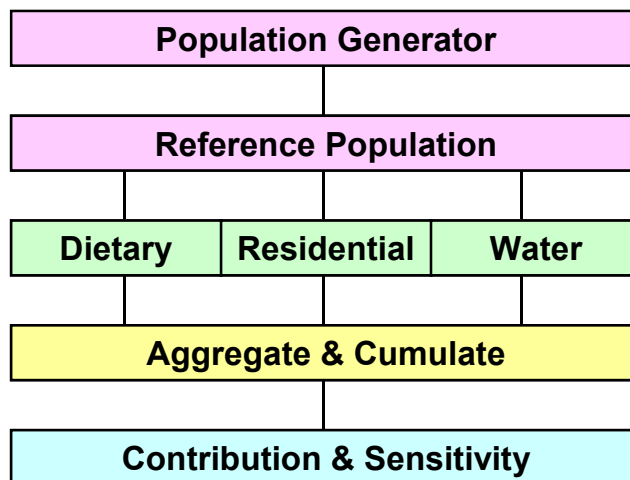
The Toxicity Equivalency Factor approach has been successfully used when one chemical provides a reference point for all members of a class of chemicals sharing a common mechanism. For example, the toxic equivalency of dioxin congeners has been expressed relative to TCDD (Brown et al., 1997).

The Margin of Exposure (MOE) approach (Whalen et al., 1997) is preferred when the benchmark doses (e.g., NOAELs) for compounds sharing a common mechanism are based upon the same toxicity endpoint or biochemical surrogate, evaluated in the same species by the same route of administration and for the same duration of exposure. Experimental error in accurately defining the NOAEL can be controlled by standardizing the magnitude of response across studies by using a benchmark dose (e.g. ED<sub>10</sub>, ED<sub>50</sub>, or Point of Departure) or a measure of relative potency (Slope Factor for non-cancer endpoints or Q<sub>1</sub>\* for cancer).

The use of the Hazard Index method (NCEA, 1996) is acceptable if the RfD for each chemical is based upon similar studies and the magnitude of the uncertainty factors are the same. When the studies or the uncertainty factors used in determining the RfD are different, then combining the hazard indices is not desirable because it is not possible to separate uncertainty from variability in the final risk distribution.

## 1.8 System Design Features

Figure 1.3 illustrates the modules that make up the CARES architecture. The Population Generator was used outside of CARES to create a reference population comprised of 100,000 individuals randomly selected from 5 million individuals who completed the long form of the 1990 U.S. Census (the PUMS dataset). Individual 365-day exposure profiles are created for each of these individuals by algorithms in the Dietary, Residential, or Drinking Water modules. The dose from exposure is aggregated and/or cumulated in the respective modules and a common risk metric is calculated using the equations provided in Table 1.2. The Contribution and Sensitivity Analysis module permits the user to explore the output from the Aggregate & Cumulate module to identify the contributing sources of exposure for individuals or subpopulations. These modules are discussed in detail in the following sections.



*Figure 1.3. - Modular Components of the CARES Architecture*

## 1.9 Reference Population Source Data

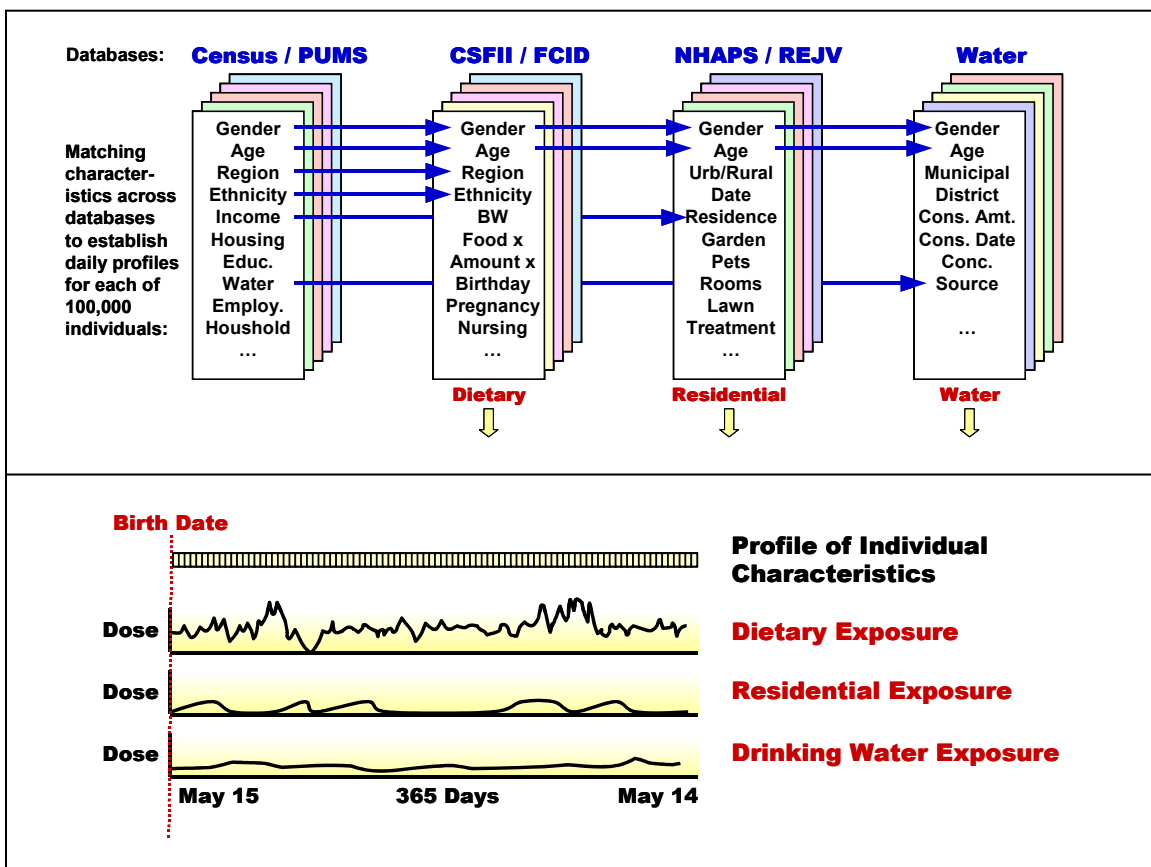
The reference population was constructed by randomly drawing 100,000 individuals from those who responded to the long form of the 1990 U.S. Census.

The 1990 U.S. Census does not provide all the attributes of individuals that are needed by CARES in order to perform aggregate or cumulative risk assessment. Therefore, data from other surveys have been incorporated into the reference population by matching Census individuals to individuals in other surveys.

## 1.10 Matching Attributes Across Surveys

A unique feature of CARES is the way in which it utilizes information from various population surveys to complete a comprehensive profile for each individual in the reference population. Selecting a set of critical attributes in the reference population and matching them to the same attributes in a second survey accomplish this. Some attributes are matched exactly for example the gender and ethnicity of subjects reported in the Census are exactly matched to the same attribute reported for subjects in CSFII/FCID food intake databases. Other attributes were matched less precisely using a measure of dissimilarity (Gower's Similarity Index) (Gower, 1971). For example age was given a high priority for closeness of matching in the age range from 1 to 12 years (exact by year up to age 12 and similar by month of birth), whereas youths were matched within a range of 12-19 years) and after age 19, age was not given a priority for matching. This is illustrated schematically in Figure 1.4.

Using this procedure, attributes not available for the reference population (e.g. daily food and water consumption) were assigned to individuals in the reference population based upon subjects in another survey, in this case CSFII/FCID.



**Figure 1.4 - Database Matching to Generate a Reference Population and to Create a 365 Day Exposure Profile for Individuals**

## 1.11 Creating a 365 Day Exposure Profiles

CARES creates a 365-day exposure profile (i.e. daily dose from exposure aggregated across all routes and pathways) for each individual in the reference population selected for inclusion in a Monte Carlo simulation (see Figure 1.4).

### Dietary Exposure Module

The daily dose from dietary exposure is calculated for individuals in CSFII/FCID that were identified as matches for individuals in the Census. These dietary doses are distributed across the calendar year. Assignment must be within the same quarter until there is dose estimate for every day in the year. This is illustrated schematically in Figure 1.5A. See Chapter 3 for details on the procedures for utilizing pesticide residue data and individual food intake records.

### Residential Exposure Module

The daily dose arising from residential exposure is calculated for up to 18 different scenarios selected based on EPA's Residential SOPs:

- Lawn Care
- Vegetable Garden Care
- Ornamental Plant Care
- Tree Care
- Pick Own Fruits/Vegetables
- Crack & Crevice Treatment
- Termite Control
- Rodent Control
- Pet Care
- Outdoor Fogger Use
- Indoor Fogger Use
- Indoor Treatment
- Paint/Wood Treatment
- Impregnated Materials
- Detergent/Handsoap Use
- Swimming Pool Use
- Golfer
- Public Use
- Custom (future)

Demographic information in the Census (e.g. region of the country, socio-economic status, housing type, pet status) is used in combination with user provided information on use (amount, frequency, and temporal pattern of use), dissipation, transfer) and human behaviors that would bring the subject in contact with the chemical. This is illustrated in Figure 1.5B. See Chapter 4 for details on the algorithms and calculations.

### Drinking Water Exposure Module

The daily dose from exposure to the chemical exposure in drinking water, is calculated by using regional and temporal specific pesticide concentrations provided by the user (based on monitoring and/or modeling), and by water intake and body weight data in the CSFII/FCID, and demographic information in the Census. This is illustrated schematically in Figure 1.5C. See Chapter 5 for details on these procedures and options.



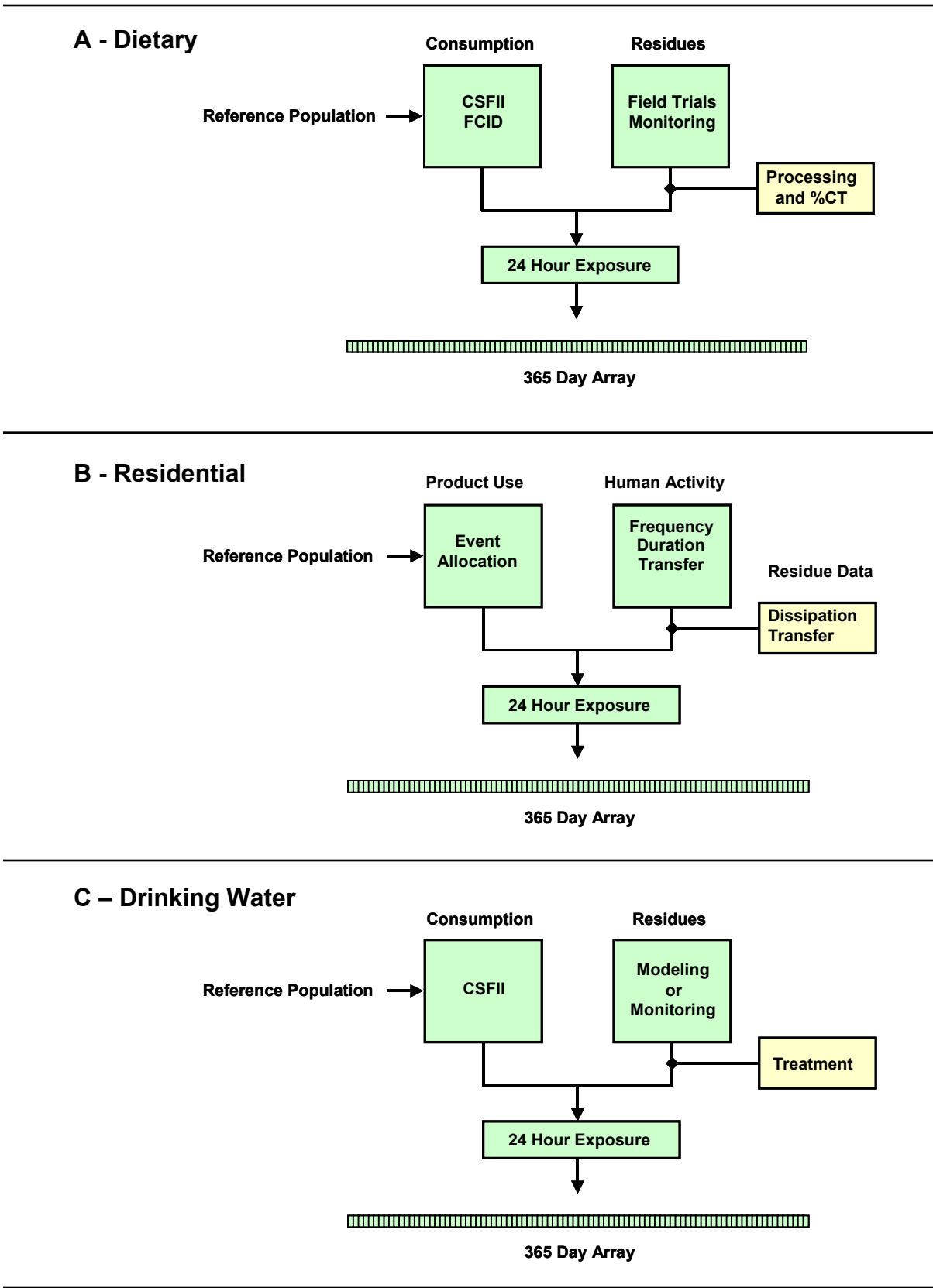
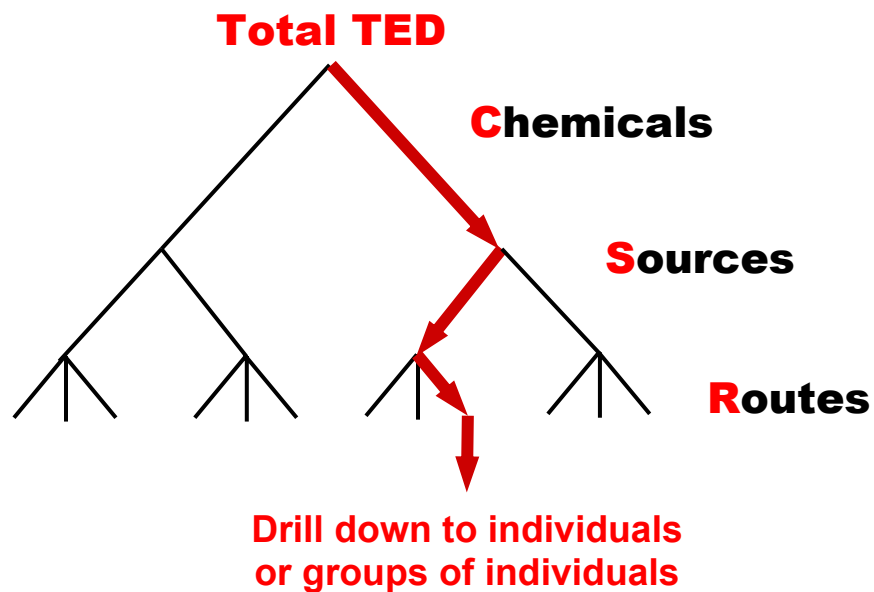


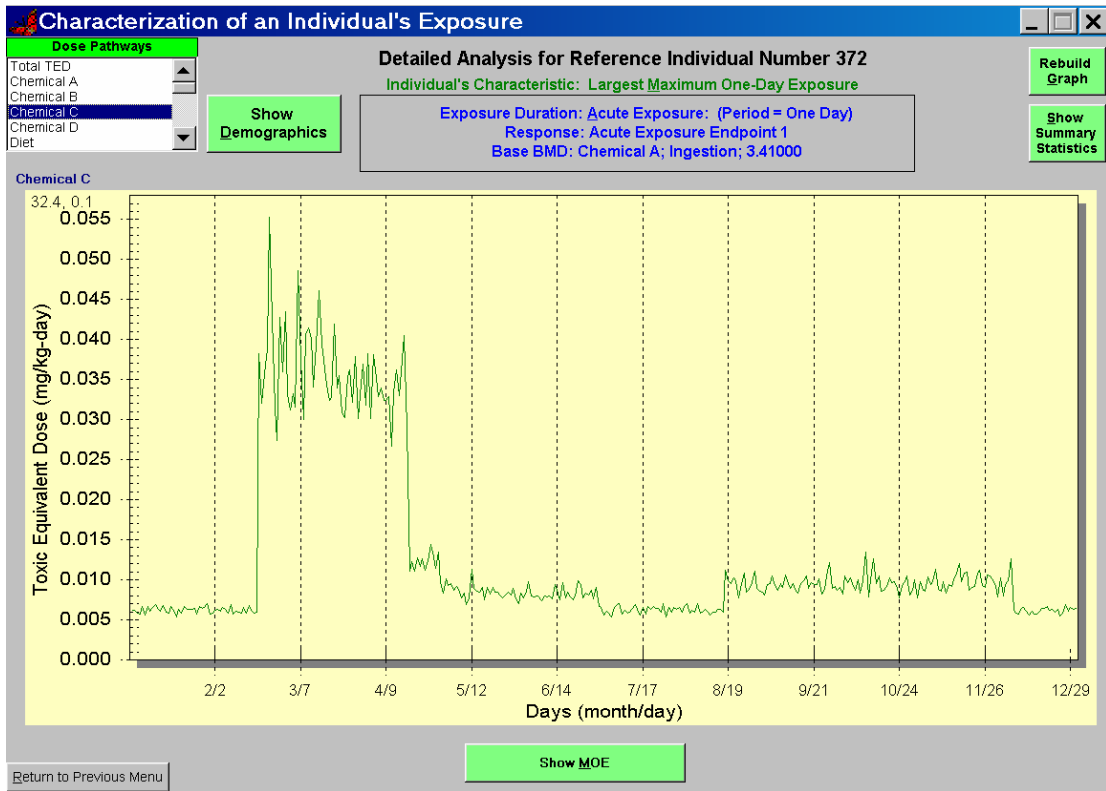
Figure 1.5 - Data Flow Diagram for the Exposure Modules

## 1.12 Viewing the Results: Contribution Analyses

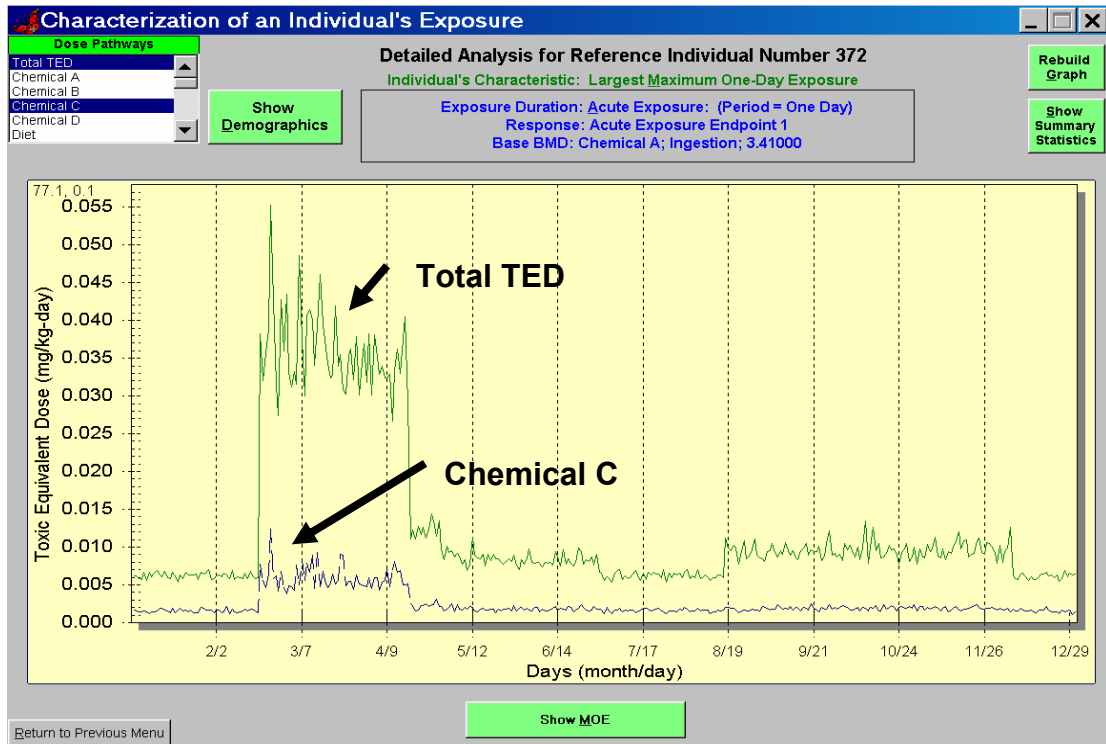
Monte Carlo simulations generate exposure and risk distributions for individuals or subpopulations of individuals that are best viewed graphically. CARES has incorporated an intuitive viewing utility which when coupled with a data explorer allows the user to query the results of the simulation in a manner that permits orderly decision-making. Figure 1.6 provides a schematic representation of how the user might structure a contribution analyses in cumulative risk assessment. Figure 1.7 provides a 365-day dose profile for one individual. The contribution of this individual's daily toxic equivalent does attributed to the chemical (Figure 1.8), pathway (Figure 1.9) or route (Figure 1.10) of exposure are shown. Similar analyses can be performed on groups of individuals in a user-defined subpopulation and statistics summarized in graphical or tabular form for all percentiles of the exposure or risk distribution are available within CARES (Figure 1.11).



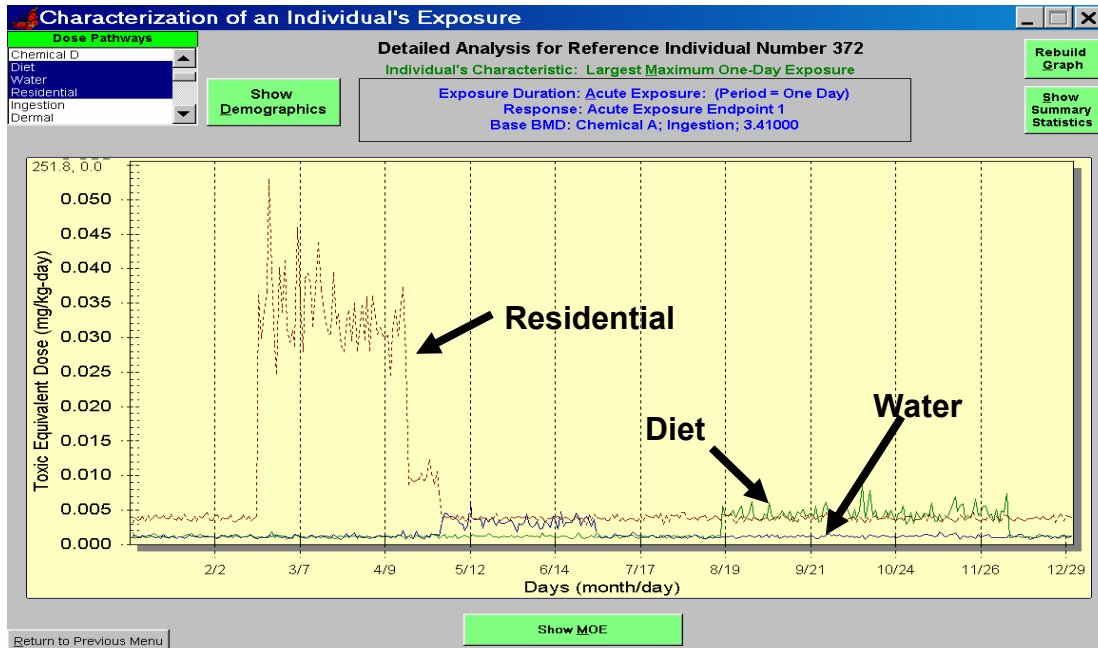
*Figure 1.6 - Schematic Representation of Decision Tree for Contribution Analyses*



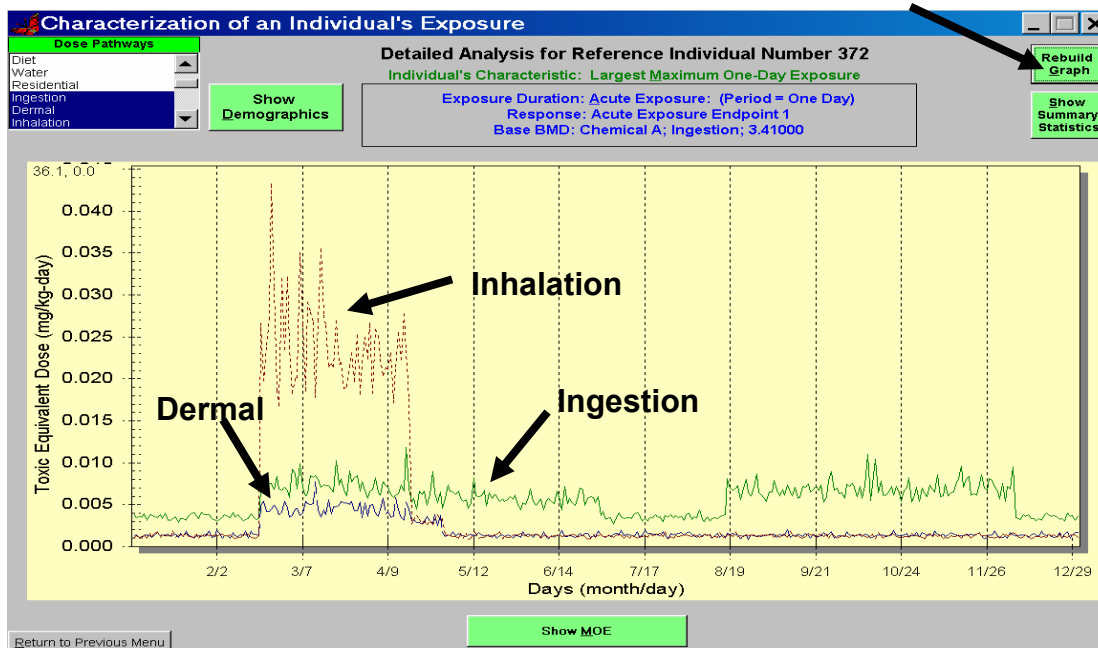
**Figure 1.7 - Total Toxic Equivalent Dose (TED) for Subject 372**



**Figure 1.8 - Chemical Contribution to the Total TED for Subject 372**



**Figure 1.9 - Pathway Contribution to the Total Toxic Equivalent Dose for Subject 372**



**Figure 1.10 - Route-Specific Contribution to the Total TED for Subject 372**

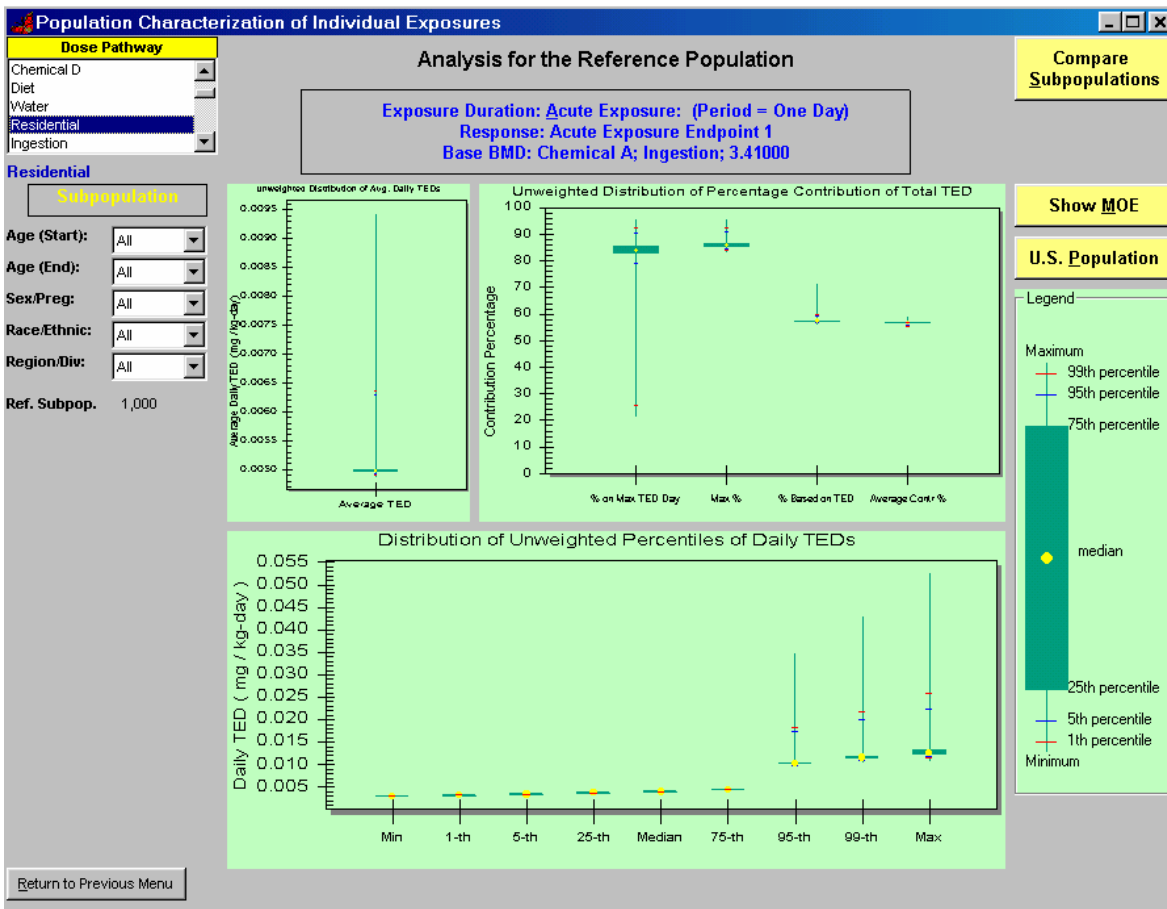


Figure 1.11 - Total Toxic Equivalent Dose for Subject 372

## 1.13 Sensitivity Analyses

The contribution analyses utility built into CARES Version 1.0 allows the user to conduct sensitivity analyses. The user can explore the consequence of changes in input parameters on the exposure or risk distribution by conducting successive simulation and comparing the results. Such an approach permits the user to determine which of the many input variables are capable of significantly impacting the risk distribution (i.e., how sensitive the risk distribution is to changes in input). Such systematic exploration of the sensitivity of the risk distribution to input parameters allows the user to allocate resources to the refinement of data that would likely have the largest impact on risk.

## 1.14 Uncertainty Analyses

The contribution analysis utility in CARES Version 1.0 can be used to conduct an uncertainty analysis. For example in an crack and crevice residential exposure assessment, the user may be uncertain about the distribution underlying of time that children come in contact with carpet and other floor surfaces in the

residence. The effect of this uncertainty can be quantified by running multiple simulations where different input distributions for this parameter are utilized while everything else about the simulation is maintained constant. The magnitude of the differences in the cumulative risk distribution (median, mean, upper percentile) between the multiple assessments constitutes a quantitative measure of the uncertainty associated with the simulation.

## 1.15 Testing, Verification, and Validation

Code testing and software verification ensure the computer code accurately represents the algorithms and solves the equations upon which it is based. Model validation determines how well the models are able to characterize hazard, exposure and risk compared to that occurring in the real world. Models that accurately and consistently predict these parameters are thought to be more valid than those that do not. CARES allows the user to compare results from lower tier (data poor) models to higher tier (data rich) models. As a result of this type of analysis, it is expected that data requirements will be further clarified and the models will come to be more representative of the real world. Thus as a result of successive improvements in the model, it is expected that the CARES software will produce results which are widely accepted as an accurate and representative estimate of a specified population's distribution of exposure and risks associated with pesticide use.

Overall validation, which includes appropriate documentation as well as testing and verification of the underlying exposure assessment models, will be conducted and documented following the system life cycle approach illustrated in Figure 1.12.

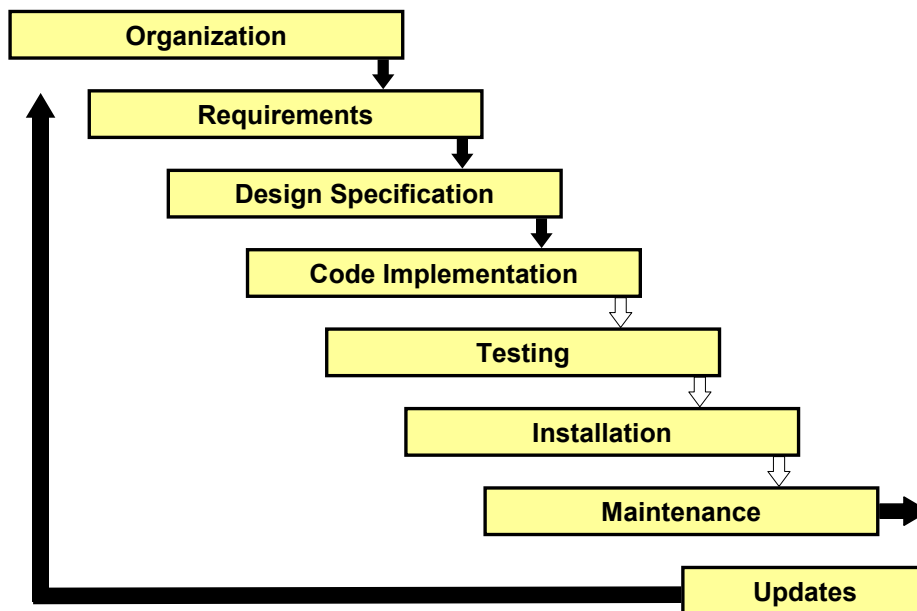


Figure 1.12 - System Life-Cycle Development and Documentation

The CARES Technical team adopted procedures to document user findings and to ensure that each component or object in the overall CARES model faithfully reproduces the physical, chemical, or biological behavior(s) of that part of the world it simulates. This iterative process was used in the developed of early, alpha versions of CARES and will continue following the official release of CARES Version 1.0. The documentation to be provided with Version 1.0 (and later versions) is summarized in Table 1.3.

**Table 1.3 - Summary of Life Cycle Documents for CARES**

System Documentation	
<b>Requirements</b>	Describe what the system does.
<b>Design Specifications</b>	Detail system architecture, logic, structures, performance specifications.
<b>Source Code</b>	Programming code with meaningful comments and illustrative diagrams.
<b>Test Documents</b>	Compilation of test plans and test results and all verification steps.
<b>System Installation</b>	Software and hardware installation details. Description of supplied files and their configuration.
<b>System Reference Manual</b>	Description of system usage including error messages and recovery procedures.
<b>User Manuals and Tutorials</b>	Introductory through advanced description of how to use the system. Presented with diagrams, screen shots, and examples. Hardcopy and on-line versions. Self-paced tutorial guides.
<b>Maintenance Procedures</b>	How to maintain and upgrade the system. Periodic test procedures. Security, backup, and recovery procedures.
<b>Change Control Procedures</b>	How to handle changes and revisions, updates and major additions. Addresses both changes to current code and procedures as well as how to handle addition of models, modules, databases and other significant evolutionary changes.
<b>Management</b>	Ongoing system management and user control procedures.

## 1.16 References

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## 2. Reference Population

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# Chapter 2 – Reference Population

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## 2.1 The Reference Population

In order to provide an accurate estimate of the potential exposure to a population, the population that is being simulated by a model must represent, as far as possible, real people and real circumstances that might result in exposure. CARES is designed to accurately simulate dietary (including drinking water) and residential exposure for representative individuals within the U.S. population based on the unique characteristics of that individual (e.g. age, gender, race/ethnicity, body weight, geographic location, income, type of residence and activity patterns). It does this by calculating exposure to a pre-selected sample of individuals using data taken from the 1990 U.S. Census. For the purposes of creating CARES Version 1.0, a single, static, reference population (RP) of 100,000 individuals was created. In the future, it is anticipated that additional special populations could be created as needed. (Note: for additional information on how the reference population was developed, please see Appendix B).

All calculations within CARES are based upon the reference population that consists of 100,000 persons selected from the 1990 Census. This RP population is static, or fixed, and is used either in total or as selected subpopulations to support all CARES evaluations. Since it is not feasible with current PC technology to simulate individual exposure to each of the approximately 250 million persons in the 1990 Census, a smaller representative subsample or RP was created by sampling the U.S. Census Public Use Micro Data Sample (PUMS).

The 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 general U.S. population. PUMS data are taken from the “long” form from the U.S. Census. PUMS 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. The long form contains many types of data on individuals who live within the United States including age, gender, location and type of residence, etc. The PUMS sample is stratified by these data to make sure that it remains representative of the U.S. population.

The CARES RP was created 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 number of persons in the RP was chosen to be able to support exposure analyses for key user-specified subpopulations. Example strata include:

#### 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 RP was designed to include sufficient numbers of individuals in each of these groups so that the probability is high that the quantiles in the RP distribution are close to the quantiles in the population distribution. Since the extremes (99th percentile and above) of the exposure distribution are of interest in doing different types of risk assessments, large numbers of individuals in each of the subpopulations of interest were required in the reference population.

A sample size of 5000 for subpopulations was determined to provide sufficient confidence that CARES would not appreciably underestimate the 99.9th population quantile and will not appreciably overestimate the 99.9th population quantile if the underlying data are accurate. Analyses can be performed with fewer persons; however, the resulting exposure estimates will not be as reliable. Of course inaccuracies in the underlying data sets will have a significant effect on the accuracy of the final estimate. In addition, conservative assumptions made in the data selection process (for example use of crop field trial data or worst case residential usage assumptions) will significantly affect how well the final estimates represent reality.

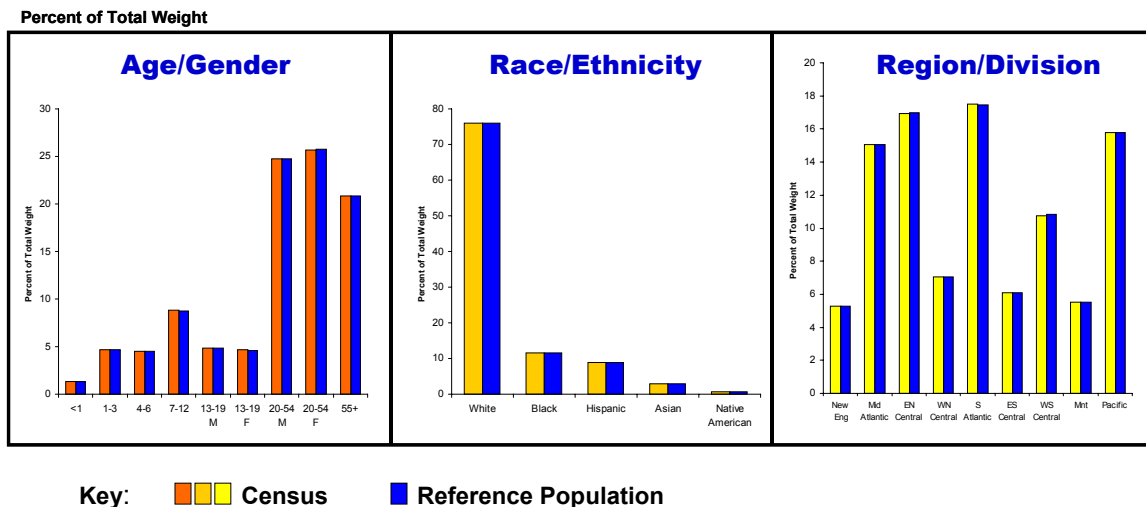
All of the random number generation used in the creation of the Reference Population was done using the random number generator in SAS, Version 8 (currently, the latest version). "The SAS® System is an integrated system of software providing complete control over data management, analysis, and presentation." SAS is published and distributed by SAS Institute Inc., SAS Circle, Box 8000, Cary, NC 27512-8000. As described in SAS Language, Reference Version 6 First Edition, 1990, page 592, the random number generator is RANUNI, which generates a random variant from a uniform distribution. The RANUNI function returns a number generated from the uniform distribution on the interval (0,1) using a prime modulus multiplicative generator with modulus 231-1 and multiplier 397204094 (Fishman and Moore, 1982). The RANUNI function is identical to the UNIFORM function. The syntax is RANUNI(seed). The seed used in sampling PUMS was 13575591. The seed used in the matching

with CSFII/FCID was 34178945. The random number streams using these seeds have been reviewed from a statistical perspective.

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 about 12 million people in the 5% PUMS. These weights are then used by CARES to provide accurate estimates of potential exposures to the entire population or subpopulations.

Because of the minimum requirement for 5000 individuals in each subpopulation group, the relative proportion of the various subpopulations within the RP is not similar to the U.S. population. For example, the proportion of infants and young children in the RP (>20%) is much higher than that in the U.S. population. The RP of 100,000 contains the statistical weights needed to convert the exposure values so that they accurately represent exposure within the U.S. population. These weights include the weights provided in the PUMS as well as the weights required by moving from the PUMS to the smaller reference population. A person in the RP may represent a thousand or more persons within the actual U.S. population; however, population level exposure estimates from CARES will be representative of exposure to the general U.S. population.

The CARES reference population was qualitatively and quantitatively compared to the Census/PUMS population to make sure that it was representative of the U.S. population. This was done using various graphical techniques to compare measured variables within each population (age, gender, location, residence type, etc.). The two populations (RP and PUMS) were found to be almost identical both quantitatively and qualitatively (see Figure 2.1 and Tables 2.1 and 2.2) for all parameters that were analyzed.



**Figure 2.1 - Quantitative Comparison of Age/Gender, Race/Ethnicity, and Locational Data for the U.S. Census and the Reference Population.**

The simulation period within CARES is one calendar year. For each person in the reference population, the calendar year begins on a selected birthday and extends through a 365-day period until the day before their next birthday. Exposures are simulated for each day (24-hour period) during the year. While less than 24-hour exposure intervals may be useful to provide more accurate estimates of exposure for some compounds, the food consumption data set (CSFII/FCID database) and residential algorithms are not sufficiently robust to support this type of analysis at this time.

**Table 2.1 - 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
<b>Age/Gender</b>		
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
<b>Race/Ethnicity</b>		
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
<b>Census Division</b>		
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

**Table 2.2 - Number of individuals in the Reference Population in each State and Comparison Between Total Weights Per State in the Reference Population and the PUMS/Census**

State FIPS Code	State Postal Code	Number of Individuals in Reference Population	Sum of Weights in Reference Population	Number of Individuals in PUMS / Census	Sum of Weights in PUMS / Census
01	AL	1,487	3,948,075	192,768	3,943,127
02	AK	541	528,034	28,593	530,149
04	AZ	1,790	3,552,611	176,223	3,572,732
05	AR	884	2,321,612	113,041	2,286,477
06	CA	12,622	28,865,598	1,426,742	28,979,354
08	CO	1,349	3,263,525	166,910	3,204,894
09	CT	1,190	3,169,011	155,261	3,181,210
10	DE	248	655,184	31,213	641,437
11	DC	225	557,175	28,854	569,188
12	FL	4,926	12,613,305	652,504	12,618,337
13	GA	2,579	6,261,801	325,923	6,293,815
15	HI	673	1,059,406	53,900	1,067,782
16	ID	408	1,000,402	48,923	970,424
17	IL	4,477	11,128,929	570,166	11,110,104
18	IN	2,104	5,346,792	271,970	5,386,194
19	IA	1,031	2,629,850	134,160	2,666,634
20	KS	990	2,354,311	122,484	2,388,985
21	KY	1,327	3,513,812	175,195	3,566,755
22	LA	1,632	4,154,997	204,087	4,083,282
23	ME	475	1,150,067	61,072	1,189,760
24	MD	1,904	4,667,413	240,038	4,666,963
25	MA	2,338	5,845,623	300,738	5,801,791
26	MI	3,627	9,119,092	449,575	9,073,623
27	MN	1,825	4,246,797	222,882	4,248,953
28	MS	1,024	2,468,751	130,191	2,490,972
29	MO	1,951	4,992,682	248,226	4,957,008
30	MT	409	758,914	38,517	773,225
31	NE	622	1,517,432	76,701	1,530,615
32	NV	544	1,178,662	60,235	1,171,696
33	NH	422	1,056,830	55,521	1,072,762
34	NJ	3,101	7,525,423	396,353	7,528,251
35	NM	908	1,509,655	77,568	1,478,820
36	NY	7,072	17,243,101	892,718	17,377,131
37	NC	2,615	6,374,680	327,330	6,387,570
38	ND	287	594,476	30,107	610,945
39	OH	4,110	10,627,708	528,847	10,571,637
40	OK	1,680	3,025,126	151,782	3,044,117
41	OR	1,172	2,899,697	138,418	2,768,199
42	PA	4,416	11,537,717	584,028	11,506,836
44	RI	371	957,330	47,683	964,180
45	SC	1,262	3,376,446	163,374	3,364,914
46	SD	343	635,323	33,121	667,731
47	TN	1,827	4,745,574	239,324	4,733,052
48	TX	7,025	16,657,844	869,399	16,558,412
49	UT	791	1,623,526	88,238	1,693,064
50	VT	216	519,674	27,495	538,449
51	VA	2,303	5,944,524	291,032	5,975,784
53	WA	2,108	4,714,636	239,857	4,722,693
54	WV	635	1,724,997	86,789	1,749,311
55	WI	1,938	4,742,974	241,664	4,747,601
56	WY	196	437,611	22,581	442,630
	Total	100,000	241,344,737	12,240,321	241,469,575

## 2.2 Matching of Census Data with other Databases

While the U.S. Census contains many descriptive variables for each of the person in the population, it does not contain many variables that are needed to be able to estimate exposure. For example, dietary consumption, drinking water consumption, and human activity patterns are not included in the U.S. Census data. In order to calculate exposure, these variables must be obtained from other current databases which can be “matched” to the U.S. Census data. In this way the Reference Population deals with real people at the time the databases are assembled. For example, seventy-year-old people are described “today” rather than trying to describe what they might be like at a point seventy years in the future.

It is impossible to match an individual in the Census with the exact same individual in another database. The identities of person in most surveys are generally unknown or are hidden from users for reasons of confidentiality. Also, the same individuals are unlikely to be present or represent the same age groups in samples taken at different times. It is possible, however, to match persons in the U.S. Census with similar persons in the other datasets. For example, the U.S. Census may contain data for a four-year old, Hispanic, female. This information can then be matched with dietary and drinking water consumption and activity data for a 4 year old, Hispanic, female from other datasets to be able to estimate exposure.

The Census based characteristics for each individual that are used by any component of CARES are saved in a “Vector of Individual Characteristics” (VIC) for each member of the reference population. The VIC contains the individual’s age, gender, income, residence type, etc. as well as the characteristics derived from this information through matching that might lead to exposure such as food and drinking water consumption and the frequency and duration of various activities. In practice there are two components of the VIC: the VIC kernel and the VIC augmentation. The VIC kernel represents the information for each individual that never changes from one CARES analysis to another. For example, a person’s age or residence location remains the same for all CARES analyses. Or for the CARES Version 1.0, the matching between the Census and CSFII (Continuing Survey of Food Intake by Individuals) individuals has already been done as part of the VIC. The VIC augmentation contains data that may change between analyses. For example, a user may wish to change the probability that a person has a dog or other type of pet between analyses. The VIC for each person is stored for each analysis and can be easily retrieved if needed to facilitate data analyses.

Matching between the Census data and other databases is done using distance (or dissimilarity) measurements for a set of variables present in both databases. The idea is to match similar persons as much as possible between datasets. The databases were matched using simple Euclidean distances for some qualitative variables (region, etc.) and Euclidean distances along with multidimensional scaling for quantitative variables such as household size, etc. (Cox and Cox, 1994) Then Gower’s dissimilarity index (Gower, 1971) was used to combine individual characteristic differences. The following list contains characteristics that were used in matching an individual from PUMS to individuals contained in CSFII database.



- Region
- Urban vs. Rural status
- Household Size
- Gender
- Age
- Race/Ethnicity
- Household Income
- Percent of Poverty Level
- Poverty Category
- Employment Status
- Educational Level
- Home Ownership Status

Some of the variables on this list received higher priority in the matching process than others. For example, gender was always matched exactly. Age, on the other hand, was matched closely for infants (exact by year, similar by month), children (exact by year to age 12), and youth (matched within a range of 12-19 years) but after age 19 did not receive any priority in matching databases. This process resulted in the selection of a “primary match” person in the CSFII to the Census data. The CSFII data adds body weight, height, and pregnancy status on a single day to the VIC and also provides food consumption data (discussed in greater detail below).

The next step in the process of creating the VIC is to create a 365-day profile for each person in the reference population. The first element of the 365-day profile represents the characteristics of the RP individual on their last birthday and the 365th element in the profile will be the day prior to their next birthday. Since neither the Census nor the CSFII contains information on birthdates, a birthday is selected consistent with the data contained in the surveys. For example, for infants there is a record of age in months in the CSFII. Thus we can “count back” from the date of the survey and assume that the birthdate occurred somewhere within a 30-day window. For older persons, it was assumed that the birthday occurred on or before the first of the two survey dates in the CSFII, but less than a year before the second date (if present). The birthdates for persons were generated randomly and uniformly within the ranges given above.

A similar method to that used for birthdays was used to create gestational age profiles for pregnant females so that associated weight gains could be simulated. The CSFII contains information on “number of months pregnant” that can be used to give an estimate of a window of when conception probably occurred. Weight gain during pregnancy was then estimated by using a simple cubic exponential model to fit the “desirable weight gain” guidelines provided by the Texas Department of Health (Garriot and Morat, 2000).

It is important to obtain height and weight measurements for individuals to be able to accurately estimate exposure. The height and weight values were reported in EPA’s Food Commodity Intake Database (FCID) that is based on the CSFII database. (The CSFII has some missing values for height and weight that were replaced by imputed values in the FCID.) For adults (20 years and greater) it was assumed that weight and height did not change during the year. For other age groups, however, it was assumed that both height and weight changed during the 365-day profile. The reported weights from FCID were compared to the distribution of weights for persons of the same age and gender as reported

by the National Center for Health Statistics (NCHS, 2000) to obtain an estimate of the percentile into which the person fell. Then it was assumed that the persons weight and height changed over time (changes monthly) in a manner similar to others in the same percentile of the overall distribution for that age.

## 2.3 Creation of Food Consumption Profiles

After the Census data has been matched to the appropriate CSFII dataset, the food consumption profile for each person in the reference population can be created. The goal is to answer the question “what did each person eat on each day during the 365-day period?” The CSFII dataset contains one or (usually) two days of consumption data for each person in the survey. It is not reasonable to assume that the person eats the same thing for 365-days as they ate during the two days in which they were surveyed. Instead, surrogate days from the CSFII/FCID are used to fill in the other 363 or 364 days of the consumption profile.

The matching between consumption days is uses the same process (Euclidean distance and Gower’s dissimilarity) as that used to match the U.S. Census and CSFII data as explained above. However, here person-specific and day-specific characteristics were compared for the person in the reference population to consumption days of other surrogates in the FCID. Parameters used in matching dietary consumption days included:

- Day of year (calendar date)
- Food Sufficiency (enough to often not enough)
- Health Status (excellent to poor)
- Smoking Level (<100 in lifetime to >40 per day)
- Vegetarian (yes or no)
- Diabetic (yes or no)
- Low Calorie Diet (yes or no)
- Low Fat Diet (yes or no)
- Low Salt Diet (yes or no)
- Low Sugar Diet (yes or no)
- Diabetic Diet (yes or no)
- Milk Allergy (yes or no)
- Egg Allergy (yes or no)
- Fish/Shellfish Allergy (yes or no)
- Peanut Allergy (yes or no)
- Breastfeeding Status (yes or no)
- Lactation Status (pregnant, lactating, preg & lactating, not any)
- Age in months (used for matching infants <1 year)
- Day of Week (Sunday through Saturday)

Conceptually, the process used in matching is straightforward. For each person in the reference population the algorithm considered one day of the consumption profile at a time. It finds the 3-5 person-days in the FCID surrogate pool that are most similar to the reference population person and profile day being filled. One of the 3-5 candidate person-days is then randomly selected and added to the profile. For most persons in the FCID there are two days of dietary consumption. If there is another person-day for the surrogate person selected, then an attempt is made to add it to the profile as well.

More specifically, for each RP individual the food consumption imputation algorithm repeats the following steps until the profile of 365 days is completely filled:

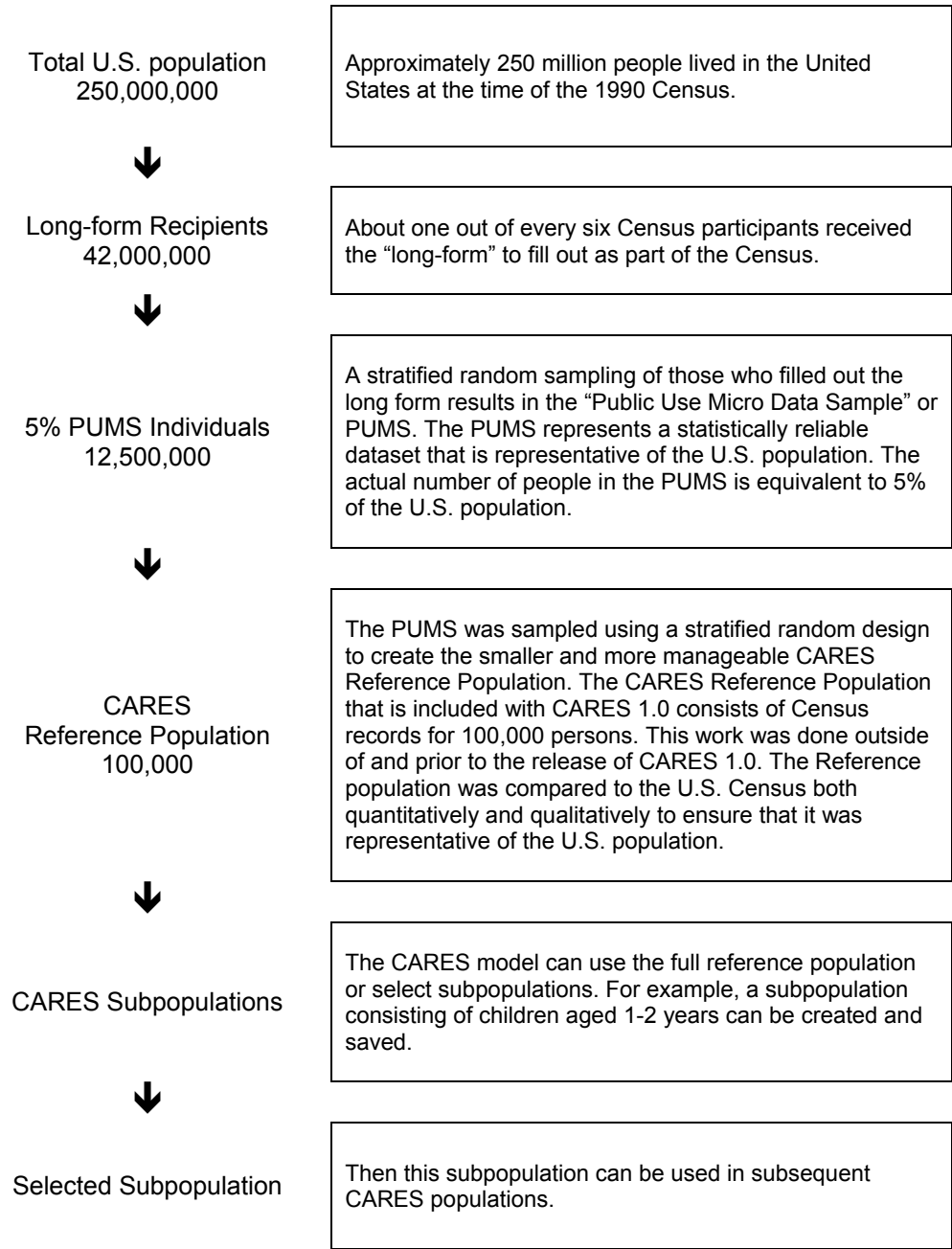
1. Pick the next day-in-age, D, in random order. If D is already assigned a CSFII person-day and there are unfilled days-in-age remaining, then pick a new day-in-age, D. (Note days are selected in random order to avoid systematic bias in filling days.)
2. Construct all matching characteristics that will 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's 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's dissimilarities.
5. Randomly select one out 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 person just selected, then continue with the next unfilled value of D at step 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 the 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-or-week for the second CSFII person-day. Randomly select day-in-age D\* from among these and assign it as the second CSFII person day.

As with the Census to CSFII matching, not all of the matching parameters were given equal weight. Primary matching characteristics included gender, pregnancy status for women, age in months for infants less than one year old, breastfeeding status (for infants < 1yr), and age in years for persons less than 20 years old. To preserve the seasonal nature of consumption data, the "matching neighborhood" was restricted to within seven days of the target date. (Whenever the +7 day restriction resulted in fewer than 3 candidate person days, the restriction was relaxed to +15 days or in a few instances to +30 days to obtain >3 candidate person days). In addition, because consumption patterns may be affected by the day of the week (weekend consumption may be different from weekday consumption, etc.), a preferred order of matching days of the week was established. The highest preferred day-of-week was always the same day-of-week that the algorithm was seeking to fill. The other days were preferred in

order of increasing Euclidean distance, however, with weekdays being set to be more similar to each other than with weekend days, etc.

## **2.4 Creation of Residential and Drinking Water Profiles**

Additional matching is done between the CARES reference population and the appropriate databases to help determine potential exposure from residential and drinking water sources. The reference population contains general information about the person's age, where they live, and what size and type of house they live in. The matching from this information to facts such as pet or lawn ownership and the likelihood of pesticide treatments occurs within the residential module and will be discussed as part of that chapter. The amount of drinking water that is consumed is part of the CSFII/FCID food matching discussed above. Additional matching, however, can also be done as part of the CARES analysis to match information on location and drinking water source (well or public water system) that may be available in the reference population with additional user supplied information on drinking water sources. This matching is discussed as part of the drinking water module (Chapter 5 and Appendix B).



**Figure 2.2 – Reference Population Flowchart**

## 2.5 References

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# 3. Dietary Module

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# Chapter 3 – Dietary Module

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## 3.1 Introduction

Five different CARES modules are used when estimating dietary exposure. The Run Specifier Module is used to provide information describing the modeling run. The Chemical Selector Module is used to designate the chemical(s) that will be used in the assessment. The Population Selector Module is used to designate the subpopulation that will be used in the assessment. The Food Selector Module is used to select the foods and residues that will be used in the assessment. The Dietary Module then carries out the actual food and residue matching and exposure calculation. Technical information on the Population Selector Module (as it relates to dietary assessment), the Food Selector Module, and the Dietary Module is included below. The relationships between all five of the modules and various input/output files are shown in Figure 3.1 (see end of Chapter).

## 3.2 Population Selector

The Population Selector is used to designate the population that will be used in the assessment. As part of the creation of the reference population, individuals within the U.S. Census were matched with similar individuals within the CSFII (Continuing Survey of Food Intake by Individuals, 1994-96,98) database to obtain food consumption data for each day within a 365-day period. This survey contains dietary consumption and other useful data for 21,662 persons. In most cases, two days of dietary consumption information were obtained for each person, thus a total of approximately 40,000 dietary days are available for use in CARES.

The CSFII database contains information on foods as eaten. For dietary exposure assessment, consumption of raw agricultural commodities (RAC) is needed. The conversion of the CSFII data to RAC data was done jointly by USDA/ARS and EPA/HED and published as the Food Commodity Intake Database (FCID, as modified by Novigen Sciences and supplied to EPA for use in probabilistic modeling using Calendex™). The FCID takes the individual eating event data from CSFII and summarizes it in 24-hour intervals for each person in the CSFII. This 24-hour time-step simplification of the CSFII data allows faster calculation of dietary exposure. However, this efficiency comes at the cost of assuming that all residues on individual units of a commodity during a day are exactly the same (which is unlikely). In addition, use of a 24-hour total value does not allow exposure or risk assessments for periods of less than 1-day. This may affect the ability of the model to accurately estimate risk for compounds such as carbamate insecticides that have effects that have been shown to be rapidly reversible.

The FCID contains data on how the food was prepared. For example a commodity such as apples may be eaten raw, peeled, cooked, juiced, etc. These data are important since residues may be affected (increased or decreased) by each of these preparation or processing steps. CARES retains this food preparation information and it can be used when assigning residue values to

different types of prepared foods as well as when determining the relative importance of various sources of dietary exposure.

The CARES Reference Population (RP) includes daily consumption of RACs for 100,000 persons. These data can be viewed (and queried) by opening the Population Selector module within CARES using the Notitia interface. In order to use CARES to estimate dietary risk, the user opens the Population Selector module and selects the population for which exposure is to be estimated. The full population, pre-selected sub-populations, or a user-selected sub-population can be selected for exposure estimates.

### **3.3 Food Selector**

The Food Selector module has three sections that are presented as “tabs” on the Notitia screen: Foods, Consumption, and Residues. Each of these sections or tabs allows the user to define and select the datasets that will be used in the dietary risk assessment.

#### **3.3.1 Foods**

The Food /Food Form database contains the basic descriptions of the potential foods and food forms that will be used in the assessment. This includes a description of the Crop Group or sub-group, the FCID Food code, a text description, and a description of food form and cooking status/methods for each food. These data form the foundation for the relationships between the consumption and residue data. In this section the user can view the underlying food consumption dataset that is being used in the assessment Table 3.1 shows a portion of the FCID database as represented in the CARES Food Selection module and Table 3.2 describes each of the columns contained in the database.

#### **3.3.2 Consumption**

The user must designate which foods will be considered in the assessment. The development of consumption files is described in the user manual. Basically the user can select either the entire FCID database (highly unlikely since no product is used on all crops) or a subset of the FCID database. Creation of the consumption database takes place in two steps. First the user defines what foods will be included in the database (either using the Notitia database or by importing data from a spreadsheet into Notitia). Then Notitia builds a “food match” consumption database for those foods based on the population that was selected in the Population Selector module. The database includes each person from the population being evaluated and a description of what they ate on day one or two of the consumption survey. It differs from the full FCID database in that it only contains the selected foods. An example of the food consumption database is shown in Table 3.3 and the columns are described in Table 3.4.

**Table 3.1 – An Example of a Portion of the FCID Database as Represented in CARES.**

Crop/Sub-Crop	Food Code	Description	Cooked Status	Food Form	Cooking Method
8	8003750	Tomato	Cooked	Not specified as to form or multiple forms	None or Not Applicable
9B	9021350	Cucumber	Salad	Not specified as to form or multiple forms	Boiled
10	10002000	Lemon, juice	Cooked	Fresh	Baked
11	11000080	Apple, peeled fruit	Cooked	Canned	None or Not Applicable
12	12000900	Cherry	Not specified as to cooked or uncooked	Not specified as to form or multiple forms	Not specified as to cooking
15	15000250	Barley, pearled barley	Cooked	Not specified as to form or multiple forms	Not specified as to cooking
15	15001210	Corn, field, meal	Cooked	Not specified as to form or multiple forms	Baked

**Table 3.2 – Description of Each Column in the FCID Database as Represented in CARES.**

Column	Description
Crop/Sub-Crop:	This designates the EPA crop grouping for each of the foods.
Food code:	This is the FCID code number for each food or food form.
Description:	This is a textual description of the food for each FCID code.
Cooked Status:	The cooked status of the food (cooked, frozen meal, not applicable, not specified, processed oil, salad, sandwich, or uncooked)
Food Form:	This is the form that the food was in before it was eaten (canned, cured, dried, fresh, frozen, not applicable, not specified or multiple forms, or other process not listed).
Cooking Method:	If the food was cooked, then this column contains a description of how it was cooked (baked, boiled, boiled or baked, fried, fried or baked, none or not applicable, not as to cooking methods).

**Table 3.3 – An Example of a Portion of the CARES Food Consumption Database.**

FCID ID	Person #	Day #	Food Code	Cooked Status	Food Form	Cooking Method	Consumed Amount (g/kg/day)
10003	1	2	Tomato	Uncooked	Fresh	None or Not applicable	1.43
10004	2	2	Tomato	Uncooked	Fresh	None or Not applicable	0.359558
10007	1	2	Tomato	Uncooked	Fresh	None or Not applicable	1.134706
10007	2	2	Tomato	Uncooked	Fresh	None or Not applicable	0.31759
10008	1	1	Tomato	Uncooked	Fresh	None or Not applicable	0.55
10008	1	2	Tomato	Uncooked	Fresh	None or Not applicable	0.256992

**Table 3.4 – Description of Each Column in CARES Food Consumption Database.**

Column	Description
FCID ID	This is the ID code for the household of each of the persons in the FCID.
Person #	This is the person number for the person within the household in the FCID.
Day #	Most FCID participants provided two days of consumption information, this value designates day one or two of consumption.
Food code:	This is the FCID code number for each food or food form.
Description:	This is a textual description of the food for each FCID code.
Cooked Status:	The cooked status of the food (cooked, frozen meal, not applicable, not specified, processed oil, salad, sandwich, or uncooked)
Food Form:	This is the form that the food was in before it was eaten (canned, cured, dried, fresh, frozen, not applicable, not specified or multiple forms, or other process not listed).
Cooking Method:	If the food was cooked, then this column contains a description of how it was cooked (baked, boiled, boiled or baked, fried, fried or baked, none or not applicable, not specified as to cooking methods).
Consumed Amount	This is the amount of food consumed during the 24 hour survey period in mg/kg bw/day.

### 3.3.3 Residues

The residue values to be associated with each food (or potentially with different food forms) are defined under the residue food tab. Residues may be single values such as tolerance values, relatively small groups of field trial data, or large monitoring databases. There are three types of values in the residue database. The first type of values are critical elements and include the CAS# (to link the residue data to a particular compound), a designation of units (usually parts-per-million), and the residue value.

A second group of values is included in the database to help the user identify the source of the residue data, but are not actually used by CARES in an analysis. For example, the “Notes” and “Data Set ID” columns are used to describe the source of the data.

A third set of values is in place for future refinements of the CARES model. These include the LOD and LOQ values that will be used as input to various “rules” on how to work with censored data. The residue database will generally be created outside of CARES using an exported template (see CARES User Guide) and then imported.

**Table 3.5 – An Example of a Portion of the CARES Residue Database.**

Data Set ID	Food Code	C S	F F	C M	CAS #	Repl icate	Sam ple	Resi due*	Notes	LOD	LOQ
ZIG-8482	8002700	0	0	0	11-1111-1	1	0	0.01	Pepper, bell, Green Peppers, California Bell, Whole Fruit, Composite Sample, Process: None, Sample: Homogenized	0.01	0.03
ZIG-8482	8002700	0	0	0	11-1111-1	2	0	0.037	Pepper, bell, Green Peppers, California Bell, Whole Fruit, Composite Sample, Process: None, Sample: Homogenized	0.01	0.03
ZIG-8482	8002700	0	0	0	11-1111-1	3	0	0.039	Pepper, bell, Green Peppers, California Bell, Whole Fruit, Composite Sample, Process: None, Sample: Homogenized	0.01	0.03
ZIG-8482	8002700	0	0	0	11-1111-1	4	0	0.057	Pepper, bell, Green Peppers, California Bell, Whole Fruit, Composite Sample, Process: None, Sample: Homogenized	0.01	0.03
ZIG-8482	8002700	0	0	0	11-1111-1	5	0	0.04	Pepper, bell, Green Peppers, California Bell, Whole Fruit, Composite Sample, Process: None, Sample: Homogenized	0.01	0.03

\* Units in ppm

**Table 3.6 – Description of Each Column in CARES Residue Database.**

<b>Column</b>	<b>Description</b>
Data Set ID	A numeric sample number; usually derived from the field trial or other data source. This description is not actually used by CARES in the analysis but may be used to sort and select data to be used in the analysis.
Food Code	This is the FCID code number for each food. Each residue value must be associated with an appropriate FCID food code. Depending on the needs of the assessment, foods can be associated at the "food/crop level (e.g. apples) or can be assigned to food codes that reflect a certain cooking status or food form.
CS	Cooking Status.
FF	Food Form.
CM	Cooking Method.
CAS #	A numeric value representing the compound to be used in the assessment. This value is used throughout CARES to represent the compound.
Replicate	A numeric sample number; usually derived from the field trial or other data source. This description is used by CARES to pool residues for the same food and food form combination to build distributions.
Sample	A numeric sample number; usually derived from the field trial or other data source. This description is used by CARES to match residues from multiple compounds present in a single analytical sample (such as when doing cumulative assessments).
Unit	Sets units for Residue, LOD, and LOQ columns. CARES assumes residue values are in "ppm" for parts-per-million.
Residue	The residue value in parts per million.
Notes	A text description of the source of the residue data; usually the food and perhaps location data. This description is not actually used by CARES in the analysis but may be used to sort and select data to be used in the analysis.
LOD	Limit of Detection. This value is not currently used in the CARES model. Future implementations will use this value when dealing with values at or below the limit of detection.
LOQ	Limit of Quantitation. This value is not currently used in the CARES model. Future implementations will use this value when dealing with values at or below the limit of quantitation.

Future versions of CARES will include a “toolbox” to be able to more effectively work with residue values. Depending on the goal of the exposure analysis, the user may select the option of calculating a mean value from the residue distribution for a given food, using individual values, or using some type of distribution of values. Mean values are used in dietary analyses when doing chronic analyses or for blended commodities such as grains. In some cases it may be best to create mathematical distributions representing possible residue values. For example, a log-normal distribution could be created based on the minimum, maximum, and typical value for a possible residue distribution. Another example of using created data distributions is when imputation techniques are used to provide estimates of residue values that lie below some point such as the limit of detection. At present these residue data distributions must be created outside of the CARES environment using the programs included in the “toolbox.”

### **3.4 Dietary Module Calculations**

After all of the appropriate data have been identified, the CARES dietary module is used to calculate the dietary exposure in two steps. The first step is to match the foods that are consumed by the population of interest with the residues in the residue database. The second step is to use all of the consumption and residue information in estimating the daily exposure for each person in the selected population.

The process of matching foods involves taking foods that are consumed and matching them with specific residue data. In most cases the consumed foods will have an exact match in the residue dataset. In many cases, however, surrogate residue data will be used for crops. For example, consumption values may be available for apples and pears, but residue data may only be available for apples. The user could then select both apples and pears in the consumption database and match them to the apple data in the residue database.

As part of the matching process in the Dietary Module, the user can enter data on the fraction of crop treated, modification factors, and the number of zeros to be included in the dataset. The fraction of crop treated value is used when CARES pulls data from the residue dataset. For example if only 10% of a given crop is treated, then approximately nine of every ten selections of the residue for a given food will be set to zero rather than using a value from the residue dataset. Different percent crop treated values can be used for each food, food form, cooked status, etc. In this manner, if there are data to support this, the percentage of crop treated for fresh tomatoes can be different than that for canned tomatoes. The inclusion of zeros in the dataset is another way of reflecting the fact that not all food items will have residues. Rather than specifying a specific percentage of crop treated, the user can specify a certain number of zeros to be included in the residue dataset. In general the percent crop treated and number of zeros options should not be used together in an assessment.

The user can enter modification factors for each of the types of residues in the database. When residue values represent residues found on “raw agricultural products,” they should be adjusted so that they represent residues on food as it is eaten. While some foods are eaten raw, much of our diet has been washed, peeled, cooked, or processed in some manner. These processing steps can significantly change the residues (increase or decrease) that may be found on a food. The FCID describes each food in terms of the cooked status and method and also the form the food was in when it was consumed. The CARES user can

enter two modification factors to describe the effects of various processing steps on the residues. The factors are simple multipliers for the residue value. For example, if cooking results in a fifty-percent reduction in residues, then the processing factor for cooking would be 0.5. If some type of processing, for example drying of fruit, results in an apparent increase in residues then the value may be greater than one.

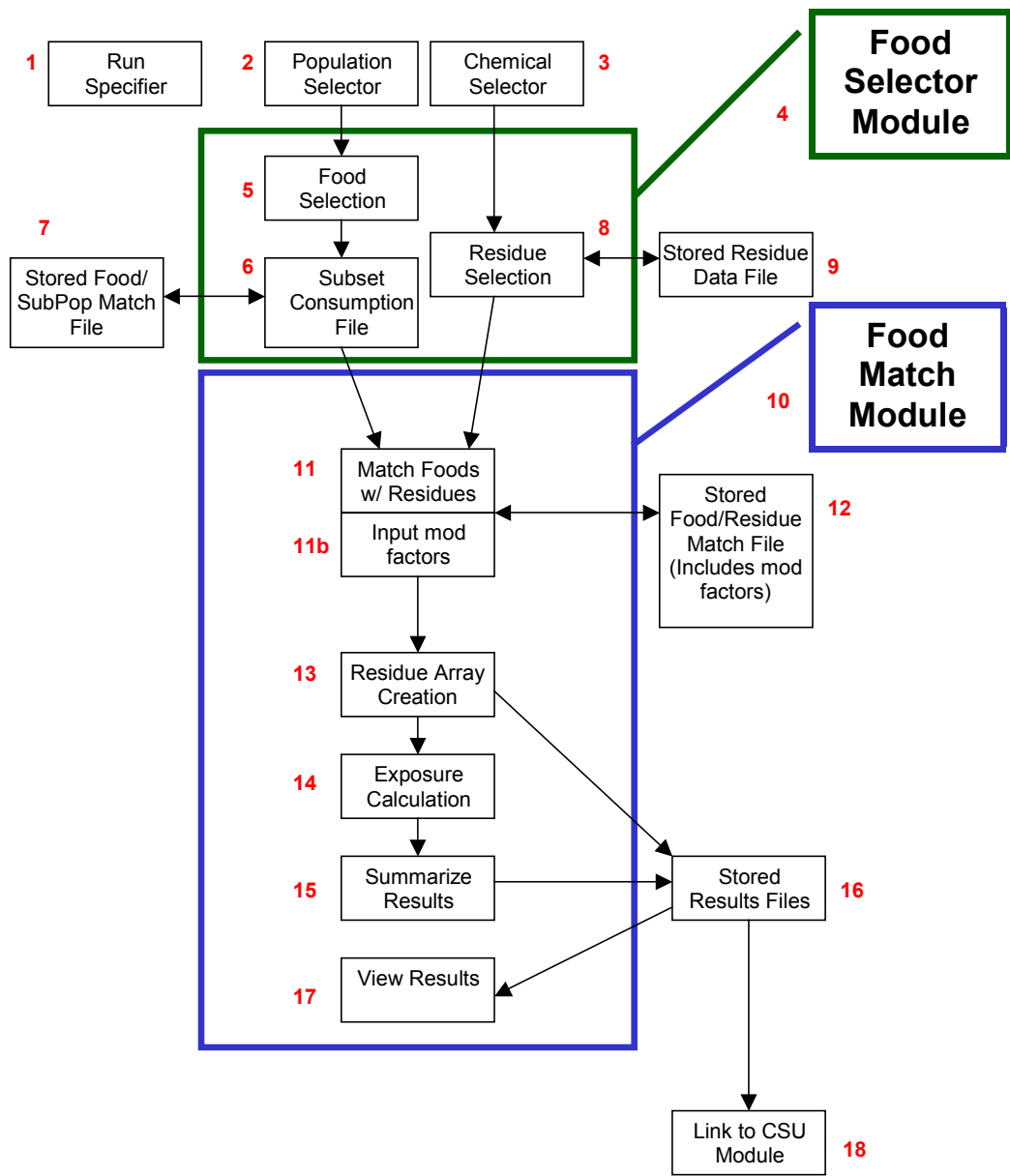
Once the consumption has been matched to the residues and values have been entered to reflect the percentage of crop treated or the effect of processing on the foods, the actual calculation of exposure is carried out according to the following process:

1. The first step is to create a Residue Distribution Array.
  - (a) A residue probability array is built that contains 101 values that represents the percentiles in the residue population ranging from the 0th percentile up to the 100th percentile. The basic algorithm used to build the residue probability array sets the highest value in the array (100th percentile) equal to the maximum residue value, the lowest value in the array (0th percentile) is equal to the minimum value in the dataset, the middle value in the array (50th percentile) is equal to the median residue. In terms of implementation of the algorithm, if the original residue file only contains a single value, then all values in the array are set equal to that value. If the original residue file contains two values, then the low value is placed in the 0th percentile in the array, the high value is placed in the 100th percentile.
  - (b) CARES then determines all percentile values at intervals of 1%. If there is not an actual value at that point, then a straight line interpolation is used to determine the value that represents that percentile.
  - (c) The array for the residue distribution is now stored for use (values for each of the percentiles can be viewed at the end of the run as one of the results tables). (e) These steps are repeated for all of the residue distributions.
2. CARES takes the first person in the selected population, opens the food match file for that person and creates an array of all the foods that are eaten over the 365 day period.
3. CARES begins with the first food that is consumed by the person. Based on the percent crop treated value, CARES determines if the food has residues or not (untreated foods do not contain residues). If not, then CARES moves to step 5. If the food is determined to contain residues, then a residue value for that food is randomly selected from the residue percentile array created in step 1 above.
4. The food consumption (g/kg bw/d) is multiplied by the residue value (ppm) and the units conversion factor (1/1000) to provide the exposure for that food in mg/kg bw/d. This value is then stored along with the day on which the exposure occurred.
5. CARES then proceeds to the next food that is consumed.



6. When all of the consumed foods for the first person in the population have been multiplied by the appropriate residue values, the food exposure array is then stored for future use.
7. The exposures from all foods for each day are then summed to provide a daily total exposure. This value is then stored in an array.
8. Three summary variables are then calculated: the maximum daily value, the "aggregate" or total exposure value for the 365-day period, and the average daily exposure (aggregate or total exposure divided by 365 days).

Data can be retrieved and viewed as part of the dietary module or retrieved and used by the CSU module. In addition, any of the data files can be exported for use in other programs such as spreadsheets or word processing programs.



**Figure 3.1 – Data Flow Among Dietary Module Components**

See next page for explanation of numbered components.

### Key to the Flow Chart for the CARES Dietary Modules

Item	Description
1	The Run Specifier module is used prior to running the dietary modules to provide identification information for files created during the assessment.
2	The Population Selector module is used prior to running the dietary modules to select the subpopulations that will be used in the assessment.
3	The Chemical Selector module is used prior to running the dietary modules to select the chemicals that will be included in the assessment.
4	The Food Selector module allows the user to specify the foods and residues that will be included in the assessment.
5	The first step in using the food selector module is to select the foods that will be considered in the assessment by opening the complete list of foods.
6	The user creates a subset of the complete list that includes only those foods that will be considered as part of the upcoming assessment.
7	This food subset file is then stored and the name added to the list of available datasets. This data file is then available for use in future assessments. The user then selects the dataset that they wish to use in the assessment.
8	The second step in running the Food Selector module is to select the residues that will be used in the assessment. This is done by selecting a pre-existing residue file, editing a pre-existing residue file, or importing data to create a new residue file.
9	The residue data can be stored for future use. The user then selects the residue dataset that they wish to use in the assessment. Once the user has reached this point, they are ready to run the dietary module. If the user only wishes to conduct a dietary analysis, then they click on the "run canvas" (rocket) button. (If the user only wishes to run an aggregate assessment that includes residential or drinking water analysis, then at this point they would enter data for those other modules before running the assessment modules.)
10	The Food Match Module contains the algorithms to match the appropriate consumption and residue values and also the exposure calculation routines.
11a	The first step in running the Food Match module is to match the consumed foods with the residues for those foods.
11b	The second step in running the Food Match module is to add any residue modification factors (% crop treated, processing factors, etc.) to the dataset.
12	This creates a file containing all of the matched foods, residues, and modification factors that can then be stored for future use.
13	Based on the residue data and modification factors, CARES creates residue distributions for each food. This file is then stored for future use.
14	The exposure for each person in the subpopulation is calculated by multiplying their consumption of each food on each day by the appropriate residue value.
15	The results are summarized to provide a daily total exposure. Three summary variables are also calculated: the maximum daily value for the year, the "aggregate" or total exposure value for the 365 day period, and the average daily exposure (aggregate or total exposure divided by 365 days).
16	The exposure values for each food on each day for each person in the subpopulation are stored along with the daily total exposure and summary variables.
17	The stored results of the dietary module can be viewed and exported by the user.
18	These results are also available for use by the CSU module.



# 4. Residential Module

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# Chapter 4 – Residential Module

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## 4.1 Introduction

This chapter provides the methodological framework for the CARES (Cumulative and Aggregate Risk Evaluation System) Residential (Non-dietary) Module. This chapter includes the following:

- Documentation of the residential exposure scenarios
- Description of calendar-based residential exposure modeling
- Residential scenario specific algorithms

Additional information regarding technical considerations in the use of the residential exposure module is provided in the  $\alpha$ -CARES Residential (Non-dietary) Module White Paper (2001).

## 4.2 Residential Exposure Scenarios

The following scenarios are currently represented in the CARES residential model:

1. Lawn Care
2. Vegetable Garden Care
3. Ornamental Plant Care
4. Tree Care
5. Pick Own Fruits/Vegetables
6. Crack & Crevice Treatment
7. Termite Control
8. Rodent Control
9. Pet Care
10. Outdoor Fogger Use
11. Indoor Fogger Use
12. Indoor Treatment
13. Paint/Wood Treatment
14. Impregnated Materials
15. Detergent/Handsoap Use
16. Swimming Pool Use
17. Golfer
18. Public Health
19. Custom (future)

The following sections provide a description of how each scenario is implemented in CARES.

### 4.2.1 Lawn Care

Potential non-occupational dermal and inhalation exposures that individuals may receive from pesticide use on turf are evaluated with this scenario. This scenario assumes that pesticides are available to be inhaled or have the potential to come

in contact with the skin of adults during the handling (i.e. mixing, loading and application) of lawn chemicals. This scenario also assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults and children during post-application activities on treated turf. The method to determine handler inhalation and dermal exposure to pesticides from turf applications relies on algorithms specified by EPA using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). The method to determine post-application inhalation and dermal exposure to pesticides from treated turf relies on exposure data from user-specified sources (U.S. EPA, 1997a; U.S. EPA 2001).

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.1 – Lawn Care Scenario Requirements**

Characteristic	Description
Mixing, Loading, Application Methods	The user must determine: 1) methods used to mix and load the product (i.e. closed or open systems), 2) methods used to apply granular formulation pesticides, such as drop-type spreaders, rotary spreaders, belly grinders, shaker cans, and dispersed by hand (spot treatment), 3) methods used to apply liquid formulations, such as hose-end sprayers, typical garden sprinkler/watering can (spot treatment), low-pressure handwands (spot treatment), and backpacks (spot treatment).
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment (full or spot treatments) and size of the treated area(s). The lawn size is estimated based on residence characteristics from the vector of individual characteristics (Sielken and Holden, 2001). Exposure estimates are based on the application rate and area treated, or the amount of formulation (as defined in the residential assessment algorithms in Appendix D).
Area Treated	The area treated is determined from the vector of individual characteristics. The U.S. EPA assumption for area treated for a deterministic assessment of this scenario is 0.5 acres.
Turf Transferable Residue (TTR)	Turf transferable residue (TTR) data are described using a degradation curve derived from empirical data or from default assumptions. Transferable residues derived from empirical TTR data are evaluated using regression analysis of the log-transformed residue data (completed by the user outside of CARES). The results are reported as a TTR algorithm, a half-life of the compound on foliage or as an estimated residue value at a specified time after application. Alternatively, EPA default assumptions may be used to estimate transferable residues over time by assuming that 5 percent of the application rate is available on the turf as transferable residue, and that the residue degrades 10% per day (U.S. EPA, 2001). The label-specified application rate and type of formulation are important predictors of turf residues that must also be considered.
Transfer Coefficient	The dermal transfer coefficient is provided by the user. The U.S. EPA assumption for dermal transfer coefficient for a deterministic assessment of this scenario is 14,500 cm <sup>2</sup> /hr (adults) and 5,200 cm <sup>2</sup> /hr (children) for short-term exposures, and 7,300 cm <sup>2</sup> /hr (adults) and



Characteristic	Description
	2,600 cm <sup>2</sup> /hr (children) for intermediate-term exposures (U.S. EPA, 2001). The dermal transfer coefficients were estimated using Jazzercise studies of adults in contact with treated surfaces for 20 minutes, resulting in a normalized hourly dermal transfer coefficient of 43,000 cm <sup>2</sup> /hr. The 20-minute Jazzercise activity represents a 1-hour activity for short-term exposure or a 2-hour activity for intermediate-term exposure.
Event Allocation	The probability that an individual is eligible for pesticide use is determined by residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used by an individual is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Exposure Algorithm – Mixer, Loader, Applicator	Algorithms used to estimate handler dermal and inhalation exposures are defined in Appendix D. The U.S. EPA assumption for mixer, loader, applicator dermal and inhalation exposures for a deterministic assessment of this scenario relies on the Pesticide Handlers Exposure Database (PHED) to describe route-specific unit exposures using measures of central tendency from the PHED database (milligrams exposure per pound active ingredient mixed, loaded or applied). The user may also specify a distribution of empirical exposure rate values (empirical or parametric).
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D.
Duration	Duration is based on the 75 <sup>th</sup> percentile value (i.e., 120 minutes) for playing on grass for ages 1-4 years and ages 5-11 years (Tsang and Klepeis 1996 as cited on pg. 15-79 of U.S. EPA 1997b, Exposure Factors Handbook, EFH). The data were truncated at the 75 <sup>th</sup> percentile. 23% of children ages 1-4 years played on grass more than 2 hours/day (p. 15-78). In comparison, the 95 <sup>th</sup> percentile for playing outdoors is 3.5 hours, the 95 <sup>th</sup> percentile for time spent on school grounds/playgrounds is 2.9 hours, while the 95 <sup>th</sup> percentile for time spent at home in the yard or other areas outside the home is 5.75 hours for children 1-4 years (p. 15-96, 15-124 and 15-136 of U.S. EPA, 1997b).
Market Share	Market share for each active ingredient (AI) is specified in the

Characteristic	Description
	residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion treating a lawn), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.2 Vegetable Garden Care

This procedure provides a method for estimating potential non-occupational dermal and inhalation exposures that individuals may receive from pesticide use on gardens. Garden applications include insect and weed treatments around walkways, driveways, foundations, vegetables, and ornamentals. Garden applications are also made to control plant diseases. This scenario assumes that pesticides are available for inhalation or have the potential to come in contact with the skin of adults during the mixing/loading and application of pesticides used around the garden. This scenario also assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults and children during post-application activities around the garden. The method to determine handler inhalation and dermal exposure to pesticides from turf applications relies on algorithms specified by EPA using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). The method to determine post-application inhalation and dermal exposure to pesticides from treated turf relies on using exposure data from user-specified sources (U.S. EPA, 1997a; U.S. EPA 2001).

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.2 – Vegetable Garden Care Scenario Requirements**

Characteristic	Description
Application Methods	The user must determine: 1) application methods for granular formulation pesticides include drop-type spreaders, rotary spreaders, belly grinders, shaker cans, and dispersed by hand (spot treatment), 2) application methods for liquid formulations include hose-end sprayers, typical garden sprinkler/watering can (spot treatment), low-pressure handwands (spot treatment), and backpacks (spot treatment), 3) application methods for ready-to-use products include trigger pump applications.
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment (full or spot treatments), and

Characteristic	Description
	size of the garden. The garden size is estimated based on residence characteristics from the vector of individual characteristics (Sielken and Holden, 2001).
Area Treated	The area treated is determined from the vector of individual characteristics. The U.S. EPA assumption for the amount handled is based on 10,000 ft <sup>2</sup> or 1/4 acre (i.e. large garden in a farm-type setting) for treatments based on area, and 5 gallons of spray diluent (i.e., two 2.5 gallon handwand treatments) for treatments based on concentrations.
Event Allocation	The probability that an individual is eligible for pesticide use is determined by residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used by an individual is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Mixer, Loader, Applicator Exposure Algorithms	Algorithms used to estimate handler dermal and inhalation exposures are defined in Appendix D.
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D.
Transfer Coefficient	The dermal transfer coefficient must be provided by the user. The U.S. EPA assumption for dermal transfer coefficient is 10,000 cm <sup>2</sup> /hr for adults and 5,000 cm <sup>2</sup> /hr for youth (age 10-12 years) (e.g., tomato harvesting). Transfer coefficients describing a variety of post-application activities can be found in the Science Advisory Council for Exposure policy number 003.1 agricultural transfer coefficient (revised August 7, 2000).
Duration	The U.S. EPA assumption for the duration of exposure used in a deterministic assessment is assumed to be 0.25 hours per day for youths (age 10-12 years) and 0.67 hours per day for adults (age 18-64 years), based on the 95 <sup>th</sup> percentile values for time spent working in a garden or other circumstances working with soil (U.S. EPA, 1997b). The U.S. EPA assumption of the timing of re-entry (days post-application) used in a deterministic assessment is based on re-entry the day of application.

Characteristic	Description
Dislodgeable Foliar Residues (DFR)	Dislodgeable Foliar Residue (DFR) data are described using a degradation curve derived from empirical data or from default assumptions. Residues derived from empirical data are evaluated using regression analysis of the residue data (completed by the user outside of CARES). The results are reported as a DFR algorithm, a half-life of the compound on foliage or as an estimated residue value at a specified time after application. Alternatively, DFR data may be based on default assumptions: 1) estimated dislodgeable residue on the day of application based on 20 percent of the application rate, with DFR on subsequent days estimated based on a daily dissipation rate of 10%, or 2) measured dislodgeable residue on the day of application, with DFR on subsequent days estimated based on a daily dissipation rate of 10% (U.S. EPA 1997a). The label-specified application rate and type of formulation are important predictors of DFR that must also be considered.
Market share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion treating vegetable gardens), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

### 4.2.3 Ornamental Plant Care

This procedure provides a method for estimating potential non-occupational dermal and inhalation exposures that individuals may receive from pesticide use on ornamental plants such as flowers, shrubs (e.g., rose bushes) and trees. Ornamental plant care application includes treatments to control insects, weeds, and plant diseases. This scenario assumes that pesticides are available for inhalation or have the potential to come in contact with the skin of adults during the mixing/loading and application of pesticides used during ornamental plant care activities around the residence. This scenario also assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults and children during post-application activities around treated ornamental plants. The method to determine handler inhalation and dermal exposure to pesticides from applications relies on algorithms specified by EPA using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). The method to determine post-application inhalation and dermal exposure

to pesticides from treated ornamental plants relies on using exposure data from user-specified sources (U.S. EPA, 1997a; U.S. EPA 2001).

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.3 – Ornamental Plant Care Scenario Requirements**

Characteristic	Description
Application Methods	The user must determine: 1) application methods for granular formulation pesticides including drop-type spreaders, rotary spreaders, belly grinders, shaker cans, and dispersed by hand (spot treatment), 2) application methods for liquid formulations including hose-end sprayers, typical garden sprinkler/watering can (spot treatment), low-pressure handwands (spot treatment), and backpacks (spot treatment), 3) application methods for ready-to-use products including trigger pump applications.
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment (full or spot treatments), and the number and size of plants treated. The number and size of ornamental plants is estimated based on residence characteristics from the vector of individual characteristics (Sielken and Holden, 2001).
Event Allocation	The probability that an individual is eligible for pesticide use is determined by residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used by an individual is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Exposure Algorithm – Mixer, Loader, Applicator	Algorithms used to estimate handler dermal and inhalation exposures are defined in Appendix D.
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal and inhalation exposures are defined in Appendix D.
Dislodgeable Foliar	Dislodgeable Foliar Residue (DFR) data are described using a degradation curve derived from empirical data or from default

Characteristic	Description
Residues (DFR)	assumptions. Residues derived from empirical data are evaluated using regression analysis of the residue data (completed by the user outside of CARES). The results are reported as a DFR algorithm, a half-life of the compound on foliage or as an estimated residue value at a specified time after application. Alternatively, DFR data may be based on default assumptions: 1) estimated dislodgeable residue on the day of application based on 20 percent of the application rate, with DFR on subsequent days estimated based on a daily dissipation rate of 10%, or 2) measured dislodgeable residue on the day of application, with DFR on subsequent days estimated based on a daily dissipation rate of 10% (U.S. EPA 1997a). The label-specified application rate and type of formulation are important predictors of DFR that must also be considered.
Transfer Coefficient	The dermal transfer coefficient must be provided by the user. The U.S. EPA assumption for dermal transfer coefficient for harvesting fruit from fruit trees is 10,000 cm <sup>2</sup> /hr for adults and 5,000 cm <sup>2</sup> /hr for youth (age 10-12 years). Transfer coefficients describing a variety of post-application activities can be found in the Science Advisory Council for Exposure policy number 003.1 agricultural transfer coefficient (revised August 7, 2000).
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion treating ornamental plants), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.4 Tree Care

This procedure provides a method for estimating potential non-occupational dermal and inhalation exposures that individuals may receive from pesticide use on trees (e.g., fruit and nut trees). Tree care application includes treatments around trees to control insects, weeds, and plant diseases. This scenario assumes that pesticides are available for inhalation or have the potential to come in contact with the skin of adults during the mixing/loading and application of pesticides used during ornamental plant care activities around the residence. This scenario also assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults and children during post-application activities around treated trees. The method to determine handler inhalation and dermal exposure to pesticides from applications relies on algorithms specified by EPA using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). The method to determine post-application

inhalation and dermal exposure to pesticides from treated trees relies on using exposure data from user-specified sources (U.S. EPA, 1997a; U.S. EPA 2001).

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.4 – Tree Care Scenario Requirements**

Characteristic	Description
Application Methods	Application methods include: 1) drop-type spreaders, broadcast spreaders, shaker cans, and dispersed by hand (spot treatment) for granular formulation pesticides, 2) hose-end sprayers, typical garden sprinkler/watering can (spot treatment), low-pressure handwands (spot treatment), and backpacks (spot treatment) for liquid formulations, 3) trigger pump applications for ready-to-use products.
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment (full or spot treatments), and the number and size of trees treated. The number and size of plants is estimated based on residence characteristics from the vector of individual characteristics (Sielken and Holden, 2001).
Event Allocation	The probability that an individual is eligible for pesticide use is determined by residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used by an individual is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups (U.S. EPA, 1997b).
Exposure Algorithm – Mixer, Loader, Applicator	Algorithms used to estimate handler dermal and inhalation exposures are defined in Appendix D.
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal and inhalation exposures are defined in Appendix D.
Dislodgeable Foliar Residues (DFR)	Dislodgeable Foliar Residue (DFR) data are described using a degradation curve derived from empirical data or from default assumptions. Residues derived from empirical data are evaluated using regression analysis of the residue data (completed by the user

Characteristic	Description
	<p>outside of CARES). The results are reported as a DFR algorithm, a half-life of the compound on foliage or as an estimated residue value at a specified time after application. Alternatively, DFR data may be based on default assumptions: 1) estimated dislodgeable residue on the day of application based on 20 percent of the application rate, with DFR on subsequent days estimated based on a daily dissipation rate of 10%, or 2) measured dislodgeable residue on the day of application, with DFR on subsequent days estimated based on a daily dissipation rate of 10% (U.S. EPA 1997a). The label-specified application rate and type of formulation are important predictors of DFR that must also be considered.</p>
Transfer Coefficient	<p>The dermal transfer coefficient must be provided by the user. The U.S. EPA assumption for dermal transfer coefficient is 10,000 cm<sup>2</sup>/hr for adults and 5,000 cm<sup>2</sup>/hr for youth (age 10-12 years) (e.g., tomato harvesting) (U.S. EPA, 1997a). Transfer coefficients describing a variety of post-application activities can be found in the Science Advisory Council for Exposure policy number 003.1 agricultural transfer coefficient (revised August 7, 2000).</p>
Market Share	<p>Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion treating trees), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.</p>



## 4.2.5 Pick Own Fruits/Vegetables

This procedure provides a method for estimating potential non-occupational dermal and inhalation exposures that individuals may receive from handling fruits and vegetables that have previously been treated with pesticides. This scenario assumes that pesticide residues are transferred to the skin of adults/youth who enter treated fields/orchards during "pick your own" fruit and vegetable harvesting. For the purposes of this procedure, "pick your own" facilities are considered commercial farming operations that allow public access for harvesting fruits and vegetables in large-scale fields treated with commercially labeled pesticides. The method for estimating post-application dermal exposure from pesticides on fruits and vegetables is based on exposure data from user-specified sources.

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.5 – Pick Own Fruits/Vegetables Scenario Requirements**

Characteristic	Description
Dislodgeable Foliar Residues (DFR)	Dislodgeable Foliar Residue (DFR) data are described using a degradation curve derived from empirical data or from default assumptions. Residues derived from empirical data are evaluated using regression analysis of the residue data (completed by the user outside of CARES). The results are reported as a DFR algorithm, a half-life of the compound on foliage or as an estimated residue value at a specified time after application. Alternatively, DFR data may be based on default assumptions: 1) estimated dislodgeable residue on the day of application based on 20 percent of the application rate, with DFR on subsequent days estimated based on a daily dissipation rate of 10%, or 2) measured dislodgeable residue on the day of application, with DFR on subsequent days estimated based on a daily dissipation rate of 10% (U.S. EPA 1997a). The label-specified application rate and type of formulation are important predictors of DFR that must also be considered.
Duration	The duration of exposure must be specified. EPA assumes that the duration of exposure is 2.0 hours per day for youth (age 10-12 years) and 4.0 hours per day for adults (age 18-64 years), based on the 50th percentile values for time spent outdoors at a farm (U.S. EPA, 1997b, U.S. EPA, 1997b).
Transfer Coefficient	The user must specify activity-specific transfer coefficients based on empirical data. Transfer coefficients describing a variety of post-application activities can be found in the Science Advisory Council for Exposure policy number 003.1 agricultural transfer coefficient (revised August 7, 2000). Alternatively, EPA assumes a dermal transfer coefficient of 10,000 cm <sup>2</sup> /hr for adults and 5,000 cm <sup>2</sup> /hr for youth (age 10-12 years) (U.S. EPA, 1997a).
Event Allocation	The probability that an individual participates in this activity is determined from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used by an individual

Characteristic	Description
	is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D. Post-application exposure may be assessed on the same day the pesticide is applied and/or on subsequent days after application. EPA assumes that individuals could enter a "pick your own" site immediately after application.
Active Ingredient	Pesticide products not labeled for the residential/home garden market may also be considered for this scenario. All exposures occur post-application. Therefore, the amount of formulation handled, the treatment method, size of the area treated, application rate and type of formulation are not pertinent to this scenario <i>except</i> as predictors of DFR.
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion picking their own fruits/vegetables), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.6 Crack & Crevice Treatment

This procedure provides a method for estimating potential exposures that homeowners may receive from inhalation and dermal contact during pesticide

crack and crevice and broadcast treatments indoors. This scenario also provides a method for estimating oral exposures in children contacting treated surfaces, assuming that pesticide residues are transferred to the skin of children during post-application contact with treated indoor areas and are subsequently ingested as a result of hand-to-mouth transfer.

This scenario assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults during the mixing/loading and application of pesticides used indoors. The method to determine handler inhalation and dermal exposure to pesticides from crack and crevice and broadcast treatments relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). This procedure also provides a method for estimating exposures among adults and children from dermal contact with indoor surfaces that have previously been treated with pesticides. This scenario assumes that pesticide residues are transferred to the skin of adults and children who come in contact with treated surfaces for recreation, housework, or other residential activities. The method to determine dermal exposure to pesticides from treated indoor surfaces relies on using exposure data from user-specified sources. This procedure allows the user to evaluate handler and post-application exposures.

Label information is important for specifying appropriate data inputs for the exposure assessment. The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.6 – Crack and Crevice Treatment Scenario Requirements**

Characteristic	Description
Mixing, Loading, Application Methods	The user must determine: 1) methods to apply solid formulation pesticides include using dusters, bait guns, syringe applicators and other equipment by broadcast, band, edge, spot, crack and crevice treatment, 2) methods to apply liquid formulation pesticides include using low-pressure handwand sprayers, backpack sprayers, ready-to-use products including trigger pump applicators, aerosol sprayers and foggers and other equipment by broadcast, band, edge, spot, and crack and crevice treatment.
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment (full or spot treatments) and size of the treated area(s). The treated area is estimated based on residence characteristics from the vector of individual characteristics (Sielken and Holden, 2001). Exposure estimates are based on the application rate and area treated, or the amount of formulation (as defined in the residential assessment algorithms in Appendix D).
Area Treated	The user must specify the size of the treated area. The U.S. EPA assumptions for a deterministic assessment for crack and crevice treatment are based on the amount handled to treat baseboards or carpets used by two aerosol cans and/or 2 gallons of diluted spray for low-pressure handwands (U.S. EPA, 1997a).
Atmospheric Concentration	Atmospheric concentrations are described using empirical data or default assumptions based on computer modeling. The Screening-Level Consumer Inhalation Exposure Software (SCIES) and/or the

Characteristic	Description
	<p>Multi-Chamber Concentration and Exposure Model (MCCEM) are used to calculate concentration values to which individuals will be exposed (U.S. EPA, 1997a).</p> <p>Five percent of termiticides applied by foundation/soil injection techniques penetrate the foundation of a house to become a source for off-gassing in a Chinn-type emission. One hundred percent of all pesticides applied indoors are assumed to be available for emission (U.S. EPA, 1997a).</p>
Inhalation Coefficients	<p>The hourly inhalation rate used by EPA for a deterministic assessment of post-application inhalation exposures is 0.4 m<sup>3</sup>/hour for adults at rest, 0.5 m<sup>3</sup>/ hour for adults engaged in sedentary activity, 1 m<sup>3</sup>/ hour for adults engaged in light activity, and 1.6 m<sup>3</sup>/ hour for adults engaged in moderate activity (U.S. EPA, 1997b), and are intended for assessing short-term scenarios of a few hours in duration (e.g. post-application activities).</p> <p>The daily inhalation rate used by EPA for a deterministic assessment of post-application inhalation exposures is 11.3 m<sup>3</sup>/day for adult females, 15.2 m<sup>3</sup>/day for adult males, 13.3 m<sup>3</sup>/day for average of adult males and females, 8.7 m<sup>3</sup>/day for children 1-12 years old, and 4.5 m<sup>3</sup>/day for children less than 1 year old (U.S. EPA, 1997a).</p>
Transferable Residue	<p>Transferable residue data are described using a degradation curve derived from empirical data or from default assumptions. Transferable residues derived from empirical data are evaluated using regression analysis of the log-transformed residue data (completed by the user outside of CARES). The results are reported as a regression equation, a half-life of the compound on foliage or as an estimated residue value at a specified time after application. Alternatively, EPA default assumptions may be used to estimate transferable residues over time by assuming that an average of 5 percent of the application rate are available on the carpet and 10% of the application rate on hard surfaces are available as dislodgeable residue (from broadcast or crack and crevice treatments) (U.S. EPA, 2001). Post-application transferable residues after the day of application may be based on: 1) measured degradation rate based on chemical-specific data, or 2) measured residue on the day of application and a daily degradation of 10 % per day. The label-specified application rate and type of formulation are important predictors of residues that must also be considered.</p>
Transfer Coefficient	<p>The dermal transfer coefficient must be provided by the user. The U.S. EPA assumption for dermal transfer coefficient for a deterministic assessment of this scenario is 16,700 cm<sup>2</sup>/hr (adults) and 6,000 cm<sup>2</sup>/hr (children) for short- and intermediate- term exposures (U.S. EPA, 2001). The dermal transfer coefficients were estimated using Jazzercise studies of adults in contact with treated surfaces for 20 minutes, resulting in a normalized hourly dermal transfer coefficient of 200,000 cm<sup>2</sup>/hr. The 20-minute Jazzercise activity represents a 4-hour activity for short- and intermediate-term exposure.</p>
Event Allocation	<p>The probability that an individual is eligible for pesticide use is determined by residence information from the vector of individual</p>

Characteristic	Description
	characteristics (Sielken and Holden, 2001). The probability of pesticide use is specified in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups (U.S. EPA, 1997b).
Exposure Algorithm – Mixer, Loader, Applicator	Algorithms used to estimate handler dermal and inhalation exposures are defined in Appendix D. The U.S. EPA assumption for mixer, loader, applicator dermal and inhalation exposures for a deterministic assessment of this scenario relies on the Pesticide Handlers Exposure Database (PHED) to describe route-specific unit exposures using measures of central tendency from the PHED database (milligrams exposure per pound active ingredient mixed, loaded or applied) (U.S. EPA, 1998). The user may also specify a distribution of empirical exposure rate values (empirical or parametric).
Exposure Algorithm – Post-Application	<p>Algorithms used to estimate post-application dermal exposures are defined in Appendix D.</p> <p>The assumed mean surface area used by EPA for a deterministic assessment of hand-to-mouth transfer is 20 cm<sup>2</sup> based on the insertion of 3 fingers by a child (age ≤ 4 years) (U.S. EPA Science Advisory Council for Exposure, 2001). Replenishment of the hands with pesticide residues is assumed to be an implicit factor in this assessment. It is assumed that there is a one-to-one relationship between the dislodgeable residues on the indoor surface and the surface area of the skin after contact (i.e., if the dislodgeable residue on the indoor surface is 1 mg/cm<sup>2</sup>, then the residue on the human skin is also 1 mg/cm<sup>2</sup> after contacting the surface).</p> <p>The removal efficiency of residues from the hands used by EPA for a deterministic assessment of hand-to-mouth transfer is assumed to be 50%, based on removal of pesticides chlorpyrifos, piperonyl butoxide, pyrethrin from the hands of volunteers using surgical sponges wetted with human saliva (U.S. EPA Sci. Adv. Council for Exposure, 2001).</p>
Duration	The user must specify the duration of exposure. The duration of exposure to indoor surfaces used by EPA for a deterministic assessment of post-application dermal exposure during indoor crack and crevice and broadcast treatment is 8 hours for carpets and textile surfaces and 4 hours on hard surfaces (U.S. EPA 1997a).

Characteristic	Description
	<p>The duration of exposure to indoor surfaces used by EPA for a deterministic assessment of hand-to-mouth transfer is assumed to be 2 hours/day. This value represents the mean of the 75<sup>th</sup> percentile values for time playing on grass for ages 1-4 years and ages 5-11 years (U.S. EPA Science Advisory Council for Exposure, 2001). The mean rate of hand-to-mouth activity used by EPA for a deterministic assessment of hand-to-mouth transfer is 20 times per hour for short-term exposure scenarios and 9.5 times per hour for intermediate term exposure scenarios in children (age ≤ 4 years) (U.S. EPA Science Advisory Council for Exposure, 2001).</p>
Market Share	<p>Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion households with crack and crevice treatment), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.</p>

#### 4.2.7 Termite Control

This procedure provides a method for estimating potential non-occupational inhalation exposures in adults and children.

This scenario assumes that pesticides are available to be inhaled during post-application of pesticides used for termite control. The method to determine handler inhalation and dermal exposure to pesticides relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). This procedure also provides a method for estimating dose among adults and children from inhalation and from dermal contact with indoor surfaces that have previously been treated with pesticides. This scenario assumes that pesticide residues are transferred to the skin of adults and children who come in contact with treated surfaces for recreation, housework, or other residential activities. The method to determine dermal exposure to pesticides from treated indoor surfaces relies on using exposure data from user-specified sources. This procedure allows the user to evaluate handler and post-application exposures.

Label information is important for specifying appropriate data inputs for the exposure assessment. The following information must be determined to estimate daily inhalation and dermal mixer/loader/applicator doses.

**Table 4.7 – Termite Control Scenario Requirements**

Characteristic	Description
Mixing, Loading, Application Methods	Methods to apply solid formulation pesticides include using bait stations, syringe applicators and other equipment by broadcast, band, edge, spot, crack and crevice treatment. Methods to apply liquid formulation pesticides include using low-pressure handwand sprayers, backpack sprayers, ready-to-use products including trigger pump applicators, and other equipment by broadcast, band, edge, spot, and crack and crevice treatment.
Active Ingredient	The amount of active ingredient handled is based on the label-specified application rate, the type of treatment (full or spot treatments), and the size of the treated area(s).
Area Treated	The area treated is estimated based on residence characteristics from the vector of individual characteristics (Sielken and Holden, 2001).
Atmospheric Concentration	<p>Atmospheric concentrations are described using empirical data or default assumptions based on computer modeling. An EPA deterministic assessment of post-application inhalation exposures from termite treatment assumes that the Screening-Level Consumer Inhalation Exposure Software (SCIES) and/or the Multi-Chamber Concentration and Exposure Model (MCCEM) are used to calculate indoor atmospheric concentration values (EPA, 1997a).</p> <p>Five percent of termiticides applied by foundation/soil injection techniques penetrate the foundation of a house to become a source for off-gassing in a Chinn-type emission. One hundred percent of all pesticides applied indoors are assumed to be available for emission (U.S. EPA, 1997a).</p>
Inhalation Coefficients	<p>The hourly inhalation rate used by EPA for a deterministic assessment of post-application inhalation exposures is 0.4 m<sup>3</sup>/hour for adults at rest, 0.5 m<sup>3</sup>/ hour for adults engaged in sedentary activity, 1 m<sup>3</sup>/ hour for adults engaged in light activity, and 1.6 m<sup>3</sup>/ hour for adults engaged in moderate activity (U.S. EPA, 1997b), and are intended for assessing short-term scenarios of a few hours in duration (e.g. post-application activities).</p> <p>The daily inhalation rate used by EPA for a deterministic assessment of post-application inhalation exposures is 11.3 m<sup>3</sup>/day for adult females, 15.2 m<sup>3</sup>/day for adult males, 13.3 m<sup>3</sup>/day for average of adult males and females, 8.7 m<sup>3</sup>/day for children 1-12 years old, and 4.5 m<sup>3</sup>/day for children less than 1 year old (U.S. EPA, 1997a).</p>
Event Allocation	The probability that an individual is eligible for pesticide use is determined by residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used by an individual is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a

Characteristic	Description
	reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal and inhalation exposures are defined in Appendix D.
Duration	The user must specify the duration of exposure.
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion households with termite treatment), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.8 Rodent Control

Potential non-occupational post-application oral exposures that individuals may receive from pesticide use for rodent control are evaluated with this scenario. This scenario assumes that pesticides used for rodent control have the potential to be ingested by children during post-application activities involving contact with solid pesticide formulations (granules, pellets or dry materials).

The following information must be determined to build the CARES canvas and estimate daily post-application exposures from incidental ingestion:

**Table 4.8 – Rodent Control Scenario Requirements**

Characteristic	Description
Active Ingredient	The amount of formulation handled is based on the percentage of active ingredient in the product, and the type, number and size of



Characteristic	Description
	products encountered. The user must determine the type, number, and size of products encountered.
Area Treated	An EPA deterministic assessment of incidental ingestion of rodenticides by children (age 1-6 years) assumes that the amount of material ingested is 0.3 grams per day (U.S.EPA, 1997a).
Event Allocation	The probability that an individual is eligible for pesticide exposure is determined by product use and residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used in the residence is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. The user must determine if the frequency of occurrence should rely on the default assumption of daily occurrence, or on product use information supplied by the user.
Body Weight	Body weights of children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment for toddlers (3 years old as representative of the 1 to 6 year old age group) is 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997a).
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D.
Duration	The user must specify the duration of exposure. An EPA deterministic assessment of incidental ingestion exposures of rodenticides by children assumes that a single ingestion event occurs each day.
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion treating a residence for rodents), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.9 Pet Care

This procedure provides a method for estimating potential exposures that homeowners may receive from inhalation and dermal contact during treatment of pets. This scenario also provides a method for estimating post-application dermal and oral exposures in children contacting treated pets, assuming that pesticide residues are transferred to the skin of children during post-application contact

with treated pets and are subsequently ingested as a result of hand-to-mouth transfer.

This scenario assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults during the mixing/loading and application of pesticides to treat pets. The method to determine handler inhalation and dermal exposure to pesticides from pet treatments relies on algorithms specified by EPA (U.S. EPA, 1997a) using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). This procedure also provides a method for estimating exposure among adults from dermal contact with pets that have previously been treated with pesticides. This procedure also provides a method for estimating exposure among children from dermal contact with pets that have previously been treated with pesticides, and from ingestion resulting from hand-to-mouth transfer of pesticides from exposed skin surfaces in contact with treated pets. This scenario assumes that pesticide residues are transferred to the skin of adults and children who come in contact with treated pets. The method to determine dermal exposure to pesticides from treated pets relies on using exposure data from user-specified sources. This procedure allows the user to evaluate application and post-application exposures.

Label information is important for specifying appropriate data inputs for the exposure assessment. The following information must be determined to build the CARES canvas and estimate application and post-application exposures:

**Table 4.9 – Pet Care Scenario Requirements**

Characteristic	Description
Mixing, Loading, Application Methods	The user must determine the 1) type of formulation (e.g. liquid, solid/dust, impregnated material), 2) method used to apply liquid formulation pesticides such as shampoos, dips and ready to use treatments including trigger pump applicators, and aerosol sprayers, 3) method used to apply dry formulation pesticides such as dusts, 4) method used to handle/apply impregnated formulation of pesticides such as flea collars.
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment (full or spot treatments) and the size and number of pet(s) treated.
Area Treated	The user must specify the treatment area (i.e. the number and size of pets treated). The size and number of pet(s) treated are estimated based on the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumptions for a deterministic assessment for treatment of pets are based on the amount handled for a single pet treatment event per day. Exposure estimates are based on the application rate, the size and number of pet(s) treated, and the amount of formulation (as defined in the residential assessment algorithms in Appendix D).
Transferable Residue	Transferable Residue (TR) data are described using a degradation curve derived from empirical data or from default assumptions. Residues derived from empirical data are evaluated using regression analysis of the residue data (completed by the user outside of CARES). The results are reported as a TR algorithm, a half-life of the compound or as an estimated residue value at a specified time after

Characteristic	Description
	application. Alternatively, TR data may be based on default assumptions: 1) twenty percent of the application rate is retained on the pet as dislodgeable residue on the day of application, 2) ten percent of the available dislodgeable residues are transferred during contact with the treated animals, 3) TR remains constant over time (U.S. EPA, 1997a).
Event Allocation	The probability that an individual is eligible for pesticide exposure is determined by product use and residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used in the residence is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. The user must determine if the frequency of occurrence should rely on the default assumption of a single pet treatment event per day, or on product use information supplied by the user.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age group (U.S. EPA, 1997b).
Exposure Algorithm – Mixer, Loader, Applicator	<p>Algorithms used to estimate applicator dermal and inhalation exposures are defined in Appendix D.</p> <p>An EPA deterministic assessment of exposures from dip, shampoo, dust and collar pet treatments assume that: 1) ten percent of the active ingredient applied to the pet are assumed to be the amount the homeowner is exposed to during dipping, dusting, and shampooing, 2) one percent of the active ingredient applied to the pet is assumed to be available for dermal and inhalation exposure from handling flea collars (U.S. EPA, 1997a).</p> <p>An EPA deterministic assessment of exposures from ready-to-use aerosol spray pet treatments assume that: 1) a single pet treatment event per day, 2) the amount handled during each treatment is the maximum application rate on the label, or one-half can of spray, 3) dermal and inhalation unit exposure rates are based on PHED aerosol can applicator scenario, 4) the density of an organic spray solution contained in a single use pressurized can is assumed to be 0.80 g/mL unless a product-specific value is provided (U.S. EPA, 1997a).</p>
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal and oral exposures are defined in Appendix D.

Characteristic	Description
	<p>An EPA deterministic assessment of dermal exposures from pet treatments assume that: 1) twenty percent of the application rate is retained on the pet as dislodgeable residue on the day of application, 2) ten percent of the available residues are transferred during contact with the treated animals, 3) post-application activities are assessed on the same day that the pesticide is applied, 4) one animal is contacted per day (U.S. EPA, 1997a).</p> <p>An EPA deterministic assessment of oral exposures from pet treatments assume that pesticide residues are transferred to the skin of toddlers from the handling/touching of treated pets and are subsequently ingested as a result of hand-to-mouth transfer. The deterministic assessment also assumes that: 1) twenty percent of the application rate is retained on the pet as dislodgeable residue on the day of application, 2) ten percent of the available residues are transferred during contact with the treated animals, 3) post-application activities are assessed on the same day that the pesticide is applied, 4) for subsequent days after application, it is assumed that the pesticide will not dissipate since it is desirable to maintain a specific level of pesticide on the pet (i.e., flea collars), 5) the exposed skin surface area of both hands is 350 cm<sup>2</sup> for a toddler (age 3 years), 6) replenishment of the pesticide residues on the hands is assumed to be infinite, 7) an average pet is assumed to have a body surface area of approximately 6,000 cm<sup>2</sup>, based on an assumed body weight of a medium size dog of 30 lbs (U.S.EPA, 1997a), 8) there is a one-to-one relationship between the transferable residue on the surface of the pet and on the surface area of the skin after contact, 9) the mean rate of hand-to-mouth activity and duration of exposure (U.S. EPA, 1997a).</p>
Duration	<p>An EPA deterministic assessment of oral exposures from pet treatments assume that the mean rate of hand-to-mouth activity is 1.56 events/hr for toddlers (3 to 5 year olds), and the duration of exposure for toddlers is assumed to be 2 hours per day, based on the time children play outside per day (U.S. EPA, 1997a).</p>
Market Share	<p>Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion households with pet treatment), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.</p>

## 4.2.10 Outdoor Fogger Use

This scenario provides a method for estimating post-application exposures in adults and children following outdoor fogger treatments. This procedure addresses the use of several types of products including typical single use aerosol foggers, multi-use insecticide candles and torches, and other single use, slow-release products (e.g., impregnated solids that slowly burn over a given duration and emit pesticide). This scenario assumes that pesticides in outdoor foggers are instantaneously released in a specific volume of air, that the air is mixed to produce a uniform concentration of the pesticide throughout the air. Label information is important for specifying appropriate data inputs for the exposure assessment. The method to determine post-application inhalation and dermal exposure to pesticides relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources.

The following information must be determined to build the CARES canvas and estimate daily inhalation post-application exposures:

**Table 4.10 – Outdoor Fogger Use Scenario Requirements**

Characteristic	Description
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment, the amount of active ingredient, and the size of the treated area.
Area Treated	The user must specify the area treated. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on an outdoor living space with dimensions of 20 ft long x 20 ft wide x 8 ft high (i.e. 3,200 ft <sup>2</sup> or 90.62 m <sup>3</sup> ).
Atmospheric Concentration	The user must specify the atmospheric concentration in the treated area. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on: 1) an "instant release" of the active ingredient (e.g. all active ingredient is instantaneously released into the air, 2) the chemical is assumed to be diluted in outdoor air at a ratio of 1 to 100 (i.e., 1 percent of the product released is available for inhalation), 3) the pesticide is assumed to remain in the air at this concentration for the entire duration of exposure (U.S. EPA, 1997a).
Event Allocation	The probability that a pesticide is used in the residence is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. The user must determine if the frequency of occurrence should rely on the default assumption, or on product use information supplied by the user. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on the outdoor living space treated with two single-use, ready-to-use products such as a fogger (U.S. EPA, 1997a).
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a

Characteristic	Description
	<p>reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).</p>
<p>Exposure Algorithm – Post-Application</p>	<p>Algorithms used to estimate post-application dermal and oral exposures are defined in Appendix D.</p> <p>The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on: 1) a specific gravity of 0.80 g/mL is assumed in all calculations unless a product specific value is available, based on a mean value of various organic solvents, 2) the adult inhalation rate is 13.3 m<sup>3</sup>/day or 0.55 m<sup>3</sup>/hour, 3) the child inhalation rate is 8.7 m<sup>3</sup>/day or 0.36 m<sup>3</sup>/hour (U.S. EPA, 1997a).</p>
<p>Duration</p>	<p>The user must specify the duration of exposure. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on occupancy of the treated outdoor living space of 5 hours/day for adults (age 18-64 years) and 3 hours/day for toddlers (age 1-4 years).</p>
<p>Market Share</p>	<p>Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion households with outdoor fogger treatment), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.</p>

## 4.2.11 Indoor Fogger Use

This scenario provides a method for estimating post-application exposures in adults and children following indoor fogger treatments. This procedure addresses the use of several types of products including typical single use aerosol foggers, multi-use insecticide candles and torches, and other single use, slow-release products (e.g., impregnated solids that slowly burn over a given duration and emit pesticide). This scenario assumes that pesticides in indoor foggers are instantaneously released in a specific volume of air, and that the air is mixed to produce a uniform concentration of the pesticide throughout the specified volume of air. The method to determine inhalation and dermal exposure to pesticides from indoor fogger applications relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). Label information for each product should be reviewed for specific data inputs.

The following information must be determined to build the CARES canvas and estimate daily inhalation post-application exposures:

**Table 4.11 – Indoor Fogger Use Scenario Requirements**

Characteristic	Description
Mixing, Loading, Application Methods	Application methods for pesticides applied as indoor foggers include aerosol cans, multi-use insecticide candles, and other single use, slow-release products (e.g., impregnated solids that slowly burn over a given duration and emit pesticide).
Active Ingredient	The amount of formulation handled is based on the label-specified application rate, the type of treatment, the amount of active ingredient, and the size of the treated area.
Area Treated	The user must specify the area treated. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on an outdoor living space with dimensions of 20 ft long x 20 ft wide x 8 ft high (i.e. 3,200 ft <sup>2</sup> or 90.62 m <sup>3</sup> ).
Atmospheric Concentration	The user must specify the atmospheric concentration. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on: 1) an "instant release" of the active ingredient (e.g. all active ingredient is instantaneously released into the air, 2) the chemical is assumed to be diluted in outdoor air at a ratio of 1 to 100 (i.e., 1 percent of the product released is available for inhalation), 3) the pesticide is assumed to remain in the air at this concentration for the entire duration of exposure (U.S. EPA, 1997a).
Transferable Residue	Transferable residue data are described using a degradation curve derived from empirical data or from default assumptions. Transferable residues derived from empirical data are evaluated using regression analysis of the log-transformed residue data (completed by the user outside of CARES). The results are reported as a regression equation, a half-life of the compound on foliage or as an estimated residue value at a specified time after application. Alternatively, EPA default assumptions may be used to estimate transferable residues over time by assuming that an average of 5 percent of the application rate are

Characteristic	Description
	available on the carpet and 10% of the application rate on hard surfaces are available as dislodgeable residue (from broadcast or crack and crevice treatments) (U.S. EPA, 2001). Post-application transferable residues after the day of application may be based on: 1) measured degradation rate based on chemical-specific data, or 2) measured residue on the day of application and a daily degradation of 10 % per day. The label-specified application rate and type of formulation are important predictors of residues that must also be considered.
Transfer Coefficient	The dermal transfer coefficient must be provided by the user. The U.S. EPA assumption for dermal transfer coefficient for a deterministic assessment of this scenario is 16,700 cm <sup>2</sup> /hr (adults) and 6,000 cm <sup>2</sup> /hr (children) for short- and intermediate- term exposures (U.S. EPA, 2001). The dermal transfer coefficients were estimated using Jazzercise studies of adults in contact with treated surfaces for 20 minutes, resulting in a normalized hourly dermal transfer coefficient of 200,000 cm <sup>2</sup> /hr. The 20-minute Jazzercise activity represents a 4-hour activity for short- and intermediate-term exposure.
Event Allocation	The probability that a pesticide is used in the residence is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. The user must determine if the frequency of occurrence should rely on the default assumption, or on product use information supplied by the user. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on the outdoor living space treated with two single-use, ready-to-use products such as a fogger (U.S. EPA, 1997a).
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Exposure Algorithm – Mixer, Loader, Applicator	Algorithms used to estimate handler dermal and inhalation exposures are defined in Appendix D.
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal and oral exposures are defined in Appendix D.  The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on: 1) a specific gravity of 0.80 g/mL is assumed in all calculations unless a product



Characteristic	Description
	specific value is available, based on a mean value of various organic solvents, 2) the adult inhalation rate is 13.3 m <sup>3</sup> /day or 0.55 m <sup>3</sup> /hour, 3) the child inhalation rate is 8.7 m <sup>3</sup> /day or 0.36 m <sup>3</sup> /hour (U.S. EPA, 1997a).
Duration	The user must specify the duration of exposure. The U.S. EPA assumptions for a deterministic assessment for treatment of outdoor fogger treatment are based on occupancy of the treated outdoor living space of 5 hours/day for adults (age 18-64 years) and 3 hours/day for toddlers (age 1-4 years) (U.S. EPA, 1997a).
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion households with outdoor fogger treatment), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.12 Indoor Treatment

See Indoor Fogger Use and/or Crack And Crevice Treatment.

#### 4.2.13 Paint/Wood Treatment

Potential non-occupational dermal and inhalation exposures that individuals may receive from pesticide use in paint/wood treatment are evaluated with this scenario. This scenario assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults during the handling (i.e. mixing, loading and application) of paint/wood products. This scenario assumes that aerosols and/or vapors are available to be inhaled or contact dermal surfaces while spraying, brushing, and rolling. Spray paint aerosols are assumed to be similar to aerosols produced during applications using a pressurized spray can containing insecticides. All brush and roller paints and stains are assumed to be similar regardless of the paint type (e.g., alkyd or latex paints and stains).

This scenario also assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults and children during post-application activities on treated surfaces. This scenario also assumes that pesticides are available to be ingested by children during post-application activities. The method to determine handler inhalation and dermal exposure to

pesticides from paint/wood applications relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). The method to determine post-application inhalation and dermal exposure to pesticides from treated surfaces relies on exposure data from user-specified sources.

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.12 – Paint/Wood Treatment Scenario Requirements**

Characteristic	Description
Mixing, Loading, Application Methods	The user must determine the methods used to mix, load and apply ready-to-use liquid formulations including spraying, brushing, and rolling.
Active Ingredient	The user must specify the amount of active ingredient considered in the assessment based on label information and the size of the treated area. An EPA deterministic assessment of exposures in paint/wood treatments assumes that: 1) three cans (12 ounces each) are used per aerosol spray paint event, 2) two gallons of paint are used per brush application event, 3) two gallons of paint are used per roller brush application event, 4) five gallons of paint are used for painting/staining with a low-pressure sprayer per event, 5) fifteen gallons of paint are used for painting/staining with an airless sprayer per event for treating a house size of 40 ft. x 30 ft. x 20 ft. with a painted surface area of 2800 ft <sup>2</sup> , 6) the density of spray paint is 1.24 g/mL (U.S. EPA 1997a).
Area Treated	The user must specify the area treated based on label information and the size of the treated area. An EPA deterministic assessment of exposures in paint/wood treatments assumes that: 1) three cans (12 ounces each) are used per aerosol spray paint event, 2) two gallons of paint are used per brush application event, 3) two gallons of paint are used per roller brush application event, 4) five gallons of paint are used for painting/staining with a low-pressure sprayer per event, 5) fifteen gallons of paint are used for painting/staining with an airless sprayer per event for treating a house size of 40 ft. x 30 ft. x 20 ft. with a painted surface area of 2800 ft <sup>2</sup> , 6) the density of spray paint is 1.24 g/mL (U.S. EPA 1997a).
Atmospheric Concentration	Atmospheric concentrations are described using empirical data or default assumptions based on computer modeling. An EPA deterministic assessment of post-application inhalation exposures from paint/wood treatments assume that the Screening-Level Consumer Inhalation Exposure Software (SCIES) and/or the Multi-Chamber Concentration and Exposure Model (MCCEM) are used to calculate indoor atmospheric concentration values (EPA, 1997a). X percent of paint/wood treatments applied to outdoor surfaces penetrate the house to become a source for off-gassing in a Chinn-type emission. All paint/wood treatments applied indoors are assumed to 100 percent available for emission.
Inhalation Coefficients	The hourly inhalation rate used by EPA for a deterministic assessment of post-application inhalation exposures is 0.4 m <sup>3</sup> /hour for adults at rest, 0.5 m <sup>3</sup> /hour for adults engaged in sedentary activity, 1 m <sup>3</sup> /hour

Characteristic	Description
	<p>for adults engaged in light activity, and 1.6 m<sup>3</sup>/hour for adults engaged in moderate activity (U.S. EPA Exposure Factors Handbook, 1997b), and are intended for assessing short-term scenarios of a few hours in duration (e.g. post-application activities).</p> <p>The daily inhalation rate used by EPA for a deterministic assessment of post-application inhalation exposures is 11.3 m<sup>3</sup>/day for adult females, 15.2 m<sup>3</sup>/day for adult males, 13.3 m<sup>3</sup>/day for average of adult males and females, 8.7 m<sup>3</sup>/day for children 1-12 years old, and 4.5 m<sup>3</sup>/day for children less than 1 year old.</p>
Dermal Contact	<p>The user must specify the exposed skin surface area. An EPA deterministic assessment of post-application dermal exposures in paint/wood treatments assume that dose should be based on a surface area of the body that is relevant to the impregnated material being assessed (e.g., 1 m<sup>2</sup> for adults or 0.35 m<sup>2</sup> for toddlers (age 3 years) for dermal contact with a vinyl mattress). These values represent one half the 90<sup>th</sup> percentile body surface area for adults and children. For products where a smaller percentage (i.e., 10 percent) of the body may come into contact with the product (e.g., vinyl shower curtain), lower skin surface areas may be reasonable (i.e., 0.2 m<sup>2</sup> for adults and 0.07 m<sup>2</sup> for toddlers) (U.S. EPA 1997a).</p>
Transferable Residue	<p>The user must specify the transferable residue. An EPA deterministic assessment of post-application dermal exposures in paint/wood treatments assumes that: 1) the flux rate through impregnated materials can be estimated based on the guidance provided in EPA Document 560/5-85-015 or the "AMEM: Polymer Migration Estimation Model," by Arthur D. Little (U.S. EPA, 1997a), 2) chemical/polymer-specific inputs such as media selection (air, water, or solid), exposure to external phase (single- or double-sided), polymer thickness; migration period; diffusion coefficient (cm<sup>2</sup>/sec), polymer type (e.g., PVC, rubber), and molecular weight.</p> <p>An EPA deterministic assessment of post-application oral exposure in paint/wood treatments assumes that 20 percent of the active ingredient is remaining in paint and is available for ingestion via paint chips.</p>
Ingestion Rate	<p>The user must specify the ingestion rate of paint chips containing pesticides. An EPA deterministic assessment of post-application oral exposures from paint/wood treatments due to ingestion of paint chips containing pesticide residue assumes that the ingestion rate for paint chips containing pesticides is 0.04 gram/day for children (age 6 months to 1-1/2 year), based on a child ingesting a paint chip with an overall size of 1 in<sup>2</sup> (6.25 cm<sup>2</sup>) and an average weight of 6.5 mg/cm<sup>2</sup> for a paint chip that is one layer thick (U.S. EPA, 1997a).</p>
Event Allocation	<p>The probability that an individual is eligible for pesticide exposure is determined by product use and residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used in the residence is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. The user must determine if the frequency of occurrence should rely on the default assumption, or on product use information supplied by user.</p>

Characteristic	Description
Body Weight	<p>Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).</p>
Exposure Algorithm – Mixer, Loader, Applicator	<p>Algorithms used to estimate dermal and inhalation exposures are defined in Appendix D. The U.S. EPA assumption for mixer, loader, applicator dermal and inhalation exposures for a deterministic assessment of this scenario relies on the Pesticide Handlers Exposure Database (PHED) to describe route-specific unit exposures using measures of central tendency from the PHED database (milligrams exposure per pound active ingredient mixed, loaded or applied). The user may also specify a distribution of empirical exposure rate values (empirical or parametric).</p>
Exposure Algorithm – Post-Application	<p>Algorithms used to estimate post-application dermal and inhalation exposures are defined in Appendix D.</p>
Duration	<p>The user must specify the duration of exposure. An EPA deterministic assessment of post-application exposures in paint/wood treatments assumes that: 1) daily exposure from application is based on the amount of active ingredient handled per day and not the exposure duration (i.e., a single painting event per day), 2) dermal dose from post application should be based on a duration of exposure that is relevant to the impregnated material being assessed (e.g., 8 hours per day of contact would be reasonable for vinyl mattresses based on the median value for the amount of time sleeping, or 0.5 hours for contact with a shower curtain (U.S. EPA, 1997a)).</p>
Market Share	<p>Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion using a paint/wood treatment), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share only for AIs included in the analysis.</p>

## 4.2.14 Impregnated Material

Potential non-occupational dermal and oral exposures that individuals may receive from pesticides in impregnated materials are evaluated with this scenario. This scenario assumes that pesticides have the potential to come in contact with the skin of adults and children during post-application activities involving contact with impregnated materials including pet collars and impregnated pest strips. This scenario also assumes that pesticides have the potential to be ingested by children during post-application activities involving contact with impregnated materials. The method to determine post-application dermal exposure to pesticides from impregnated materials relies on exposure data from user-specified sources. Potential non-occupational inhalation doses that individuals may receive from pesticides in impregnated materials are evaluated with the crack and crevice scenario. The method to determine post-application dermal exposure relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources.

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.13 – Impregnated Material Scenario Requirements**

Characteristic	Description
Active Ingredient	The amount of formulation handled is based on the percentage of active ingredient in the product, and the type, number and size of products encountered. The user must determine the type, number, and size of products encountered.
Area Treated	<p>The user must specify the area treated based on label information and the size of the treated surface area. An EPA deterministic assessment of dermal exposures from impregnated materials assumes that the total surface area of the impregnated material is based on the exposed surface area of the body relevant to the product and the expected contact with the product. The entire surface of the product is impregnated. For example, dermal exposure from impregnated vinyl mattresses assume that 1 m<sup>2</sup> (adults) or 0.35 m<sup>2</sup> (toddlers age 3 years) would be reasonable estimates of exposed surface areas and treated surfaces. For products such as vinyl shower curtains, where a smaller percentage (i.e., 10 percent) of the body may come into contact with the product, lower skin surface areas may be reasonable (i.e., 0.2 m<sup>2</sup> for adults and 0.07 m<sup>2</sup> for toddlers) (U.S.EPA, 1997a).</p> <p>An EPA deterministic assessment of incidental ingestion exposure from impregnated materials assumes that the total surface area of the impregnated material is 500 cm<sup>2</sup> (e.g., the surface area of an impregnated toy), and that the entire product is impregnated (U.S.EPA, 1997a).</p>
Flux Rate	An EPA deterministic assessment of dermal and incidental oral exposures from impregnated materials assumes that the flux rate through impregnated materials can be estimated based on media (air, water, or solid), exposure to external phase (single- or double-sided), polymer thickness, migration period, diffusion coefficient (cm <sup>2</sup> /s), polymer type (e.g., PVC, rubber), and molecular weight. (EPA

Characteristic	Description
	Document 560/5-85-015, U.S. EPA, 1992).
Event Allocation	An EPA deterministic assessment of post-application dermal and incidental ingestion exposures assumes that the event occurs each day. The user must determine if the frequency of occurrence should rely on the default assumption or on product use information supplied by the user.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). The U.S. EPA assumption of body weight for a deterministic assessment for toddlers (3 years old as representative of the 1 to 6 year old age group) is 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997a).
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D.
Duration	An EPA deterministic assessment of dermal exposures from impregnated materials assume that the dose should be based on a duration of exposure that is relevant to the impregnated material being assessed. For example, 8 hours per day of contact would be reasonable for vinyl mattresses based on the median value for the amount of time sleeping (U.S. EPA, 1997b). Materials, such as shower curtains, would have shorter contact periods (e.g., 0.5 hours).
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion using impregnated material), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.15 Detergent/Handsoap Use

This procedure provides a standard method for estimating exposures to handlers from dermal contact with detergent, bar soap, and other consumer products using the U.S. EPA Office of Pollution Prevention and Toxics, Economics, Exposure, and Technology Division DERMAL model. The model also provides a method for estimating post-application (i.e., passive) exposure to laundry detergent. The model is used primarily in screening-level assessments of dermal

exposure to the components of consumer products. The model estimates dermal exposures for the following types of consumer products: 1) general purpose cleaner, 2) liquid laundry detergent, 3) rug and upholstery cleaners, 4) floor cleaners, 5) spray paint, 6) exterior latex paint, 7) interior latex paint, 8) oil-based paint, 9) used motor oil, 10) lubricating greases, 11) bar soap, 12) diesel fuel, 13) gasoline, 14) news ink, 15) vinyl upholstery cleaner, 16) wax strippers. The method to determine exposure relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources.

This procedure also provides a standard method for estimating dermal exposures to adults and children from post-application exposure of exposed skin surfaces in contact with materials (e.g. clothing) treated with detergents containing the active ingredient. Dermal post-application exposures are estimated using the DERMAL model using the weight fraction of the chemical in the product of interest and assuming a certain film thickness of product on the skin and surface area exposed. In addition, default values are used for the frequency of events per year, exposure duration, and body weight.

The following information must be determined to build the CARES canvas and estimate daily handler and post-application inhalation exposures:

**Table 4.14 – Detergent/Handsoap Use Scenario Requirements**

Characteristic	Description
Active Ingredient	The amount of formulation handled is based on the percentage of active ingredient in the product. The user must determine the type, number, and size of products encountered.
Area Treated	The user must specify the area treated based on label information and the size of the treated surface area. An EPA deterministic assessment of dermal post-application exposure assumes default values for the skin surface area. Alternatively, the exposed skin surface area may be estimated using body weight and height from the vector of individual characteristics using algorithms from the Exposure Factors Handbook (U.S. EPA, 1997b).
Event Allocation	The probability that an individual is eligible for pesticide exposure is determined by product use and residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used in the residence is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. The user must determine if the frequency of occurrence should rely on the default assumption, or on product use information supplied by the user.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). The U.S. EPA assumption of body weight for a deterministic assessment for toddlers (3 years old as representative of the 1 to 6 year old age group) is 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997a).

Characteristic	Description
Exposure Algorithm – Mixer, Loader, Applicator	Algorithms used to estimate applicator dermal exposures are defined in Appendix D.
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D.
Duration	The user must specify the duration of exposure. An EPA deterministic assessment of dermal post-application exposure assumes default values for the frequency of events per year and exposure duration (U.S. EPA, 1995).
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion using impregnated material), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.



## 4.2.16 Swimming Pool Use

Potential non-occupational dermal and inhalation exposures that individuals may receive from pesticide use in swimming pools are evaluated with this scenario. This scenario assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults during the handling (i.e. mixing, loading and application) of swimming pool chemicals. This scenario also assumes that pesticides are available to be inhaled or have the potential to come in contact with the skin of adults and children during post-application activities in treated swimming pools. The method to determine handler inhalation and dermal exposure to pesticides from swimming pool applications relies on algorithms specified by EPA (U.S. EPA, 1997a; U.S. EPA 2001) using exposure data from user-specified sources, including PHED (U.S. EPA, 1998). The method to determine post-application inhalation and dermal exposure to pesticides from treated swimming pools relies on exposure data from user-specified sources.

The following information must be determined to build the CARES canvas and estimate daily inhalation and dermal mixer/loader/applicator and post-application exposures:

**Table 4.15 – Swimming Pool Use Scenario Requirements**

Characteristic	Description
Mixing, Loading, Application Methods	The user must determine: 1) methods used to apply ready to use dry formulation pesticides, such as pouring and/or placing solids and water soluble packets, 2) methods used to mix, load and apply ready-to-use liquid formulations including open pouring of liquids and placing of water soluble gel packets
Active Ingredient	The amount of formulation handled based on the label-specified application rate, and size of the treated area(s). Exposure estimates are based on the application rate and area treated, or the amount of formulation (as defined in the residential assessment algorithms in Appendix D).
Area Treated	The area treated (pool capacity) is determined from the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption for size of pool treated for a deterministic assessment of this scenario is 20,000 gallons (U.S. EPA, 1997a).
Available Residue	The user must determine: 1) the initial concentration of the product in swimming pool water, 2) the daily degradation rate of the product in swimming pool water over time. Alternatively, an EPA deterministic assessment of post-application exposures in swimming pools assumes that: 1) 100 percent of the application concentration is available in the pool water for dermal contact, ingestion and inhalation since biocides are typically maintained in pool water at specified levels, 2), the pesticide will not dissipate for subsequent days after application since it is desirable to maintain a specified level of biocide in the water.
Dermal Contact	The user must specify the exposed skin surface area. An EPA deterministic assessment of post-application exposures in swimming pools assumes that: 1) the surface area is 20,900 cm <sup>2</sup> for adults and

Characteristic	Description
	9,000 cm <sup>2</sup> for children (age 6 years) (U.S. EPA, 1997a), and 2) the permeability coefficient (K <sub>p</sub> ) is a chemical specific value (cm/hr). K <sub>p</sub> may be measured or predicted from octanol-water partition coefficient (K <sub>ow</sub> ) values and molecular weight (U.S. EPA, 1997a).
Event Allocation	The probability that an individual is eligible for pesticide use is determined by residence information from the vector of individual characteristics (Sielken and Holden, 2001). The probability that a pesticide is used by an individual is specified by the user in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. An EPA deterministic assessment of post-application dermal and incidental ingestion exposures assumes that the event occurs each day.
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Exposure Algorithm – Mixer, Loader, Applicator	Algorithms used to estimate dermal and inhalation exposures are defined in Appendix D. The U.S. EPA assumption for mixer, loader, applicator dermal and inhalation exposures for a deterministic assessment of this scenario relies on the Pesticide Handlers Exposure Database (PHED) to describe route-specific unit exposures using measures of central tendency from the PHED database (milligrams exposure per pound active ingredient mixed, loaded or applied) (U.S. EPA, 1998). The user may also specify a distribution of empirical exposure rate values (empirical or parametric).
Exposure Algorithm – Post-Application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D. An EPA deterministic assessment of post-application exposures in swimming pools assumes that the mean ingestion rate for adult and children swimmers is 0.05 L/hour (U.S. EPA, 1997a). The assumed mean inhalation rate is 1.7 m <sup>3</sup> /hour for adults (i.e., over 18 years) and 1.2 m <sup>3</sup> /hour for children (i.e., under 18 years), based on a moderate activity level (U.S. EPA, 1997a). Gas phase concentrations are based on an ideal gas model and Raoult's Law (U.S. EPA, 1997a).
Duration	The user must specify the duration of exposure. An EPA deterministic assessment of post-application exposures in swimming pools assumes that the duration of exposure is 5 hours per day for both children (age 6 years) and adults (18-64 years) (U.S. EPA, 1997a).
Market Share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be

Characteristic	Description
	based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion treating a swimming pool, then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.17 Golfer

Potential non-occupational dermal exposures that individuals may receive from pesticide use on golf course turf are evaluated with this scenario. This scenario assumes that pesticides have the potential to come in contact with the skin of adults and children during post-application activities on treated turf on golf courses. The method to determine post-application dermal exposure to pesticides from treated turf relies on exposure data from user-specified sources (U.S. EPA, 1997a; U.S. EPA 2001).

The following information must be determined to build the CARES canvas and estimate daily dermal post-application exposures:

**Table 4.17 – Golfer Scenario Requirements**

Characteristic	Description
Turf transferable residue (TTR)	Turf transferable residue (TTR) data are described using a degradation curve derived from empirical data or from default assumptions. Transferable residues derived from empirical TTR data are evaluated using regression analysis of the log-transformed residue data (completed by the user outside of CARES). The results are reported as a TTR algorithm, a half-life of the compound on foliage or an estimated residue value at a specified time after application. Alternatively, default assumptions may be used to estimate transferable residues over time by assuming that 0.1 to 0.5 percent of the application rate is available on turf as transferable residue, and that the residue degrades 10% per day (U.S. EPA 2001). The label-specified application rate and type of formulation are important predictors of turf residues that must also be considered.
Transfer Coefficient	The user provides the dermal transfer coefficient. The U.S. EPA assumption for dermal transfer coefficient for a deterministic assessment of this scenario is 200 to 760 cm <sup>2</sup> /hr (U.S. EPA, 2001a).
Event allocation	The user specifies the probability that an individual is eligible for a golf activity involving pesticide exposure in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. U.S. EPA default assumptions on the

Characteristic	Description
	percentage of golf courses treated and the percentage of the population playing golf are based on survey information from Doane and GolfTrak (DOANE Marketing Research, Inc. GolfTrak, 1998-1999) as reported by U.S. EPA (2001a).
Body Weight	Body weights of adults are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b).
Exposure algorithm – post-application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D.
Duration	The user must specify duration of exposure on turf. EPA default assumptions for the duration of exposure for golfers on treated turf ranges from 2 to 4 hours based playing an 18-hole round of golf and the extent of golf course treatment. The higher value represents playing on courses where only tees and greens have been treated; the higher value represents playing on courses where fairways, tees and greens have been treated (U.S. EPA 2001a)
Market share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion of golf courses treated), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.18 Public Health

Potential non-occupational dermal exposures that individuals may receive from pesticide use for public health use in residential areas are evaluated with this scenario. This scenario assumes that pesticides have the potential to come in contact with the skin of adults and children during post-application activities on turf and other treated surfaces. The method to determine post-application dermal exposure to pesticides from treated surfaces relies on exposure data from user-specified sources (U.S. EPA, 1997a, U.S. 2001).

The following information must be determined to build the CARES canvas and estimate daily dermal post-application exposures:

**Table 4.18 – Public Health Scenario Requirements**

Characteristic	Description
Transferable residue	Transferable residue (TR) on turf or other surfaces are described using a degradation curve derived from empirical data or from default assumptions. Transferable residues derived from empirical data are evaluated using regression analysis of the log-transformed residue data (completed by the user outside of CARES). The results are reported as a regression equation (slope and intercept), a half-life of the compound, or an estimated residue value at a specified time after application. Alternatively, EPA default assumptions may be used to estimate transferable residues over time by assuming that 0.1 to 0.5 percent of the application rate is available on turf as transferable residue, and that the residue degrades 10% per day (U.S. EPA, 2001). The label-specified application rate and type of formulation are important predictors of residues that must also be considered.
Transfer Coefficient	The user provides the dermal transfer coefficient. The U.S. EPA assumptions for dermal transfer coefficient for a probabilistic assessment of this scenario are 700 to 16000 cm <sup>2</sup> /hr for children and 1930 to 13200 cm <sup>2</sup> /hr for adults, based on studies by Vaccaro et al., 1996, and Black, 1993 (U.S. EPA, 2001a).
Event allocation	The user specifies the probability that an individual is eligible for an activity involving pesticide exposure in the event allocation data entry screen. The frequency of pesticide use is specified in the event allocation data entry screen. The U.S. EPA assumptions for public health use of pesticides for public health are based on various sources including reports from the Florida Coordination Council on Mosquito Control and the Outdoor Residential Exposure Task Force (U.S. EPA, 2001a).
Body Weight	Body weights of adults and children are specified in the vector of individual characteristics (Sielken and Holden, 2001). The U.S. EPA assumption of body weight for a deterministic assessment is 71.8 kg for adults (60 kg for females when the selected endpoint is from a reproductive or developmental study). A body weight of 71.8 kg represents the mean body weight for all adults (i.e., male and female, ages 18 years and older) and is the value recommended in U.S. EPA (1997b). A body weight of 60 kg represents the mean body weight for females between ages 13 and 54 years (U.S. EPA, 1997b). Toddlers (3 years old), used to represent the 1 to 6 year old age group, are assumed to weigh 15 kg, based on the mean of the median body weights for male and female toddlers. (U.S. EPA, 1997b). Infants (age 6 months to 1-1/2 year) are assumed to weigh 10 kg, based on the mean of the median values for male and female children in the 6-11 month and 1-year age groups. (U.S. EPA, 1997b).
Exposure algorithm – post-application	Algorithms used to estimate post-application dermal exposures are defined in Appendix D.
Duration	The user must specify duration of exposure on treated surfaces. EPA default assumptions for the duration of exposure on outdoor treated surfaces ranges from 0 to 3.5 hours/day for children, and 0 to 2.1 hours/day for adults (U.S. EPA, 1997b).

Characteristic	Description
Market share	Market share for each active ingredient (AI) is specified in the residential product list (input residential screen). Market share may be based on % of total market share for all AIs used for the selected treatment scenario, including AIs with different toxicological endpoints that are excluded from the analysis. Alternatively, market share may be based on % of total market share for only those AIs used for the selected treatment scenario that are included in the analysis (input chemical screen). The market share information provided by the user will depend on the nature of the residential scenario probabilities. If scenario probabilities are generic (e.g. proportion of golf courses treated), then the user may need to specify total market share for all AIs including those with different toxicological endpoints that are excluded from the analysis. However, if the scenario probabilities are specific for products included in the analysis, then the user may need to specify total market share for only those AIs included in the analysis.

#### 4.2.19 Custom

Future versions of the CARES residential model will allow the user to create custom scenarios using user-defined algorithms. This capability is not functional in CARES Version 1.0.

## 4.3 Calendar Based Residential Exposure Modeling

### 4.3.1 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 at infrequent intervals, while other events such as treating a lawn with a weed control product may occur at frequent intervals of a few times per year. Below is a description of the method used in the CARES model 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 4.16 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 4.16 – A Sample Table for “Ingredients & Products”**

Active Ingredient	Product
Ingredient 1	Product 1
Ingredient 1	Product 4
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 4.17 shows this dependency of efficacy period on product.

**Table 4.17 – A Sample Table for “Products & Efficacy Periods”**

Product	Efficacy Period (Days)
Product 1	Period 1
Product 2	Period 2
.....	.....
Product n	.....

Products are used for specific scenarios. Scenarios include “Lawn Care”, “Ornamental Plant Care”, “Indoor Fogger Use”, etc. Table 4.18 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 4.18 – A Sample Table for “Products & Scenarios”**

Product	Scenario
Product 1	Scenario 1
Product 1	Scenario 2
Product 2	Scenario 3
Product 3	Scenario 3
.....	.....
Product n	Scenario n

Given a sub-population (i.e.doer vs. non-doer), there are finite probabilities whether the individuals live in residences where any of the product use scenarios occur. These probabilities are tabulated in Table 4.19. 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 4.19 – 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
.....	.....	.....
Scenario n	.....	.....

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 4.20 lists the products and applicators types.

**Table 4.20 – A Sample Table “Products & Professional vs. Consumer Use”**

Product	Application Type
Product 1	Professional
Product 2	Consumer
.....	.....
Product n	.....

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 4.21 shows the distributions of product use scenarios as a function of month. Each row in this table must add to 1.0.

**Table 4.21 – A Sample Table for “Scenarios & Seasonal Use”**

Product Use Scenario	Jan	Feb	.....	Dec
Scenario 1	0.05	0.1	.....	0.05
Scenario 2	0.01	0.01	.....	0.01
.....	.....	.....	.....	.....
Scenario n	.....	.....	.....	.....

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 4.22 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 4.22 – A Sample Table for “Senarios & Day of Week Use”**

Product Use Scenario	Sun	Mon	.....	Sat
Scenario 1	0.2	0.1	.....	0.2
Scenario 2	0.15	0.15	.....	0.15
.....	.....	.....	.....	.....
Scenario n	.....	.....	.....	.....

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 4.23 lists the products and re-entry periods.

**Table 4.23 – A Sample Table for “Products/Scenario & Re-Entry Periods”**

Product Use Scenario	Re-Entry Period (Days)
Product 1/Scenario 1	0.5
Product 1/Scenario 2	0.33
.....	.....
Product n/Scenario n	.....

When certain product(s) are 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 24 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 4.24 – A Sample Table for “Scenarios & Co-Occurrences of Use”**

Product Use Scenario	Scenario 1	Scenario 2	.....	Scenario N
Scenario 1	0.0	0.2	.....	.....
Scenario 2	0.1	0.0	.....	.....
.....	.....	.....	.....	.....
Scenario n	.....	.....	.....	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 4.25.

**Table 4.25 – A Sample Table for “Scenarios & Numbers of Annual Users”**

Product Use Scenario	Number Of Annual Use
Scenario 1	12
Scenario 2	8
.....	.....
Scenario n	.....

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 4.26, below, all the cells should add to 1.0.

**Table 4.26 – A Sample Table for “Market Share”**

Product Use Scenario	Ingredient 1	Ingredient 2	.....	Ingredient N
Product 1	0.1	0.0	.....	.....
Product 2	0.0	0.05	.....	.....
.....	.....	.....	.....	.....
Product n	.....	.....	.....	.....

### 4.3.2 Stochastic, Calendar-Based Product Use Event Allocation Algorithms

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.

#### The Distribution of the Number of Scenario Events

The general algorithms presented in Appendix D are applicable to any irregularly used pesticide product. There are several important sources of information available to the user to assign necessary information. First, the frequency of the scenario, defined as the number of episodes of occurrence across the year, is known. Table 4.27 displays a hypothetical use distribution. Note that this is only for persons encountering the event scenario. For example, fogger use information from 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 4.27 – Fogger Use Frequency for People 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 are reported (e.g. 10-25 times), it may be 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 may be assumed that the frequencies between 101 and 122 are equally likely. This assigns zero probability to use frequencies in excess of the maximum (e.g. > 122 times a year, or more than every third day use). This last probability assignment may be 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.

#### Distributing Events over the Year

The temporal structure of application events over the year must also be determined. Table 4.28 gives a hypothetical use pattern for product use.

**Table 4.28 – Hypothetical Percentage of Product Use by Month of Year**

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 event is under consideration, the data in Table 4.28 can be directly used to assign this event to a particular month. Once the event has been assigned 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 January 1 is  $0.034 \div 31$  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.

### 4.3.2.1 Assigning the Number of Products Used Per Event

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

**Table 4.29 – Number of Products Used Per Event**

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

Table 4.29 shows that 16% (0.16) of scenario 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, it may be assumed that the 39% for the 4+ category, 13% was for the use of 4 products, 13% for 5 products, and 13% for 6 products.

### 4.3.2.2 Assigning 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 provided by the model user be used to assign events to products. That is, if Product X has 33% market share, 1/3 of all events will be assigned to this product. Note that this assumes that all products used in a given event are the same formulation. However, products are assigned randomly according to market share for each scenario event. That is, it is not assumed that a given individual might preferentially use a specific product.

## 4.3.3 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 scenario events per year.
2. Randomly distributing these events over the year.
3. Randomly generating the number of products used per event.
4. Randomly picking the 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. Once an individual is selected, the four steps presented above are performed to generate an annual scenario exposure profile, which incorporates the temporal distribution of events, the number of products used per event and the type of products used in each event.

## 4.4 Algorithms

Algorithms used for estimating exposures are defined in Appendix D and include the following:

Dermal 101 – Unit Exposure, Area Treated  
Dermal 102 – Unit Exposure, Amount of Formulation Used  
Inhalation 101 – Unit Exposure, Area Treated  
Inhalation 102 – Unit Exposure, Amount of Formulation Used  
Multiple 101 – Unit Exposure, Area Treated (Dermal + Inhalation)  
Multiple 102 – Unit Exposure, Amount of Formulation Used (Dermal + Inhalation)

Algorithms used for estimating post-application exposures are defined in Appendix D and include the following:

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

## 4.5 References

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# 5. Water Module

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# Chapter 5 – Water Module

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## 5.1 Introduction

The CARES-water module links 365 daily water consumption values for each individual in the reference population to daily water residue values provided by the user in order to calculate the contribution to daily dose from pesticides in drinking water. Each person in the CARES reference population is identified by a profile of individual characteristics (gender, age, state of residence, etc.). Based on these characteristics, each individual in the reference population can be linked to a water consumption pattern and a corresponding water residue level.

## 5.2 Water Consumption

CARES provides the user with 4 different options to characterize the water consumption of the people in reference population:

- water consumption based on USDA/CSFII-data
- two liters of water per day per 70 kg BW
- EPA/WHO constants for water consumption
- Age adjusted constant water consumption

### 5.2.1 Water Consumption Based on the CSFII

The CSFII (Continuing Survey of Food Intake by Individuals; 1994-96; 1998) does not contain complete information on water consumption. Therefore EPA developed a methodology to construct a companion water consumption database for FCID that was incorporated into CARES Version 1.0. The listing of water intake in FCID takes into account the different sources of dietary water intake. For example, a person might regularly drink tap water from home as well as at work, school or other locations outside the home. Individuals may consume water from sources other than tap water including bottled water, and water in beverages. Since there is limited data on chemical residues in bottled water and beverages, these sources of dietary water are not included in CARES Version 1.0.

The quantity of direct and indirect water ingestion can be determined from CSFII. Direct water ingestion is the amount of water directly ingested as plain water. Direct water intake can be further subdivided into direct water consumed while at home from non-bottled sources (tap water), direct water consumed while away from home from non-bottled sources (tap water), direct bottled water consumed on a day while at home, direct bottled water consumed on a day while away from home.

Indirect water ingestion represents the intake of non-commercial water added locally to food and beverages. As there was no CSFII question that isolates indirect water, the EPA identified all food items that can be prepared with locally added water. The fraction of indirect water was determined for every CSFII food

item and adjusted for the amount of water lost during cooking. This amount reported in FCID then represented the amount of indirect water consumed.

### 5.2.2 Creating a 365-Day Water Consumption Profile

Each individual in the CARES reference population has a 365-day food consumption profile that was created from birthday to birthday. This profile does not contain actual consumption values but rather each profile is a list of 365 pointers to surrogate person-days in the CSFII-database using the matching procedure described in Chapter 2. Daily water consumption as discussed previously is part of the 365-day profile created for each individual in the reference population.

### 5.2.3 Default Water Consumption

The user has the option of setting a constant water consumption for each day. The liter drinking water intake per day is a historical figure set by the U.S. Army in determining the amount of water needed for each person in the field and is an overestimate for most people. This value corresponds to a 90th percentile water consumption rate from earlier studies (Patulin, 1983; Cantor et al, 1987). Combined data from CFSII 1994-96 provide a further refinement of default water intake by gender and/or age as shown in Table 5.1.

**Table 5.1 – Default Water Intake by Gender and Age**

Age-group	Water Consumption
Adult male	2L/ 70 kg bw
Adult Female	2L/ 60 kg bw
Child (1-12 year), M/F	1L/ 10 kg bw
Infant (0-11 months), M/F	0.75 L/ 5kg bw

## 5.3 Linking Residue Data to Water Intake

A 365-day profile of water consumption for individuals in the reference population is linked to a 365-day residue profile. This residue profile must be spatially and temporally specific. The temporal resolution in CARES is by day and the maximum spatial resolution is by state although in theory the resolution may be down to the level of the FIPS code. CARES Version 1.0 is capable of differentiating between ground and surface water but not between direct or indirect water or between water consumed at home and water consumed away from home.

The user faced with the difficult task of providing residue data for ground or surface water having a a different level of spatial and temporal resolution has several choices. The user can assume constant values derived from Tier 1 models such as SCIGROW for ground water and FIRST for surface water. In Tier 2 assessments PRZM/EXAMS (Index Reservoir) can be used to generate estimates for residues in surface water. There currently are no suitable Tier 2 models for predicting ground water concentration. When available, residues in surface or ground water can be derived from regionally specific monitoring data where the temporal profile is filled in by interpolation. Alternatively, for surface

water the user can create a hybrid model using a combination of information from modeling and monitoring studies. Modeling data can be entered into a spreadsheet and monitoring data can be imported from a CARES compatible database. At this time, CARES doesn't allow a correction for water treatment within the program, but such corrections can be done by the user before the residue file is imported into CARES.

For situations where there are multi-year residue data, CARES randomly draws one year of data (365-day residue profile) and assigns it to one individual in the reference population. This is repeated for all individuals until each person has an assigned 365-day residue profile. The daily water intake for the individual is multiplied by the daily residue level to give a 365-day dose profile for each person.

## 5.4 Monitoring vs. Modeling

### 5.4.1 Strengths and Weaknesses

The CARES Water Module accepts 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 are used to estimate exposure for different geographic regions or different types of water sources in the same region as specified by the user. The strengths and weaknesses of monitoring versus modeling approaches to establishing probable ground and surface water residue concentrations are summarized in Table 5.2.

**Table 5.2 – Relative Strengths and Weaknesses of Modeling and Monitoring**

Modeling	Monitoring
<p><b>PRO</b></p> <ul style="list-style-type: none"> <li>• Cost Effective (generally less expensive than monitoring)</li> <li>• Ability to predict concentrations over a continuum in space and time</li> <li>• Comparative exposure assessments are possible</li> <li>• Relatively quick - days to months</li> <li>• Can evaluate “what-if” scenarios and sensitivities (e.g. climate, soil, application date)</li> <li>• Can incorporate effectiveness of possible mitigation alternatives</li> <li>• Not constrained by analytical LOD</li> <li>• Can quantify relative to “benchmarks”</li> </ul>	<p><b>CON</b></p> <ul style="list-style-type: none"> <li>• Costly</li> <li>• Time involved is weeks to several years</li> <li>• Difficult to design cost effective AND technically viable sampling programs</li> <li>• May require many years of monitoring and/or paired studies to evaluate effectiveness</li> <li>• Handling non-detects is difficult</li> <li>• Results are accepted as “true” values</li> <li>• Sampling represents discrete points in space and time that can only be put into context with modeling</li> <li>• Study only represents one unique combination of conditions</li> <li>• Can be constrained by analytical precision and LOD</li> <li>• Difficult to interpret results in a</li> </ul>

Modeling	Monitoring
	probabilistic fashion <ul style="list-style-type: none"> <li>• Subject to distortion by “unusual” weather</li> <li>• Difficult to interpret probabilistically</li> <li>• Cause &amp; effect difficult to assign – especially with biological monitoring</li> </ul>
<b>CON</b> <ul style="list-style-type: none"> <li>• Simplifications required in the representation of prototype systems</li> <li>• There is general public reluctance to accept predicted data</li> <li>• Calibration/validation is needed to assess how closely predicted values match reality</li> <li>• Many of the input values have high uncertainties associated with them</li> <li>• The selected input parameters may not be environmentally feasible</li> <li>• Model algorithms may oversimplify or misrepresent compound behavior</li> <li>• Tends to use conservative assumptions</li> <li>• Levels of uncertainty in inputs not obvious</li> <li>• Data on pesticide use unavailable</li> <li>• Useful watershed and flowing water scenarios not currently available</li> </ul>	<b>PRO</b> <ul style="list-style-type: none"> <li>• Provides an actual measurement of chemical residue concentration, hydrologic response etc</li> <li>• Avoids conservatism resulting from compounding conservative assumptions</li> <li>• When done well it is an excellent tool</li> <li>• Accounts for the inherent heterogeneity of the system</li> <li>• There is a greater acceptance of measured data</li> <li>• There is public confidence in monitoring data</li> <li>• Real world hydrology</li> <li>• Accounts for actual pesticide usage</li> <li>• Does not require algorithm/ model development &amp; validation</li> </ul>

#### 5.4.2 Monitoring Studies: Effect of Scale

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 (e.g., the Mississippi River at New Orleans). As indicated in Table 5.3, residue values from watersheds of basin scale or larger are likely to be more realistic than are those derived from smaller scale reservoirs.

#### 5.4.3 Computer Modeling Tiers

A brief description of the exposure assessment tiers of water modeling is given in Table 5.4. In order to account for the most common sources of drinking water a distinction can be made between private wells (dug or drilled) and community water systems (CWS) using groundwater, extracting water from a reservoir or pumping water out of a flowing water body.

**Table 5.3 – Effect of Scale on the Interpretation of Modeling and Monitoring Data**

<b>Factor</b>	<b>Small-Scale Test Plots</b>	<b>Sub-basins</b>	<b>Basins</b>
Drainage area size	<0.05 hectare	10 to 40 hectare	10 to >100 km <sup>2</sup>
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	Label use	Include asrRealist
Focus	Research, idealized system	Label use	Reality
Calibration w/ transport model	Event based	Continuous simulation	Multiple segments, continuous simulation
Extrapolating model to field scale	Questionable	Inherent	Difficult to verify w/o observations
Extrapolating model to other fields	Questionable	Questionable	Questionable

**Table 5.4 –Exposure Assessment Tiers for Water Modeling**

Tier	Dug wells	Drilled wells	Community Water System		
			Ground Water	Reservoir	Flowing Water
1	SCIGROW	SCIGROW	SCIGROW	FIRST	FIRST
2	Calibrated dataset 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 regression-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	Multiple regional datasets with aquifer dilution and 36-year weather			Population-weighted selection of IR scenarios of varying DANC, PCA, and hydraulic residence times. DANC, PCA, and HR based on regional distributions derived from CWS analysis (for each region produces x 36 scenario-years)	Population-weighted selection of river scenarios of varying PCA and hydrologic conditions. Characteristics based on regional distributions derived from CWS analysis.
4		Multi-dimensional regional fate and transport model?	Multi-dimensional regional fate and transport model?	MC or JPM assessment varying DANC, PCA, and hydraulic residence times. Other permutations could include use rates and treatment plant reductions.	MC or JPM assessment varying DANC, PCA, and hydraulic residence times. Other permutations could include use rates and treatment plant reductions.



#### **5.4.4 Tiered Models for Ground Water**

Tier-1 risk assessment for groundwater in general is based on the EPA 's "Screening Concentration in Ground Water" (SCIGROW) model. This model is based on prospective ground water monitoring studies and reflects shallow ground water sources under highly permeable soils, where leaching is the principal mode of transport for the pesticide.

A more refined approach (Tier 2) for private dug wells may be based on data from prospective groundwater studies (Prospective Groundwater Study,1995-2000). This study was initiated to monitor the potential impact of the maize herbicide acetochlor on shallow groundwater. In general shallow groundwater is not representative for drinking water. For this reason an aquifer dilution factor may be employed to extrapolate the groundwater data to the aquifer level.

Tier 3 assessment for dug wells may incorporate regional datasets, embodying detailed spatial and temporal factors. Tier-2 level residue data for private drilled wells and Community Water System (CWS) groundwater may be sampled from regional monitoring databases of wells.

#### **5.4.5 Tiered Models for Surface Water**

Tier-1 assessment for CWS surface water is often modeled using the "FQPA Index Reservoir Screening Tool" (FIRST), which is based upon an existing extremely vulnerable drinking water reservoir adjusted for crop coverage. Tier-2 level residue data for CWS drinking water can be obtained from regional monitoring databases for reservoirs, rivers and streams or can be based on the Index Reservoir model (CWS reservoir) or the Regional index river model (CWS flowing water). Tier 3 assessments for surface water sources can be based on a population weighted selection of appropriate surface water scenarios using Monte Carlo methods.

#### **5.4.6 Use of Monitoring Data**

Monitoring databases such as those based on the NAWQA and MSEA studies, and product specific studies conducted by pesticide registrants provide data on pesticide residues in water samples of various types. Although the water samples in some of these surveys are not "drinking water sources", the data can be used to estimate potential exposures via drinking water.

### **5.5 Environmental Degradates**

In general, environmental degradates should be treated as another analyte in an aggregate or cumulative assessment if they share a common mechanism of toxicity with the parent. Unfortunately, there is often limited data available for such degradates and the relationship to parent concentrations in ground and surface water is only poorly understood or described.

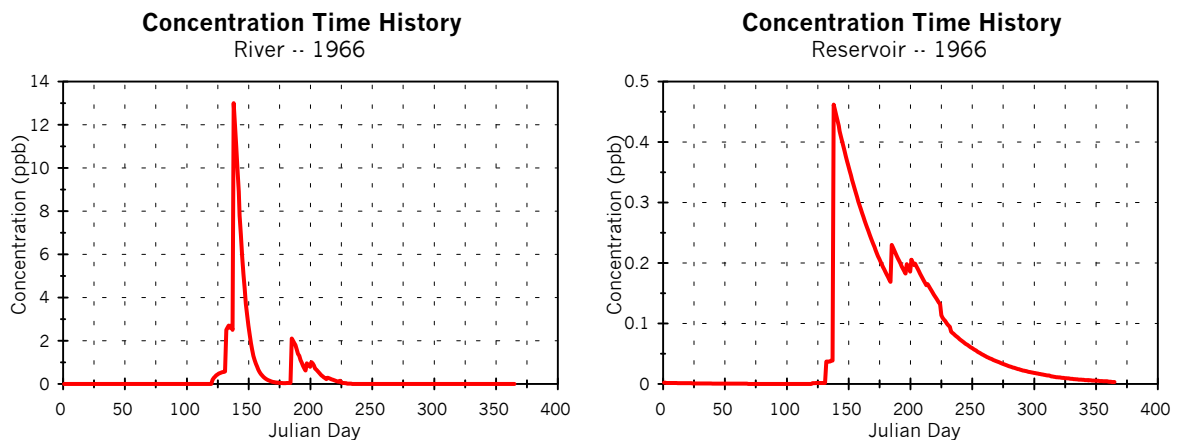
### **5.6 Spatial Surrogation of Residue Data**

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. In such cases, it will be necessary to

use “surrogate” data from a relevant nearby region. Care should be taken when using pesticide use practices, soils, climate, hydrology, and other critical factors to create a surrogate database because residues can vary dramatically even over short distances, making geographic surrogation imprecise. The user should attempt to match as many of these factors as possible. It may be wise to only use surrogate data from within larger geographic regions, such as the RAC state groupings. A future version of CARES can assign residue values to a state as a constant or as a distribution (e.g. uniform, normal or lognormal). Data for the same tap water source category can be surrogated from one state to another. Default data adjustments can be introduced by specifying a scaling factor.

## 5.7 Temporal Interpolation of Sparse Data

Temporal patterns of chemical concentrations in drinking water 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 residence times on the order weeks to months (Figure 5.1). 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 minor 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 entry to and detection in reservoirs. Chemical runoff will not occur during periods of drought and will not be at detectable levels after the chemical has undergone sufficient field degradation.



**Figure 5.1 – Effects of Hydrologic Residence Times in Rivers and Reservoirs**

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 studies.

While it may be technically possible 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 the user is allowed to choose from three methods of interpolation:

- linear
- non-linear or exponential
- step function

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.

In a future version of CARES, 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.

## 5.8 Geographic Granularity

Geographic granularity refers to the spatial resolution or smallest “geographic unit of analysis” that is 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), agronomic practices in the contributing watershed or aquifer system and the hydrodynamic response of the water body.

Assimilating this information into a risk assessment is a difficult 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 residue data is only available at county or higher level of spatial resolution.

At this time the smallest geographic unit of analysis within CARES is at the level of the State. This choice was based on the current limited availability of required input data at a higher level of resolution. 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. Other methods of dividing the country, such as the U.S. farm regions utilized by EPA in their OP cumulative assessment, are possible within CARES as long as the residue profiles are surrogated according to the desired geographic map (see Figure 5.2). Examples of each of these methods are discussed below.

- **Proximity** It is expected that the user will import into CARES an array of 365-day residue profiles based upon modeling or monitoring data. This data may represent multiple years for each state and water type (groundwater, interface water, etc.). Individuals in the CARES reference population will be mapped to this database based on proximity (i.e., an individual that resides within a state will be randomly assigned a 365-day residue profile for that state) or surrogation (see below).
- **Proportion** If an individual from the Reference Population is known to consume water from a given community water supply and there are three community water supplies within the geographic unit of analysis (A, B, and C), then 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. If A, B, and C serve 33, 47, and 20 percent of the total population served by community water supplies in the region, respectively, then, in this example, it is most likely that the individual will be assigned an annual exposure series from water supply B.
- **Surrogation** If an individual from the Reference Population is known to consume water from a domestic well, then 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.

The boundaries of six of these possible classification systems for defining granularity are depicted in Figures 5.2- 5.7. 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 have been 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 and summarized in Tables 5.5 and 5.6.

- **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 were 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 coarse 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 based entirely on public data.

At this time the smallest geographic unit of analysis within CARES is at the level of the State. This choice was based on the current limited availability of required input data at a higher level of resolution.

**Table 5.5 - 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 5.6 – Geographic Units Considered for the CARES Water Module (continued)**

<b>Geographic Unit</b>	<b>Description</b>	<b>Pros</b>	<b>Con</b>
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
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 PUMs 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

### Basin and Range

- Largest share of nonfamily farms, smallest share of U.S. cropland.
- 4% of farms, 4% of value of production, 4% of cropland.
- Cattle, wheat, and sorghum farms.

### Northern Great Plains

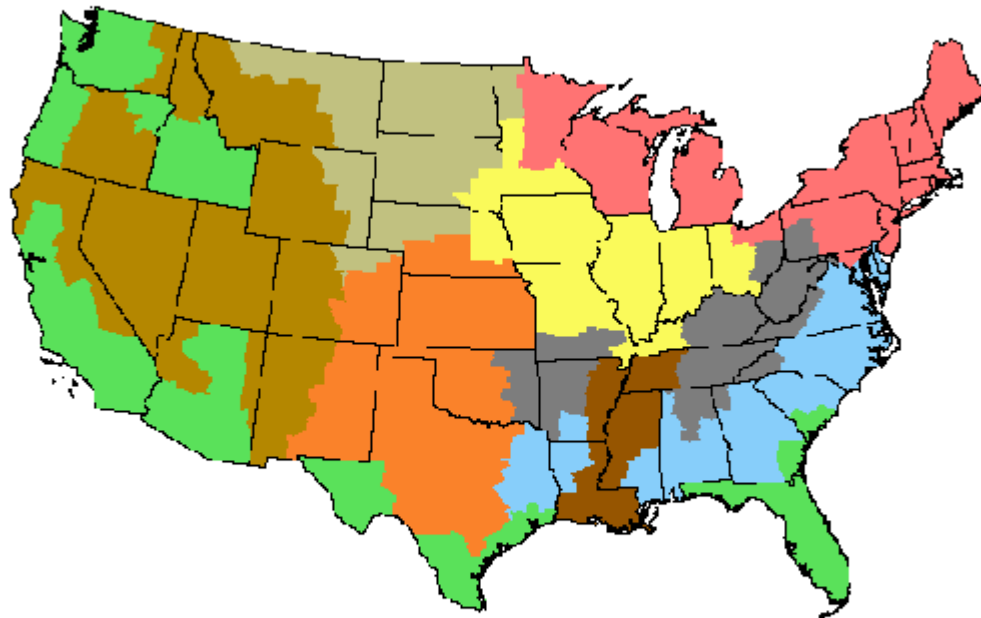
- Largest farms and smallest population.
- 5% of farms, 6% of production value, 17% of cropland.
- Wheat, cattle, sheep farms.

### Heartland

- Most farms (22%), highest value of production (23%), and most cropland (27%).
- Cash grain and cattle farms.

### Northern Crescent

- Most populous region.
- 15% of farms, 15% of value of production, 9% of cropland.
- Dairy, general crop, and cash grain farms.



### Fruitful Rim

- Largest share of large and very large family farms and nonfamily farms.
- 10% of farms, 22% of production value, 8% of cropland.
- Fruit, vegetable, nursery, and cotton farms.

### Prairie Gateway

- Second in wheat, oat, barley, rice, and cotton production.
- 13% of farms, 12% of production value, 17% of cropland.
- Cattle, wheat, sorghum, cotton, and rice farms.

### Mississippi Portal

- Higher proportions of both small and larger farms than elsewhere.
- 5% of farms, 4% of value, 5% of cropland.
- Cotton, rice, poultry, and hog farms.

### Southern Seaboard

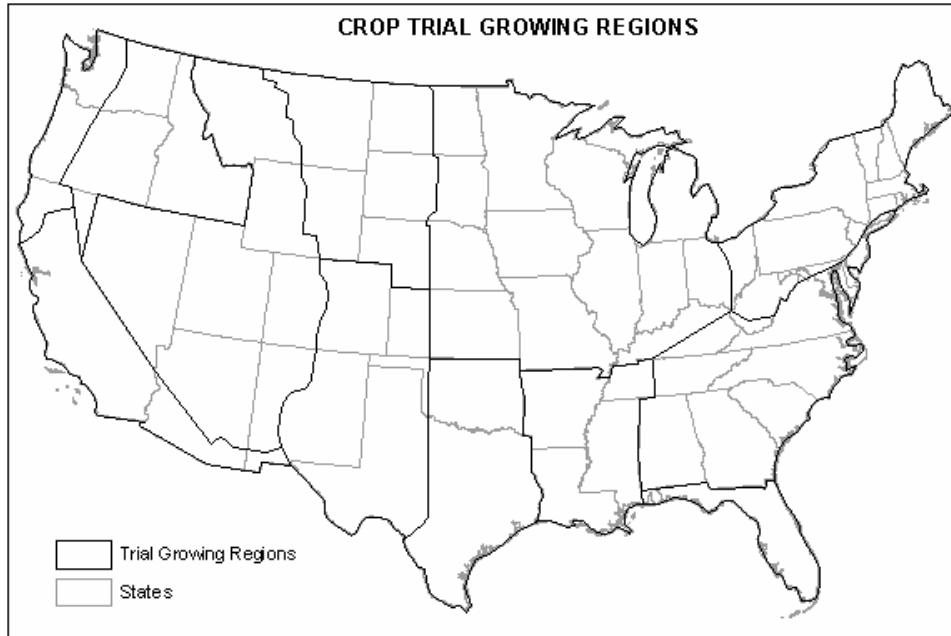
- Mix of small and larger farms.
- 11% of farms, 9% of production value, 6% of cropland.
- Part-time cattle, general field crop, and poultry farms.

### Eastern Uplands

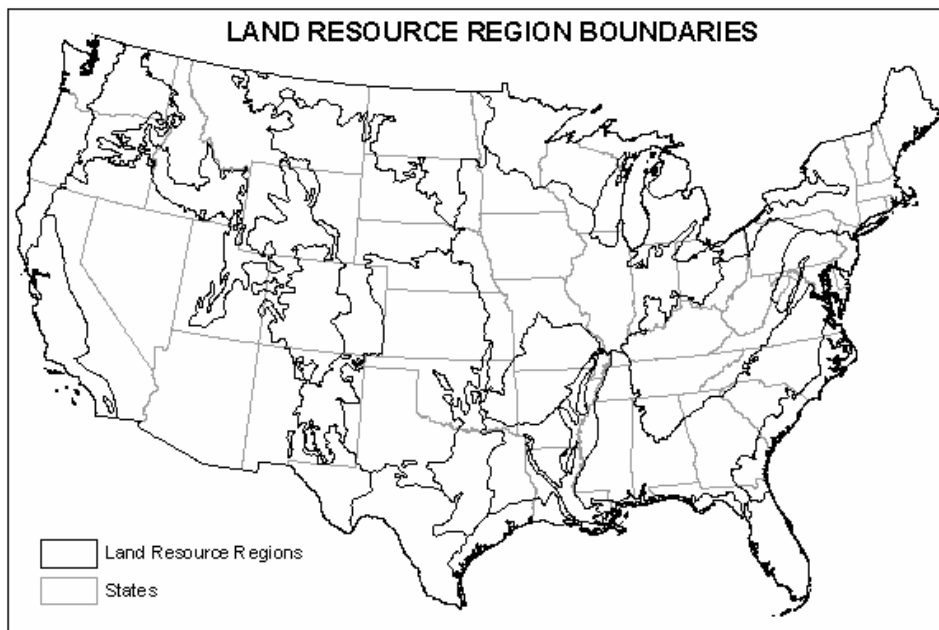
- Most small farms of any region.
- 15% of farms, 5% of production value, and 6% of cropland.
- Part-time cattle, tobacco, and poultry farms.

Figure 5.2 – US Farm Resource Regions

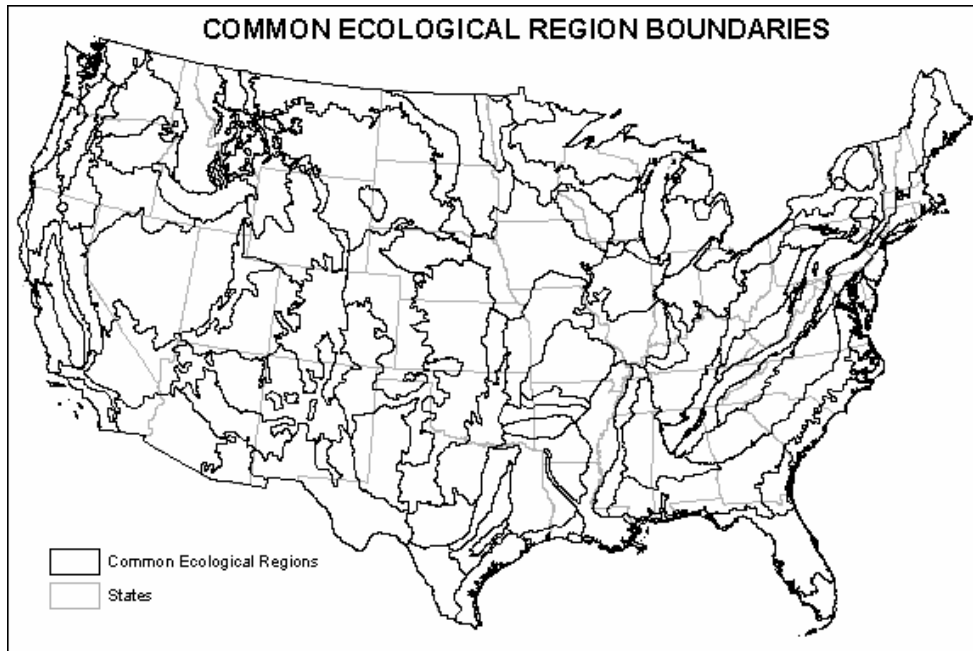




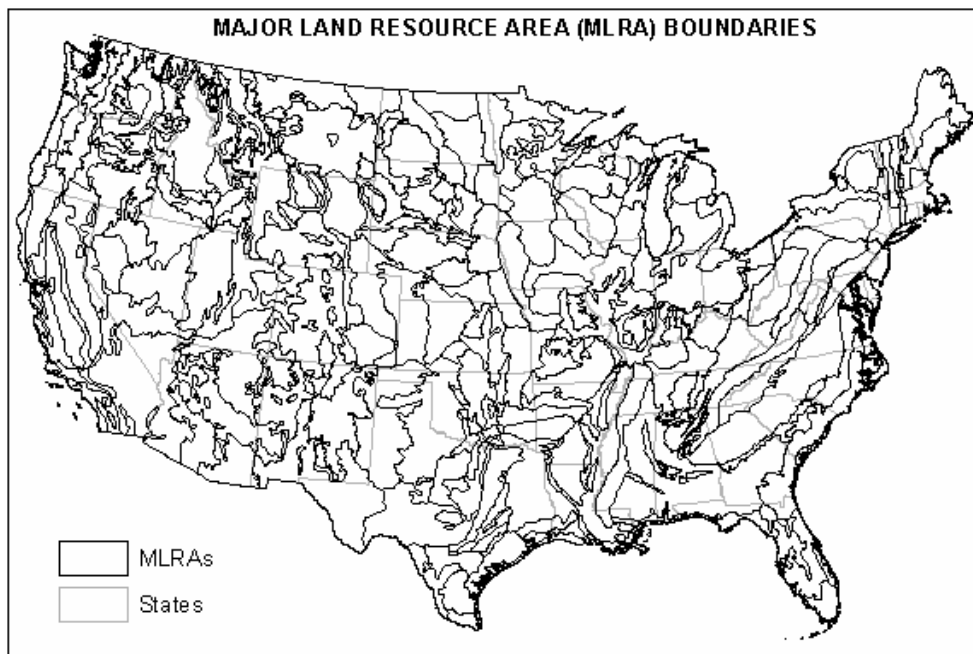
**Figure 5.3 – Crop Trial Growing Regions**



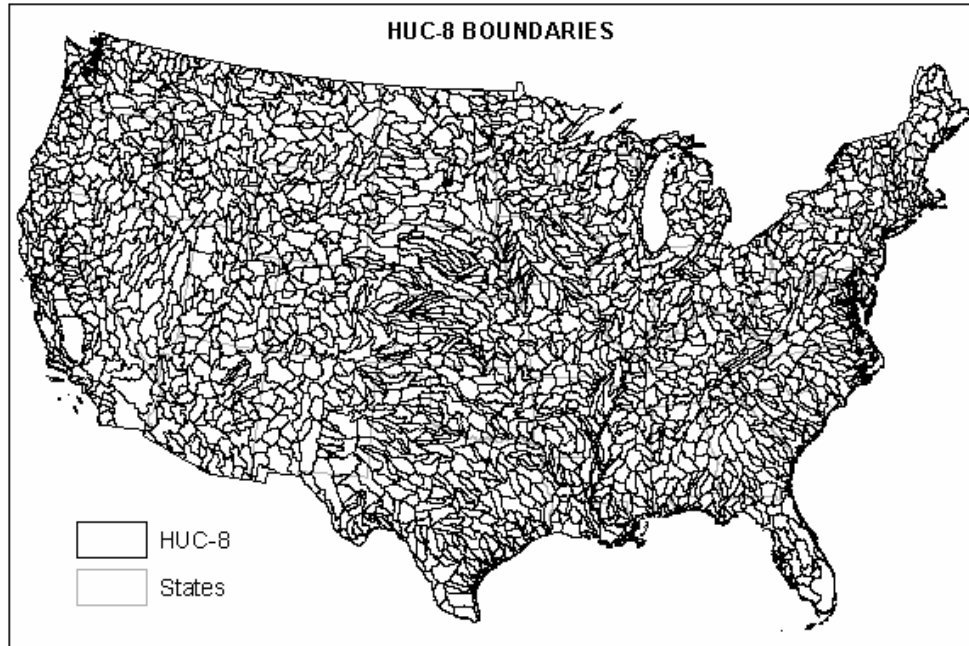
**Figure 5.4 – Land Resource Regions**



**Figure 5.5 – Common Ecological Regions**



**Figure 5.6 – Major Land Resource Areas (MLRA's)**



*Figure 5.7 – 8-Digit Hydrologic Units (HUC's)*

## **5.9 Calendarization of Residue Data Within CARES**

The residue profile for each individual will run 365 days from an individual's from birthday to his/her next birthday. The CARES Water Module attempts to preserve as much “temporal 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.

In order to ensure that no bias is introduced by the manner in which years of residue data are “sampled” 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.

## **5.10 Solution Chosen for CARES Water Module**

In this portion of the paper, the options implemented in the CARES Version 1.0. Water Module are summarized.

### **5.10.1 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.

### **5.10.2 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. This feature is not implemented in CARES Version 1.0.

### **5.10.3 Geographic Granularity**

The smallest geographic unit of analysis will be the State. Other units of organization are possible by matching individuals in the reference population to another spatial framework.

### **5.10.4 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

### **5.10.5 Dealing with Zeros**

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.

### **5.10.6 Calendarization Issues**

When sampling from multiple years of residue to fill a daily residue profile for an individual from birthday to birthday, all years in the sampled data will have equal probability of being selected. Once selected, the 365-day consumption profile will be assigned to an individual.

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.

### **5.10.7 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.

### **5.10.8 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 (see Figure 5.8).

### **5.10.9 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. Scaling factors should not be used to adjust residue levels when surrogating data.

### **5.10.10 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

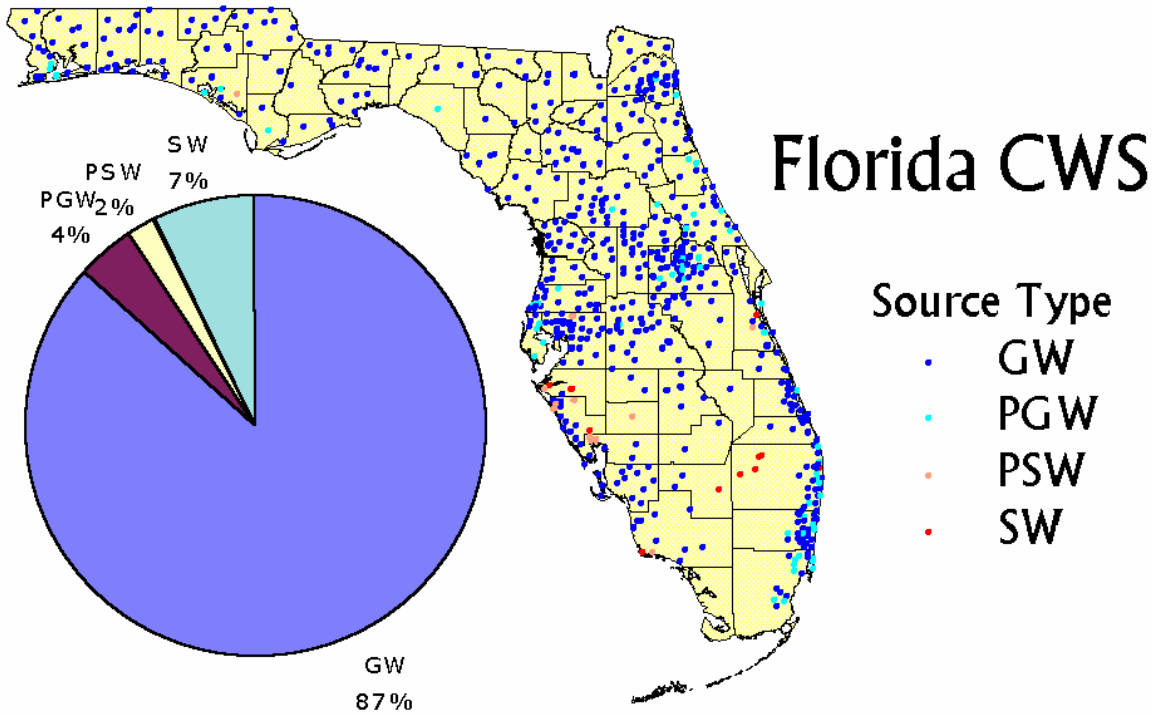
- Latitude/Longitude
- Hydrologic unit
- River vs. reservoir (for SW) Dug vs. drilled (for GW)
- Population Served
- Raw vs. Finished Water (do not apply treatment factors to finished water residues)
- Date
- Concentration of Analyte 1
- Concentration of Analyte 2
- Concentration of Analyte N

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.



**Figure 5.8 – 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.**





# 6. Aggregation and Cumulation

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# Chapter 6 – Aggregation and Cumulation

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## 6.1 Introduction

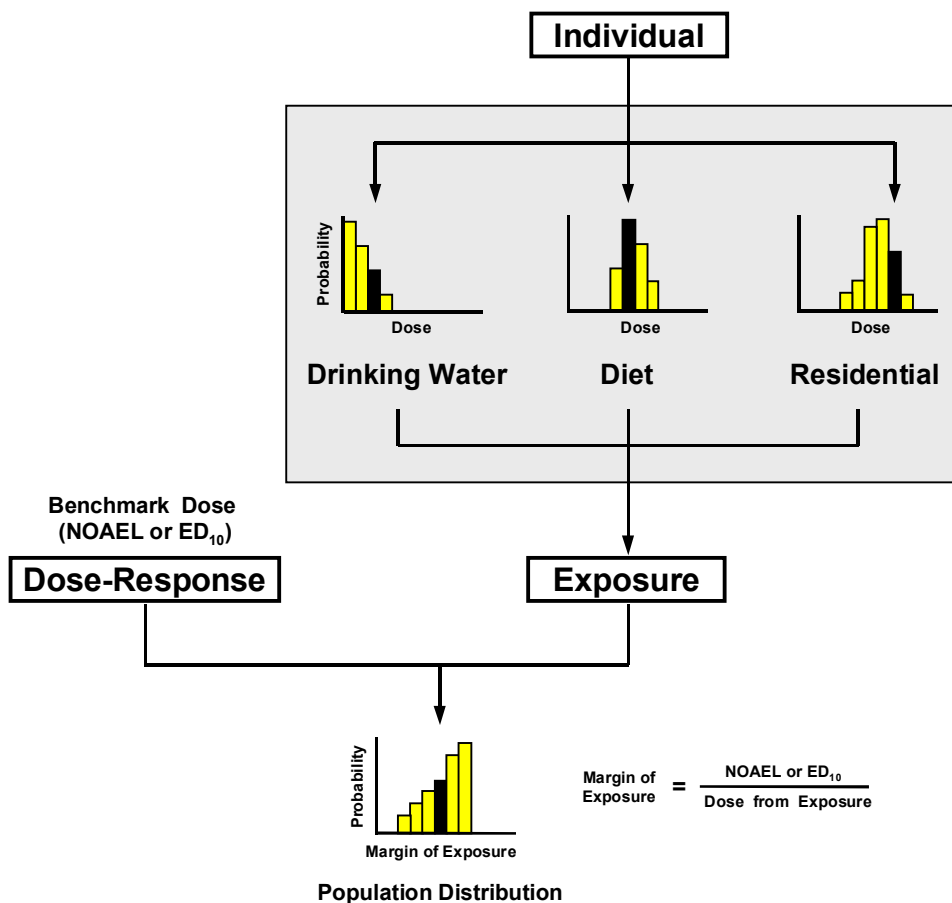
The Food Quality Protection Act (FQPA) of 1996 required that EPA consider aggregate exposure to a single pesticide when establishing pesticide tolerances and cumulative exposure to pesticides that share a common mechanism of toxicity. FQPA mandated that tolerances be set such that:

*“there is a reasonable certainty that no harm will result from aggregate exposure to the pesticide chemical residue, including all anticipated dietary exposures and other exposures for which there is reliable information.”*

## 6.2 Aggregate Risk Assessment

In aggregate risk assessments, the likelihood that an adverse health effect will occur as a result of exposure to a single chemical from all routes (oral, dermal, inhalation) and sources (dietary, water, residential) of exposure combined is determined. This is illustrated schematically in Figure 6.1. Prior to the passage of FQPA, EPA conducted independent exposure assessments for each source and did not combine doses across sources. Under FQPA, information about both exposure and hazard are brought together using a suitable risk metric to calculate the probability that an adverse effect will occur, as illustrated schematically at the bottom of Figure 6.1 where the margin of exposure is used to characterize risk.

Exposure is typically expressed as the daily dose based on either an externally applied dose or an internal dose achieved at a specific molecular or organ target. Hazard information is typically derived from animal toxicity studies and is usually expressed as a mg/kg/day dose. This can be any benchmark of toxicity selected by the risk assessor such as the no observed effect level (NOEL), the no observed adverse effect level (NOAEL), or the effective dose needed to produce a 10% response (ED<sub>10</sub>). Furthermore, the benchmark dose can be derived from any measure of toxicity such as an effect on survival, on body weight, on enzyme activity, or on molecular, biological or pathological processes. The benchmark dose can be derived from toxicity studies designed to evaluate the impact of the route of administration (e.g., oral, dermal, inhalation), specific effects on biological systems or processes (e.g., neurotoxicity, immunotoxicity, developmental toxicity), or the impact of different exposure durations (e.g. acute = 1 day, short term = 1-4 weeks, intermediate term = 4 to 13 weeks, or chronic > 13 weeks).



*Figure 6.1 – Aggregation of Exposure and Risk for a Single Chemical*

## 6.3 Temporal, Demographic and Spatial Consistency

### 6.3.1 Temporal Consistency within a Year

CARES incorporates temporality by using a “calendar-based” approach. Aggregation of the dose from exposure is done for each individual in the reference population for each day of the year being modeled by CARES. The year extends from January 1 through December 31. The CARES program also allows “moving average” time frames to be assessed for periods longer than a day. For example, the average dose during a succession of 30-day periods (e.g., Jan. 1 - Jan 30, Jan. 2 - Jan 31, Jan. 3 - Feb. 1, etc.) may be calculated and compared to an appropriate toxicity endpoint. The result would be a set of 365 thirty-day aggregate exposures or risk estimates. The first exposure period would be from Jan. 1 to Jan. 30. The second period would be from Jan. 2 to Jan. 31, and so on until the last exposure period of Dec. 31 to Jan. 29 was reached. This last period is created by “wrapping around” the exposure estimates from the end of the year to the beginning of the year.

Although CARES is able to accommodate food and water intake data and residential exposure data that are specific for each individual for each day of the year, the available food intake and residential databases generally do not possess this degree of temporal resolution.

The exception is the predicted 365-day, multiple-year pesticide residues in water from the PRZM/EXAM model. Therefore CARES employs several strategies to create the required 365-day exposure profile for each individual for each major source (dietary, water and residential) of exposure. These strategies are described in the chapters dealing with dietary (Chapter 3), water (Chapter 5) and residential (Chapter 4) exposure, as well as in the sections on the reference population (Chapter 2, Appendix B).

For example, a strategy in the residential exposure assessment to predict temporal profiles of product use across the year, is to use percent market share for each product and related exposure scenario (e.g., Lawn Care) in conjunction with the treatment intervals and conditional probabilities related to the likelihood of applying a product on a given day of the year (e.g., product use probabilities for each month of the year; probabilities for each day of the week; probabilities for professional versus consumer product application). In addition, probabilities related to co-occurrence of two or more products on the same day are assumed to be independent. Once a product use event has been predicted for a given household/individual, daily exposure estimates are calculated on the day of application and on subsequent days, until the residues in/on relevant exposure media (e.g., air, turf, and carpet) have declined or decayed to negligible levels. Thus, overlap of exposure associated with the use of two or more products could also occur during the time period of media-specific decay of one or more products. More refined strategies in temporal residential modeling include using parameter distributions and more specific temporal resolution of factors such as seasonal differences in the activity patterns and clothing configurations of individuals who may come in contact with pesticide residues in and around the home, and the use of temporal product use survey data (rather than predictive algorithms) and associated demographic information (see below).

### **6.3.2 Demographic Consistency**

The CARES program incorporates demographic characteristics into the aggregate risk assessment in a novel manner. The CARES program contains a reference population of 100,000 individuals randomly selected from the 1991 U.S. Census Public Use Microdata Sample (PUMS). Relevant characteristics of the reference population are known and are readily available to the risk assessor through the program. The age, gender, ethnicity, socio-economic status, and type of residence (apartment, house, etc.) of each individual in the reference population is known and easily referenced by the risk assessor.

In matching individuals from one survey to individuals in another such as the reference population, it is important to retain demographic consistency so that the daily aggregate dose for the individual is correctly calculated. For example, in the dietary module, a strategy was developed to match individuals in the CSFII population to individuals in the reference population who shared the same critical attributes (e.g. age, sex, and ethnicity). Once the critical matching is complete, the dietary data from the pool of matching individuals in CSFII are distributed across the 365 days such that survey data was matched to the individual's diet for that day within a maximum of 30 days (typically seven days, if possible). This matching process is described in detail in Chapter 2. This approach assured that

critical demographic consistency was maintained and that the data were distributed in an appropriate temporal manner (to accommodate season-related food consumption patterns).

Likewise, in a future version of CARES there will be a match to individuals in a temporal (12-month) pesticide use survey (e.g., Residential Exposure Joint Venture) with individuals in the reference population. In this case, location, housing type, household composition, and socioeconomic status are some likely attributes upon which the match may be based. Such matching will establish pesticide use profiles for individuals in the CARES reference population based on data from demographically similar individuals in the pesticide use survey.

### **6.3.3 Spatial Consistency**

In some situations it is important to take into account the part of the country within which the individual resides. For example, an individual in the reference population who lives in the state of Iowa, should be assigned pesticide residue data for water from sources that are modeled or monitored based on pesticide use, soil type and rainfall that is specific for that state. CARES Version 1.0 has a degree of spatial granularity (see Chapter 5) down to the level of the state. Opportunities exist in future versions of CARES to refine the level of spatial granularity that will be offered.

## **6.4 Methods for Aggregating Dose from Exposure**

CARES calculates a 365-day dose profile for each individual in the reference population or in the selected sub-population. This 365-day profile is subdivided into its constituent elements (e.g., chemical, source, and route of exposure). When an acute (single day) risk assessment is being conducted, one day is randomly selected from the 365 days available for each individual. This is repeated until a single day record has been selected for each individual. A cumulative distribution of daily doses is constructed ranging from the least to the most highly exposed individual. The percentile of the exposure distribution can thus be determined for the aggregate dose or for chemicals, source, or route sub-components. Furthermore, the relative contributions of chemical, source, or route to the total dose can also be calculated (see Chapter 7).

Aggregate risk can also be calculated using three approaches described by the EPA's Office of Pesticide Programs (OPP) describes in their 1999 Guidance document (EPA, 1999). These approaches are: (1) the Total Margin of Exposure (MOE) approach (traditionally EPA/OPP has used the MOE approach when aggregating risk from residential exposures to food and water exposures), (2) the Aggregate Risk Index (ARI) approach, and (3) the Hazard Index (HI).

The Total MOE approach is the preferred method for aggregating risk when the uncertainty factors for the different routes of exposure (oral, dermal or inhalation) are identical. The ARI approach is the preferred method for aggregating risk involving different uncertainty factors. The Hazard Index approach is described in the EPA guidance document (EPA, 1999) as being "used by other parts of the Agency" (i.e., branches other than OPP). Within CARES, the Point of Departure Index is used for either the ARI or the HI.

### Formula for the Margin of Exposure

$$MOE_{oral,dermal,inhalation} = \frac{BenchmarkDose_{oral,dermal,inhalation}}{Dose_{oral,dermal,inhalation}}$$

The Benchmark Dose (mg/kg) may be the NOAEL, ED<sub>10</sub> or other relevant measure of the toxicology endpoint describing the common mechanism of effect, and the Dose is the estimated dose (mg/kg) from the model for the specified route.

### Formula for Aggregate Margin of Exposure

$$MOE_{aggregate} = \frac{1}{\frac{1}{MOE_{oral}} + \frac{1}{MOE_{dermal}} + \frac{1}{MOE_{inhalation}}}$$

### Formula for the Aggregate Risk Index

The Aggregate Risk Index (ARI) is used when multiple MOEs must be aggregated, but different uncertainty factors have been applied to each individual MOE.

$$ARI = \frac{MOE_{calculated}}{MOE_{acceptable}}$$

The MOE<sub>acceptable</sub> is the Margin of Exposure incorporating the uncertainty factor(s) specified by the user and/or regulatory agency.

### Formula for ARI Aggregate

$$ARI_{aggregate} = \frac{1}{\frac{1}{ARI_{oral}} + \frac{1}{ARI_{dermal}} + \frac{1}{ARI_{inhalation}}}$$

The Hazard Index is a percent of the RfD and is calculated first by determining a Hazard Quotient (HQ) for each route or pathway (oral, dermal or inhalation) of exposure within each source (food, water or residential) of exposure.

### Formula for Reference Dose (RfD)

$$RfD = \frac{BenchmarkDose}{UF}$$

The Benchmark Dose (mg/kg) is typically based on the NOAEL, but the ED<sub>10</sub> or other relevant measure of the toxicology endpoint describing the common mechanism of effect, can be used. The UF is the Uncertainty Factor.

### Formula for the Hazard Quotients (HQ)

$$HQ = \frac{Exposure}{RfD}$$

Once a HQ has been calculated for each route of exposure, the routes are summed to give a HI.

### Formula for the Pathway Specific Hazard Index (HI)

$$HI_{\text{food, water or residential}} = HQ_{\text{oral}} + HQ_{\text{dermal}} + HQ_{\text{inhalation}}$$

The individual HI's for each source of exposure are summed to give a total HI:

### Formula for the Total Hazard Index

$$HI_{\text{Total}} = HI_{\text{food}} + HI_{\text{water}} + HI_{\text{residential}}$$

In the absence of uncertainty and safety factors, the three approaches described above are equivalent. Due to ease of use and familiarity, the CARES model will aggregate risk for a single pesticide using the MOE approach. Using this approach, the NOAEL or BMD is divided by the sum of exposure from food, drinking water and residential sources to yield an MOE.



## 6.5 Summary of CARES Aggregate Approach

From the previous discussion it is clear that four elements stand out as representing fundamental changes in the approach used in aggregate risk assessment required by FQPA. Temporal, demographic and spatial components have been added to the risk assessment and parameters can be point estimates or more likely are reflected by probability distributions.

These elements in an aggregate risk assessment allow the risk assessor to emphasize the principle that exposure occurs to individuals, rather than hypothetical populations. CARES uses either a deterministic method (in the lower tier assessments) or a probabilistic method (Monte Carlo, in the higher tier assessments) to determine exposures for each individual. The inclusion of these four elements, and the emphasis on individuals, is in accordance with EPA aggregate risk assessment guidance (EPA, 1999). These exposures are ultimately combined into an assessment of the entire population or defined sub-populations.

While Individuals within the reference population are real people, some of the attributes assigned to them, such as food consumption patterns, are based upon data from like individuals in other surveys (CSFII/FCID). Because the CARES model has the ability to examine exposure using demographic, spatial and temporal characteristics, the individuals have characteristics that are consistent with, and representative of, living persons. CARES performs an aggregate risk assessment for one person, then it completes a risk assessment for another, and another, until an entire reference population has been assessed. The aggregate assessment of the reference population is thus a distribution of exposures of all individuals in the population.

For each individual, aggregation is demographically, spatially and temporally consistent. The demographic, spatial and temporal elements are linked back to each individual during the aggregate risk assessment so that individual exposures more closely reflect exposures to a single person at the same time.

## 6.6 Cumulative Risk Assessment

Cumulative risk is defined as the likelihood of an occurrence of an adverse health effect resulting from exposure to multiple chemicals acting through a similar mode of action. EPA has traditionally considered exposure from single pesticides individually, with no attempt to combine exposures from pesticides with toxicologically similar modes of action. FQPA requires that EPA consider cumulative exposure to a pesticide when establishing pesticide tolerances.

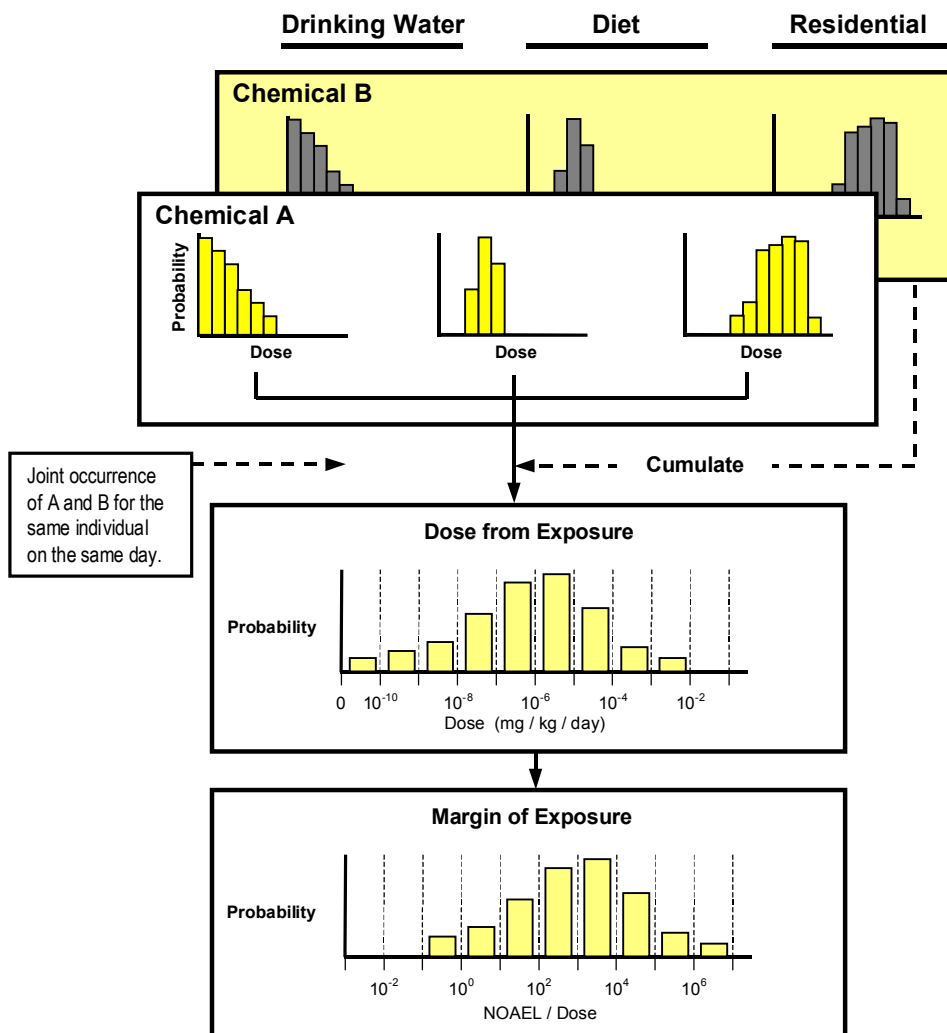
The first step in performing a cumulative risk assessment is to identify a common mechanism group. This involves selecting pesticides that display toxic endpoints associated with a common mode of action. Once a group of pesticides with a common mode of action is selected, the toxic potencies for the common effect are then estimated. The U.S. EPA has chosen to use a Benchmark Dose - most often described by the effective dose associated with a 10% response (BMD<sub>10</sub>), rather than a NOAEL or LOAEL, as their measure of toxic potency in the cumulative risk assessment process for organophosphate pesticides (SAP, 2002). EPA has developed a dose-response model to calculate the BMD for each chemical and for each route of exposure.

Once toxic potencies are determined for each pesticide in the common mechanism group, an Index Chemical is selected from the group. The purpose of the Index Chemical is to provide a point of reference from which the toxic potencies for all chemicals within the group can be standardized. With the Index Chemical as a point of reference, Relative Potency Factors (RPF) can be calculated. The RPF is calculated using the following formula:

#### Formula for RPF

$$RPF = \frac{\text{BenchmarkDose}_{\text{Chemical}_{\text{Index}}}}{\text{Dose}_{\text{Chemical}_n}}$$

The Benchmark Dose<sub>Chemical</sub> Index is the ED<sub>10</sub>, or other selected toxicology endpoint value describing the index chemical, and Dose<sub>Chemical n</sub> is the equivalent ED<sub>10</sub>, or other selected toxicology endpoint describing the *n*th Chemical. The RPF is multiplied by the exposure to chemical *n* to determine the Exposure Equivalents in terms of the Index Chemical. Cumulative exposure is the sum of all the Exposure Equivalents for each chemical in the common mechanism group, as shown in Figure 6.2.



**Figure 6.2 – Cumulative Exposure and Risk Assessment: Multiple Chemicals**

Alternatives to the index chemical approach are available within CARES if the risk assessor does not wish to establish an index chemical or to estimate toxicologically equivalent dose. These alternatives require the following three additional equations to calculate cumulative risk. Note that these are variants of the aggregate risk equations described above.

### Formula for the Cumulative Margin of Exposure

$$MOE_{Cumulative} = \frac{1}{\frac{1}{MOE_{ChemicalA}} + \frac{1}{MOE_{ChemicalB}} + \dots + \frac{1}{MOE_{ChemicalN}}}$$

### Formula for the Cumulative Risk Index

$$CRI = \frac{1}{\frac{1}{ARI_{ChemicalA}} + \frac{1}{ARI_{ChemicalB}} + \dots + \frac{1}{ARI_{ChemicalN}}}$$

### Formula for the Cumulative Hazard Index

$$HI_{Cumulative} = HI_{ChemicalA} + HI_{ChemicalB} + \dots + HI_{ChemicalN}$$

## 6.7 References

EPA, 1999. *Guidance for Performing Aggregate Exposure and Risk Assessments*. EPA/OPP, October 29, 1999.

EPA. 2002. Comparison of Acute NOAELs and Benchmark Doses for Female Brain Cholinesterase Inhibition. 6 pages. January 25, 2002

# 7. Contribution and Sensitivity

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# Chapter 7 – Contribution and Sensitivity

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## 7.1 Introduction

Assessments conducted using Monte Carlo simulation methods create exposure and risk distributions for individuals and groups of individuals (sub-populations). The relative contribution to the total exposure or risk may be different for different routes or sources, or sub-components of these. It is essential that a risk assessment tool have a utility that allow the user to determine the relative contributions to exposure and risk derived from different sources, routes or sub-components. The tool must also be able to summarize exposure and risk for sub-populations of interest that may include various demographic or geographic characteristics. This type of analysis is called contribution analysis and the process of determining the relative contributions has been called within the CARES documentation a drill-down procedure.

Sensitivity analysis is a procedure used by risk assessors to evaluate changes in the magnitude of exposure or risk that occur as a result of systematic changes in the magnitude of an identified key input parameter. Typically the risk assessor selects an input parameter to test, for example the frequency, duration or extent of hand to mouth transfer of pesticide residues for children playing on treated turf. In this case the assessor may run a simulation with a selected subset of input parameters and compare the result of the analysis to another simulation using a different subset of input parameters. This type of analysis helps the risk assessor understand the major risk drivers and may indicate where refinement of assumptions concerning input parameters could have the largest impact.

Uncertainty analysis is a special case of sensitivity analysis where the risk assessor is unsure of what value or distribution of values an input parameter may take. For example, in the example given in the previous paragraph, there may be anecdotal evidence to suggest that the frequency of hand to mouth contact in young children is very high but it is equally plausible that hand to mouth contact frequency is lower. Thus the risk assessor is uncertain about the frequency of hand to mouth contact in children. Comparing the results of Monte Carlo simulations where two or more different sets of assumptions concerning hand to mouth contact are made allows the assessor to quantify the effect of uncertainty about an input parameter on the risk assessment result.

Capability exists within CARES to conduct a range of Contribution/Sensitivity/Uncertainty (CSU) analyses. In addition, a stand-alone utility is provided with CARES Version 1.0 that is a prototype for additional CSU functionality planned for future incorporation into CARES. A routine has been written and is also included that allows the user to convert CARES output files into the format required by the prototype CSU program.

## 7.2 Contribution Analysis

CARES calculates 365-day exposure profiles expressed as mg/kg/day doses arising from major sources (dietary, water and residential use) and routes (oral, dermal, inhalation) of exposure for each individual with the reference population or subsets thereof. The Contribution/Sensitivity/Uncertainty (CSU) utility available within CARES provides the user with a tool for viewing the results of the Monte Carlo analysis. The prototype of the enhanced CSU also provided with Version 1.0 expands this capability. The enhanced CPU will be part of the final public release version of CARES.

### 7.2.1 Strategies for Conduction Contribution Analysis

Complex Monte Carlo simulations comprised of multiple chemicals, sources, routes, and scenarios for a large array of sub-populations and geographies take time to set up and run. In order to spare computer processing time and permit the user to get a sense of the relative contribution from multiple chemicals in a cumulative risk assessment and the contribution to exposure from multiple sources and routes and scenarios of exposure, it is recommend that many small simulations be run. This is illustrated schematically in the drill-down procedure shown in Figure 7.1. Using this strategy, the user could select a small sub-population of interest and ask a series of sequential questions by conducting a number of simulations. For example, the user may determine which chemical provides the largest contribution to the total Toxicologically Equivalent Dose (TED) aggregated across all sources and routes. The assessor might then determine for each chemical, which source or route is the major risk driver. Once this is known the user could determine for each chemical within the major source (e.g. dietary) which food form contributes the most or within a route (e.g. oral) which scenario (e.g. dietary or residential oral ingestion contributes the most to the total TED.

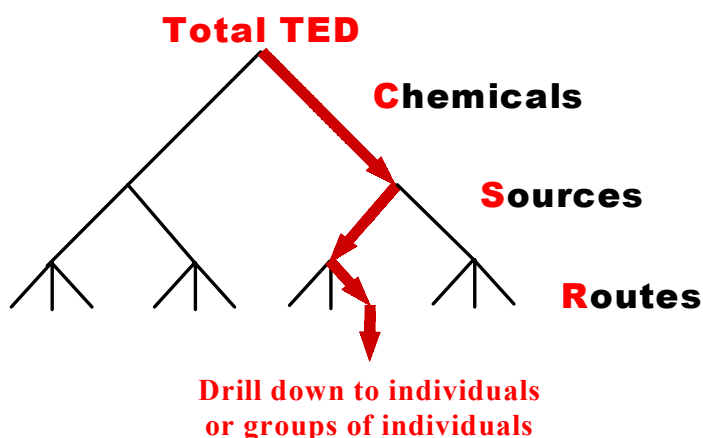


Figure 7.1 – Drill-Down Strategy for Conducting a Contribution Analysis



## 7.2.2 Components of a Contribution Analysis

### 7.2.2.1 Distribution of Daily Doses for Individuals

The CSU within CARES Version 1.0 permits the user to view exposure contributions from chemicals, routes and sources for each individual. This can be done for exposure durations ranging from a single day through one year. The 365-day exposure profile for any individual within the reference population can be viewed by the CSU. Furthermore, the records of the individuals can be sorted in the data explorer to permit the user to identify and view exposure profiles of the least or most highly exposed individuals. A sample record of such output from the CSU within CARES is illustrated in Figure 7.2. The comparable view from the prototype enhanced CSU is shown in Figure 7.3.

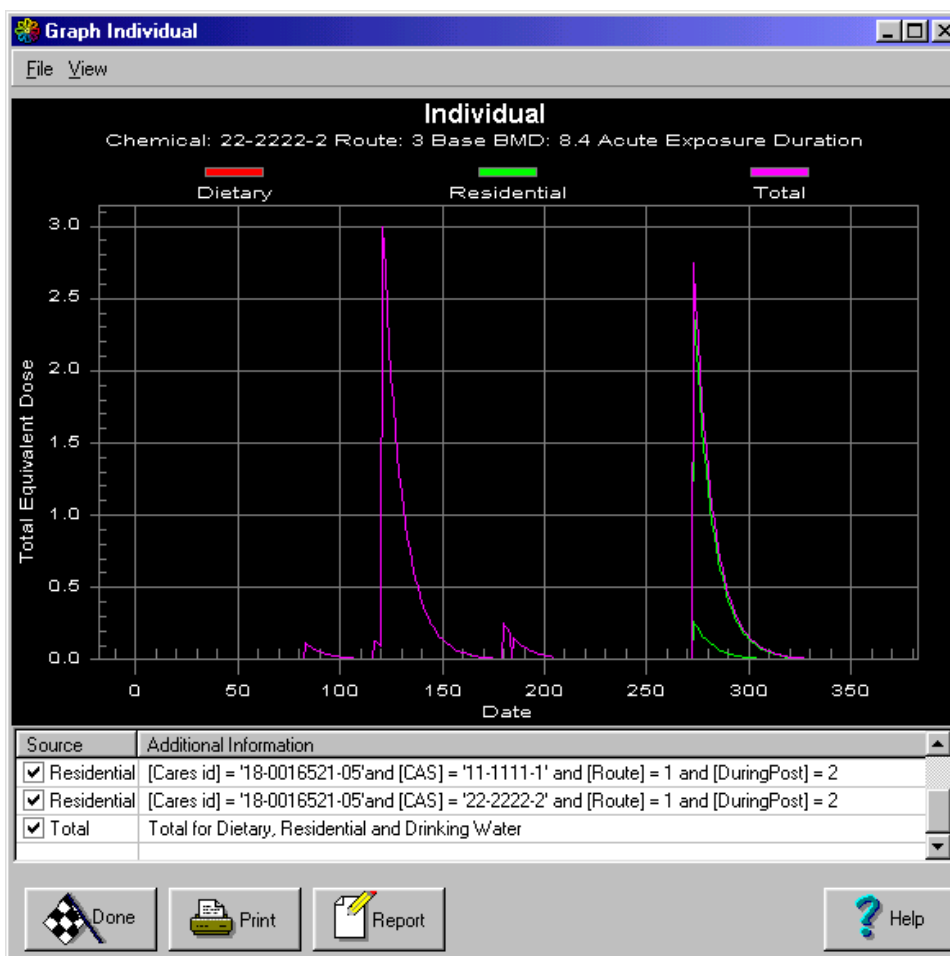
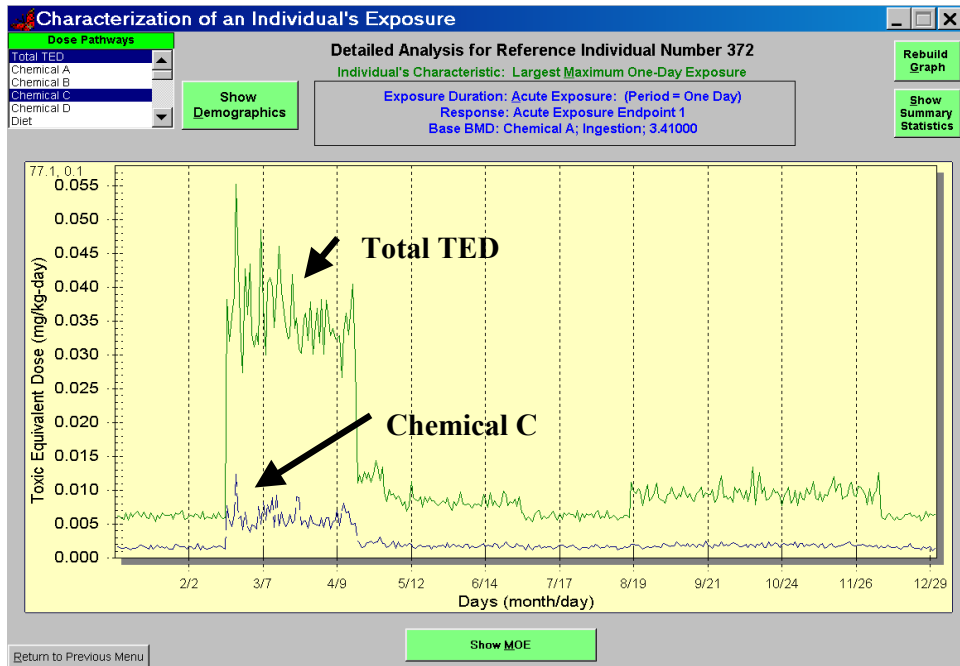


Figure 7.2 – CARES CSU Output – Individual Contribution Analysis



**Figure 7.3 – Prototype CSU Output – Individual Contribution Analysis**

#### 7.2.2.2 Distribution of Aggregated Daily Doses for Sub-populations

The CSU within CARES Version 1.0 permits the user to view the aggregate or cumulative contribution to exposure or risk for multiple chemicals, sources or routes. This is illustrated for the CSU within CARES in Figure 7.4 and in Figure 7.5 for the enhanced prototype CSU. This facility is essential for conducting the detailed drill-down contribution analysis described in section 7.2.1. Furthermore, since sub-populations can be run independently, it is possible to address the relative exposure and risk for different sub-populations of individuals using this utility.

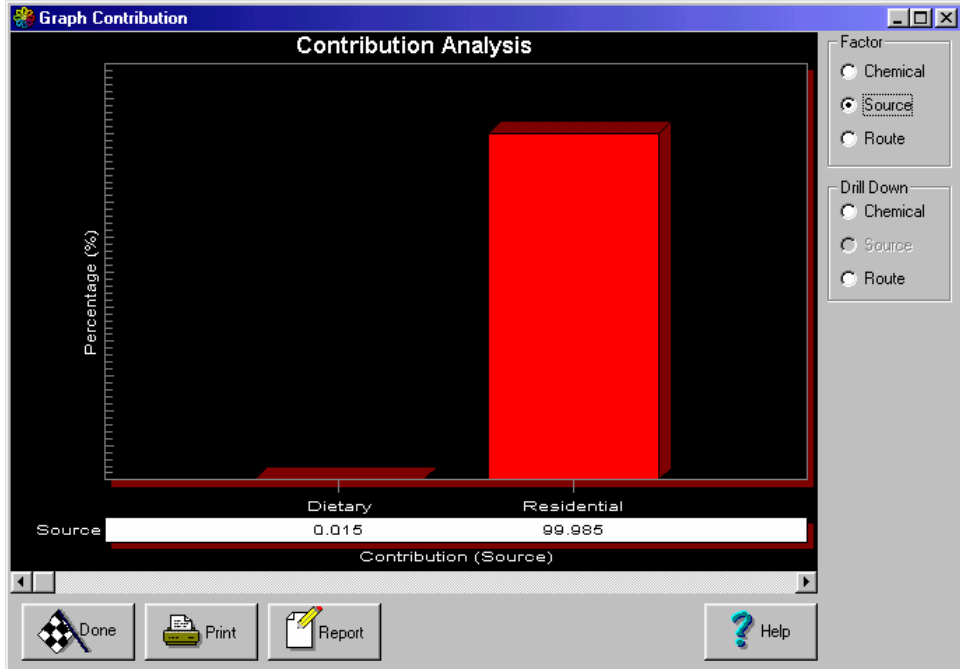


Figure 7.4 – CARES CSU Output – Group Contribution Analysis

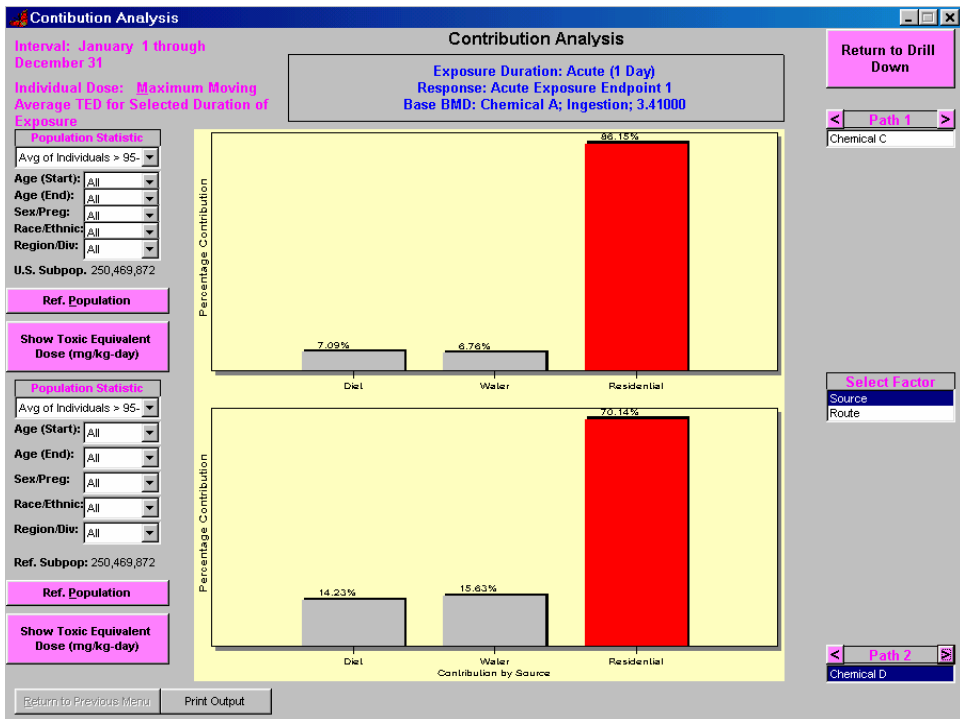


Figure 7.5 – Prototype CSU Output – Group Contribution Analysis

### 7.2.2.3 Demographic Characterization of Dose/Risk for Sub-Populations

In contribution analysis, it is not only important to be able to identify major risk drivers, but to be able to summarize them statistically. Thus for example it is common for the risk assessor to want to know the fraction of individuals who may exceed a defined standard of safety at different percentiles of the risk distribution such as the 90th, 95th, 99th or 99.9th percentile. In addition, the risk assessor may want to know what set of factors lead to an individual or a group of individuals being the most highly exposed. This may include an analysis of temporal or spatial factors that may contribute to exposure. These features have not yet been implemented in CARES Version 1.0 but work continues using the prototype CSU as a guide.

As a temporary solution, however, and as mentioned previously, we have included a utility that converts CARES output files into a form that can be read by the prototype CSU included on the accompanying CDs. The following is an illustration of the functions described above as executed by the prototype CSU.

Figure 7.6 displays a graphical representation of the Toxicological Equivalent Dose (TED) for Chemical A at different percentiles of the risk distribution for all age groups. Figure 7.7 illustrates that the same data can be viewed as box and whisker plots for all age groups combined and for selected age groups (e.g., 11-6 year) while Figure 7.8 presents the numerical data for a selected individual. Similar graphs could have been displayed for different sources or routes of exposure, or for different sub-populations.

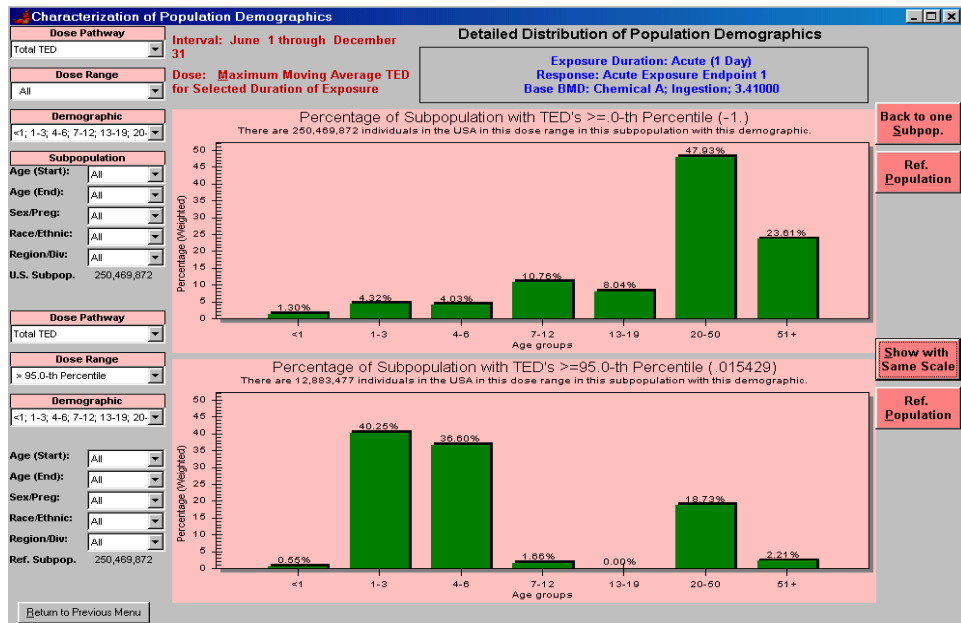


Figure 7.6 – Prototype CSU Output – Demographics / Percentiles

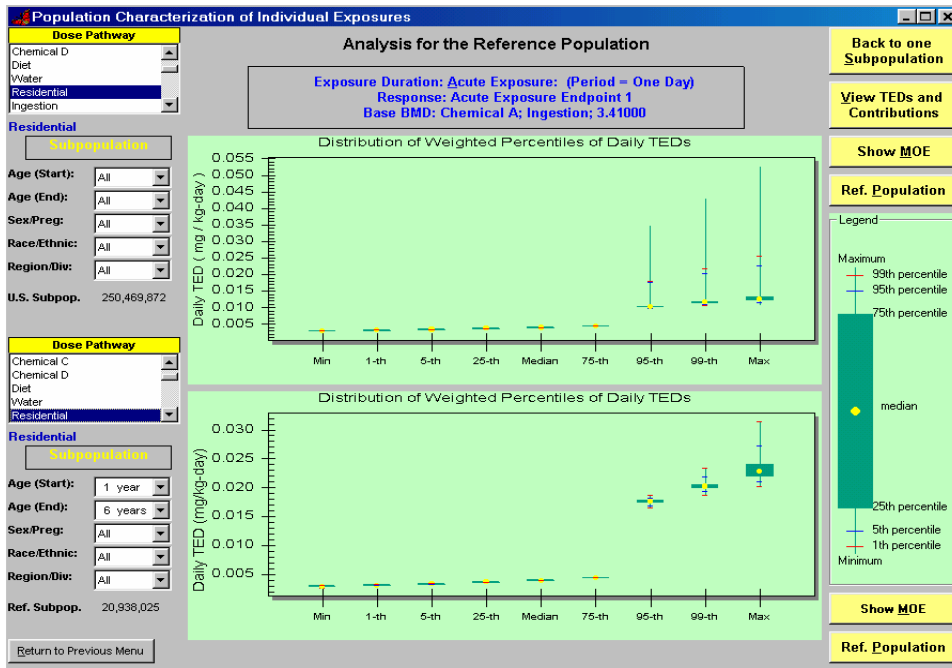


Figure 7.7 – Prototype CSU Output – Demographics / Box and Whisker Plots

**Characterization of an Individual's Exposure**

**Detailed Analysis for Reference Individual Number 372**  
 Individual's Characteristic: Largest Maximum One-Day Exposure

Exposure Duration: Acute Exposure: (Period = One Day)  
 Response: Acute Exposure Endpoint 1  
 Base BMD: Chemical A; Ingestion; 3.41000

Selected Items (double click an item or row to display the corresponding distribution of the daily toxic equivalent doses)	Daily TED: Minimum	Daily TED: 5-th Percentile	Daily TED: 10-th Percentile	Daily TED: 25-th Percentile	Daily TED: 50-th Percentile	Daily TED: 75-th Percentile	Daily TED: 90-95th Percentile
Total TED	0.005345	0.005780	0.005928	0.006511	0.008633	0.010476	
Chemical A	0.001521	0.001742	0.001851	0.002121	0.003896	0.005375	
Chemical B	0.001116	0.001382	0.001481	0.001614	0.001855	0.002226	
Chemical C	0.001088	0.001330	0.001451	0.001577	0.001805	0.002095	
Chemical D	0.000717	0.000817	0.000858	0.000948	0.001049	0.001207	
Diet	0.000749	0.000933	0.001003	0.001103	0.001262	0.003646	
Water	0.000760	0.000908	0.000965	0.001078	0.001217	0.001425	
Residential	0.002893	0.003349	0.003463	0.003652	0.003944	0.004352	
Ingestion	0.002691	0.003205	0.003343	0.003745	0.005903	0.006917	
Dermal	0.000800	0.001073	0.001149	0.001282	0.001419	0.001731	
Inhalation	0.000855	0.001016	0.001064	0.001189	0.001342	0.001574	

Figure 7.8 – Prototype CSU Output – Demographics / Tabulated Data

## 7.3 Sensitivity Analysis

As indicated in the introduction to this chapter, sensitivity analysis is a method of comparing the results of two or more Monte Carlo simulations that systematically change the magnitude or distributional characteristics of selected input parameters. The prototype CSU provided with CARES has the ability to display and compare the results of two simulations as shown in Figure 7.6 to Figure 7.8. This utility permits the user to evaluate the exposure and risk distributions for the same chemical, source, route and sub-population of interest while only changing one key input parameter. Differences in selected characteristics of the risk distribution (e.g. mean, mode, or some percentile of the risk distribution), therefore reflects the sensitivity of the risk distribution to discrete changes in the input parameters. A series of similar such analyses, in composite reflect a comprehensive sensitivity analysis that would permit the risk assessor to prioritize resources for additional data acquisition in order to refine risk or perhaps to develop a strategy for risk mitigation.

## 7.4 Uncertainty Analysis

As indicated in the introduction, uncertainty analysis is just a special case of a sensitivity analysis where the risk assessor wishes to quantify the effect of parameter uncertainty in terms of the risk distribution. Again the risk assessor must conduct a series of simulations and compare the results with each other as described in Section 7.3. The prototype CSU utility provided with CARES and illustrated in Figures 7.6 to 7.8 has this ability.

## 7.5 Summary

Previous chapters have described in general terms how an aggregate and cumulative risk assessment is conducted within CARES. This chapter lays out a strategy for conducting contribution, sensitivity and uncertainty analysis within CARES and by using a prototype utility provided with CARES.

We have developed or implemented within CARES Version 1.0 many of the critical features needed by the risk assessor to evaluate the results of a complex aggregate or cumulative risk assessment. Limitation on processing time and files storage requirements still need to be defined but we have suggested strategies that will permit the user to identify and quantify risk drivers using CARES. Additional development continues and feedback on the usefulness and the direction that CARES has taken to date will be appreciated. Feedback forms are provided in Chapter 8.

# 8. Testing and Validation

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## ***Contributing Authors***

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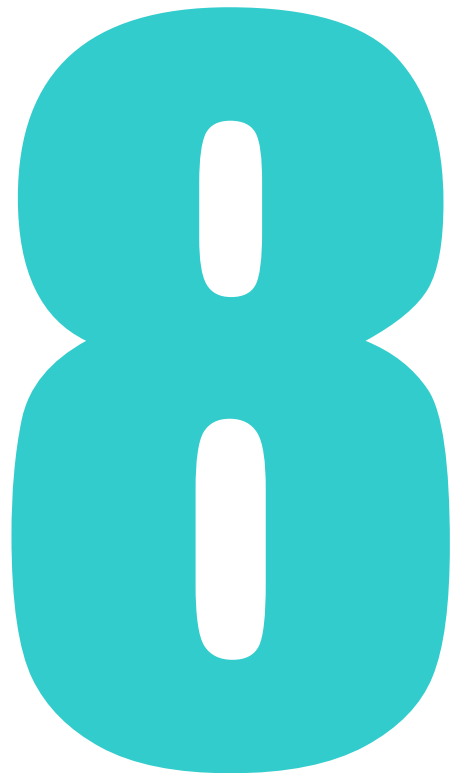
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# Chapter 8 – Testing and Validation

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## 8.1 CARES Validation Plan

A Validation Plan has been written that outlines all the required steps needed to produce a validated CARES software package. This plan (see Appendix F) defines nine types of validation categories. The first five categories cover verification, which is defined as software testing that ensures the computer code accurately represents the algorithms and solves the equations upon which it is based:

1. Test Data Sets
2. Unit Testing
3. Individual Module Testing
4. Integrated Module Testing
5. System Testing

The plan defines four additional types of validation categories:

6. Program Validation
7. Model Validation
8. Model Comparison
9. Process Validation

Some example validation projects are provided for each category to illustrate the type and scope of work needed. Thus, the Validation Plan outlines a broad coverage of testing and verification, and validation topics that is both flexible to meet the needs of the various CARES modules and satisfy broader validation requirements.

The Validation Plan (Appendix F) also includes three forms for use in tracking and managing validation activities:

- **CARES Feedback and Change Form** - Documents and tracks all testing, feedback, bugs, and subsequent changes. To be completed by all testers and returned to the CARES Technical Team.
- **CARES Validation Project Form** - Describes the exact Validation Project to be performed and includes tracking number, management information (who, where, when), and project description (objective, scope, deliverables).
- **CARES Validation Project Report** – A reporting and results form including details of the objectives, methods, and results of the completed Validation Project. The report may include appendices or reference other documentation that fully describe the project results.

The availability of the Validation Plan and the ultimate documentation of completed validation projects fulfill a necessary component in the system life-cycle documentation scheme shown in Figures 1.12 and Table 1.13 (Chapter 1).

## 8.2 CARES Version 1.0 Feedback

Several preliminary (alpha) versions of the CARES program were issued prior to CARES Version 1.0. These were prepared specifically for testing, developmental inputs, and prototype evaluation. They are not intended to demonstrate complete working software with all functional requirements met. The CARES Technical Team and one key future user reviewed these for coding errors, design and functionality issues, user-friendliness, interface issues, etc. Twenty-one sets of feedback (from one to 17 issues each) were received and processed as of January 1, 2002. All fatal errors were corrected, and the remaining issues were prioritized for correction and incorporation into CARES Version 1.0 or as potential enhancements for a future version.

The same CARES Feedback and Change Form will be available with all future releases to ensure all user feedback will be acquired and prioritized.

## 8.3 Validation Strategies

Validation projects will be completed for each module in CARES specific to the nine validation categories listed above. Table 8.1 lists the probable areas that will be covered in the validation. Because of limited resources and time constraints all validation steps have not been covered at the time of publishing this manual. Blank cells in the matrix will be defined at a later time, as well as some cells changing as more validation is completed.

**Table 8.1 – Validation Matrix**

Validation Category	Population Generator	Module	Residential Module	Water Module	Ag/Cu
<b>Verification</b>					
1. Test Data Sets	Ref Population itself	Chem A, B, Market basket	4 Workshop scenarios	3 residue sets; 3 chemicals	All previous
2. Unit Testing	by infoscientific.com				
3. Individual Module Testing	n/a	W/ output from spreadsheet	Lawn Care Stats	W/ output from spreadsheet	
4. Integrated Module Testing	n/a	W/ output from CSU		W/ output from CSU	
5. System Testing					
5a. Functional Testing	n/a	using test data sets		all menu options tested; 3 residue sets	
5b. Stress Testing	n/a	low, hi, etc.		3 residue sets	
<b>Other Validation</b>					
6. Program Validation	Documentation of standards & usability by infoscientific.com				
7. Model Validation	compare to U.S. Census	compare consumption data			
8. Model Comparison	n/a	compare to DEEM			
9. Process Validation	Life Cycle Documentation by Summit Research Services				

The Population Generator is not itself a CARES module, although the output from this software is the Reference Population database that is included in and used by CARES. Therefore, the type of validation needed here is to ensure that the population output from CARES accurately reflects the U.S. Census population data upon which the Population Generator is based. This is covered under category 7 Model Validation).

For the Residential Module, one possible data set for validation is the four scenarios from the "Scientist-To-Scientist Model Comparison Meeting of Residential Aggregate Human Exposure Models" (October, 10-11 2001, U.S. EPA Environmental Research Center, Research Triangle Park, NC). If these are not available, datasets similar to the ones proposed for the other modules will be used. Validation has been started using a Lawn Care scenario with the residential case study that was supplied with a preliminary version of CARES. Summary statistics were estimated by the CARES statistics function, and the output files were exported and compared to those obtained with an independent statistics program.

The specific strategies for validating the Dietary Module and the Water Module are included below. Strategies for Residential, CSU (Contribution and Sensitivity), and Ag/Cu (Aggregation and Cumulation) are being drafted with similar steps.

### 8.3.1 CARES Dietary Module Validation Strategy

The following provides a listing of planned or in-progress Validation Projects for each of the applicable Validation Categories (listed in section 8.1 and described in Appendix F). Additional projects may be added later.

#### ► Test Data Sets

<b>Project: Case Study Tutorial (CARES User Guide)</b>
The purpose of the first two Case Study Tutorials in the CARES User Guide is to show how a user would estimate dietary exposure for a certain sub-population. The test data sets and step-by-step tutorial procedures in the CARES User Guide will be used to perform <i>functional testing</i> on the required input routines, Dietary Module, and the CSU Module.

#### ► Individual Module Testing

For testing of the Dietary Module by itself, output will be examined from the CARES output files (Notitia data grid spreadsheets).

<b>Project: Baseline Setup and Simple Case Run</b>
<ol style="list-style-type: none"><li>1. Construct a one-person population who eats a food (apples) on many days of the year.</li><li>2. Construct a residue data set for apples that contains a single residue and no processing factors.</li><li>3. Run CARES dietary module.</li><li>4. "Hand" calculate daily exposure for that person.</li><li>5. Compare with CARES dietary module output.</li></ol>

**Project: Processing Value Check**

1. Use person and residue input files from Baseline Setup (see above).
2. Add processing factor of 2 for apples.
3. Compare CARES output with hand-calculated total.

**Project: Test for Extremely Low Values**

1. Use person and residue input files from Baseline Setup (see above).
2. Set residue values for apple to 0.000001.
3. Compare CARES output with hand-calculated total.

**Project: Test for Extremely High Values**

4. Use person and residue input files from Baseline Setup (see above)..
5. Set residue values for apple to 10000.
6. Compare CARES output with hand-calculated total.

**► Integrated Module Testing**

For integrated module testing, output is taken from the CSU Module at the end of the calculation pathway, rather than from the intermediate output from the Dietary Module alone.

**Project: Test with Multiple Food Forms**

1. Use person and residue input files from Baseline Setup (see above).
2. Change residue input files to include all food forms for apples.
3. Hand-calculate daily exposure for the single person for one year.
4. Compare with CARES dietary module results.

**Project: Test with Multiple Foods**

1. Use person and residue input files from Baseline Setup (see above).
2. Change residue input files to include multiple foods.
3. Hand-calculate daily exposure for the single person for one year.
4. Compare with CARES dietary module results.

**Project: Test with Multiple People**

1. Create population of 10 persons.
2. Use single food (apple) database.
3. Hand-calculate daily exposure for the group for one year.
4. Compare with CARES dietary module results.

**Project: Test with Multiple Residues**

1. Use the single person population from the Baseline Setup (see above).
2. Create a residue file with 10 residue points for a single food (apples).
3. Hand-calculate daily exposure range (high to low, distribution).
4. Compare with CARES dietary module results.

**Project: Test Percentage of Crop Treated**

1. Use population and residue sets from Multiple People Test (see above).
2. Use 10%CT value.
3. Hand-calculate daily exposure range (high to low, distribution).
4. Compare with CARES dietary module results.

**Project: Test Cumulative Response for Multiple Compounds**

1. Use the single person population from the Baseline Setup (see above).
2. Use single residue dataset for a single food, but create multiple residues.
3. Hand-calculate cumulative values.
4. Hand-calculate daily exposure range (high to low, distribution)
5. Compare with CARES dietary module results.

**► System Testing****Projects: These projects verify the performance of the system as a whole.**

- Limit Testing – run CARES with large amount of data or many iterations.
- Sequence Testing – run CARES using unexpected sequence of data inputs to modules, unexpected module connections, etc.
- Repetitive Testing - run CARES with and without specific modules activated, to identify where the program works correctly under most scenarios but has a problem resetting registers, pointers, etc.

**► Model Validation****Projects: These projects compare and evaluate output to reasonable experience and/or empirical data .**

- Run simulations using Crystal Ball to provide baseline estimates for consumption and compare to CARES output.
- Compare CARES consumption output to the Dietary Module White Paper (Tables 3 and Appendix 1).
- Generate a variety of results using the same analysis, e.g. mean, median, percentiles, shapes of distributions, outliers, maximum values, numbers of consumers, etc. These can then be compared to USDA reports to see if they compare qualitatively.

► **Model Comparison**

<b>Project: Compare CARES with DEEM (Single Crop, Small Population, Children)</b>
<ol style="list-style-type: none"><li>1. Set up a special population of children 1-3 in DEEM.</li><li>2. Set up a single food, single residue value.</li><li>3. Run DEEM and plot distribution</li><li>4. Set up a population of children 1-3 in CARES.</li><li>5. Set up a single food, single residue value.</li><li>6. Run CARES and plot distribution.</li><li>7. Compare the two outputs graphically, at 50th, 90th, 95th, 99th, 99.9th percentile.</li></ol>

<b>Project: Compare CARES with DEEM (Single Crop, Large Population, Youth)</b>
<ol style="list-style-type: none"><li>1. Set up a special population of youth 12-19 in DEEM.</li><li>2. Set up a single food, single residue value.</li><li>3. Run DEEM and plot distribution</li><li>4. Set up a population of youth 12-19 in CARES.</li><li>5. Set up a single food, single residue value.</li><li>6. Run CARES and plot distribution.</li><li>7. Compare the two outputs graphically, and tabular at 50th, 90th, 95th, 99th, 99.9th percentile.</li></ol>

<b>Project: Compare CARES with DEEM (Single Crop, Small Population, Adults)</b>
<ol style="list-style-type: none"><li>1. Set up a special population of adults 19+ years in DEEM.</li><li>2. Set up a single food, single residue value.</li><li>3. Run DEEM and plot distribution</li><li>4. Set up a population of adults 19+ years in CARES.</li><li>5. Set up a single food, single residue value.</li><li>6. Run CARES and plot distribution.</li><li>7. Compare the two outputs graphically, at 50th, 90th, 95th, 99th, 99.9th percentile.</li></ol>

### **8.3.2 CARES Water Module Validation Strategy**

The validation scheme as presented below has not the ambition to compare model outputs to actual measured exposure values. Rather, the purpose of this validation project is to walk the model evaluator through the technical possibilities of the model and help him or her to evaluate the impact of the different options available in the water module. His expert judgment will allow him to evaluate the realism of the model output. Therefore, this project falls under the Model Validation category. Projects for other validation categories and further details may be added later.

System Testing & Individual Module Testing - Functional testing will be completed with the following steps using test data sets. All menu options will be explored. Stress testing will be performed with a range of data from the test data sets below. With output taken from CSU, integrated testing of the water and CSU Modules will be completed as well.

### Step 1

1. A subgroup is selected in the population generator (e.g. black children younger than 6 years old).
2. Simulation is run for one compound: Compound A.
3. The consumption scenario is selected to be 2 liters/day per 70 kg BW.
4. Residue data of Set 1 from Table 8.2 is entered in the water module spread sheet.
5. The sample weight to be entered for each sample is 0.08333; this means that every sample has the same importance. This scenario could correspond to a monthly surface monitoring program during 1 year. The realistic residue values (Set 1) are rather low during the year but shoot up in April (month of application) and decrease over May and June, as run off losses are reduced.
6. Run the simulation with Set 1.
7. Repeat the exercise with Set 2 and 3. Note Set 2 and 3 are the same residue values as presented in Set 1 but are multiplied by a factor of 1000 and a factor of 0.001, respectively. The expected output should differ with a factor of 1000 as well.

**Table 8.2 Water residue data (ppm) for Step 1**

	Set 1	Set 2	Set 3
Sample 1	0.25	250	0.00025
Sample 2	0.30	300	0.0003
Sample 3	0.30	300	0.0003
Sample 4	200	200000	0.2
Sample 5	30	30000	0.03
Sample 6	5	5000	0.005
Sample 7	0.8	800	0.0008
Sample 8	0.5	500	0.0005
Sample 9	0.4	400	0.0004
Sample 10	0.25	250	0.00025
Sample 11	0.25	250	0.00025
Sample 12	0.25	250	0.00025

**Step 2**

1. The same subgroup is selected in the reference population as Step 1.
2. Simulation is run for 1 compound: Compound A.
3. The consumption scenario is selected to be based on the EPA/WHO constants for water consumption.
4. Residue data of Set 1 is entered in the water module spread sheet.
5. Run the simulation (only for Set 1).

**Step 3**

1. The same subgroup is selected in the reference population as Step 1.
2. Simulation is run for 1 compound: Compound A.
3. The consumption scenario is selected to be based on the age-adjusted constant water consumption.
4. Residue data of Set 1 is entered in the water module spread sheet.
5. Run the simulation (only for Set 1).

**Step 4**

1. The same subgroup is selected in the reference population as Step 1.
2. Simulation is run for 1 compound: Compound A.
3. The consumption scenario is derived from USDA-CSFII data.
4. Only direct tap water at home is selected.
5. Residue data of Set 1 is entered in the water module spread sheet.
6. Run the simulation (only for Set 1).

**Steps 5-19**

1. The same subgroup is selected in the reference population as Step 1.
2. Simulation is run for 1 compound: Compound A.
3. The consumption scenario is derived from USDA-CSFII data.
4. All sources of dietary intake are selected.
5. Residue data of Set 1 is entered in the water module spread sheet.
6. Run simulation (only for Set 1) for every cell of the matrix in Table 8.3.



**Table 8.3 Water data sources for Steps 5-19**

	<b>Residues in Tap Water Away From Home</b>	<b>Residues in Bottled Water</b>	<b>Residues in Indirect Water</b>
<b>Same As In Home Tap Water</b>	X	X	X
<b>Specified Multiple Of Residues In Home Tap Water</b>	Constant = 2	Constant = 0.01	Constant = 10
<b>Specified Multiple Of Residues In Home Tap Water</b>	Normal distribution Mean = 2 SD = 0.3	Normal distribution Mean = 0.01 SD = 0.05	Normal distribution Mean = 10 SD = 2
<b>Specified Constant</b>	0.8 ppm	0.005 ppm	3 ppm
<b>Specified Distribution</b>	Normal distribution Mean = 0.8 SD = 0.1	Normal distribution Mean = 0.005 SD = 0.002	Normal distribution Mean = 3 SD = 0.2

**Step 20**

1. The same subgroup is selected in the reference population as Step 1.
2. Simulation is run for 1 compound: Compound A.
3. The consumption scenario is derived from USDA-CSFII data.
4. Residues in home tap water only.
5. Residue data selected from database: e.g., 1994-data; no data assignment to states without monitoring data.
6. Set interpolation of residue data: LINEAR
7. Run simulation.
8. Repeat the simulation with Exponential interpolation.
9. Repeat the simulation with “step function” interpolation.

**Step 21**

1. The same subgroup is selected in the reference population as Step 1.
2. Simulation is run for 1 compound: Compound A.
3. The consumption scenario is derived from USDA-CSFII data.
4. Residues in home tap water only.
5. Residue data selected from database - Select e.g. 1994-data.
6. Assign a default constant residue value to all states without monitoring data as 0.05 ppm.
7. Set interpolation of residue data: LINEAR.
8. Run simulation.

## Step 22

1. A subgroup is selected in the population generator (e.g. female adults).
2. Simulation is run for 3 compounds: Chemical A, B and C.
3. The consumption scenario is selected to be 2 liters/day per 70 kg BW.
4. Residue data from Table 8.4 for all 3 chemicals is entered in the water module spread sheet.
5. Run simulation - output for all three chemicals should be identical.

**Table 8.4 Water residue data (ppm) for Step 22**

	Chem. A	Chem. B	Chem. C
Sample 1	0.25	0.25	0.25
Sample 2	0.30	0.30	0.30
Sample 3	0.30	0.30	0.30
Sample 4	200	200	200
Sample 5	30	30	30
Sample 6	5	5	5
Sample 7	0.8	0.8	0.8
Sample 8	0.5	0.5	0.5
Sample 9	0.4	0.4	0.4
Sample 10	0.25	0.25	0.25
Sample 11	0.25	0.25	0.25
Sample 12	0.25	0.25	0.25

## 8.4 Completed Validations

### 8.4.1 Reference Population

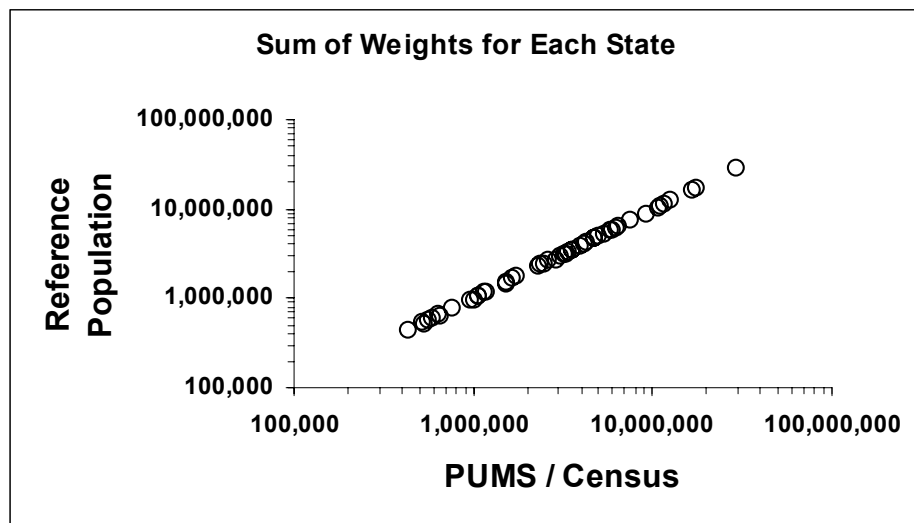
Model Validation was performed to study the demographic data and the food consumption data. First, demographics were compared for the 100,000 individuals in the Reference Population versus the 1990 U.S. Census (5% PUMS). See Appendix B for a full description of the Reference Population and how it was created. Table 2.1 (Chapter 2) 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 region/division. Figure 2.1 (Chapter 2) shows the same data in a graphical format for each age group, race, and region.

The individuals in the Reference Population can also be divided into joint age, gender, and region groups as shown in Table 8.5. Then, the region/division can be broken down into individual states for the Reference Population. Finally, a state-by-state comparison, as shown in Table 2.2 (Chapter 2), can be made to the Census/PUMS. The sum of the weights, by state, of the two populations is very similar, as seen in the fourth and sixth columns. Figure 8.1 illustrates the similarity in the weights graphically.

**Table 8.5 - Number of Individuals in the Reference Population by Age, Gender, and Region**

Age/ Gender	Region/Division*									
	NE	MA	ENC	WNC	SA	ESC	WCS	MTN	PAC	TOTAL
0	1003	2884	3384	1418	3308	1115	2299	1221	3371	20003
1 - 3	243	691	791	354	801	268	587	365	904	5004
4 - 6	240	675	815	373	779	276	601	369	881	5009
7 - 12	312	916	1141	535	1061	401	860	541	1225	6992
M 13 -19	230	700	828	357	798	311	611	347	828	5010
F 13 -19	226	699	830	352	820	313	607	343	819	5009
M 20-54	942	2652	2862	1204	3010	979	1952	1143	3319	18063
F 20-54	992	2827	3021	1249	3252	1065	2074	1204	3386	19070
55+	824	2545	2584	1207	2868	937	1630	862	2383	15840
Total	5012	14589	16256	7049	16697	5665	11221	6395	17116	100000

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



**Figure 8.1 - Total weights per state in the Reference Population and the Census/PUMS**

Next, food consumption was validated in a limited manner. The January FCID was used to show that each individual's food consumption is consistently based on multiple records (days) of consumption - i.e., an individual was not assigned the same diet over and over, and diet for multiple individuals was not based on the same subset of FCID's.

For instance, CARES individual 100 was based on 16 FCID's for January with several FCID's repeated (Table 8.4). FCID's are composed of FCID ID# + person # + day # and are the unique identifier for a daily diet record. In the next 14 CARES individuals, no FCID from individual 100 was repeated, and all 14 had similar FCID counts (from 13 to 21 FCID's). Because of the database size and CPU constraints, only these 15 individuals were examined to such a degree.

**Table 8.6 Source of Diet for Individual 100 in January**

FCID	COUNT
10317021	1
10317022	1
15144051	1
15144052	1
17416021	3
19838021	2
19838022	2
20537021	1
20537022	2
23369021	2
23369022	1
28831011	4
28831012	3
30802021	1
39814011	3
39814012	3

#### **8.4.2 Residential Module**

A lawn care scenario was used for Individual Module Testing using the "Residential Case Study (July 2001).nov" scenario supplied with an earlier, preliminary version of CARES. Extensive statistical analysis identified an issue with zeros (no exposure found) for this preliminary version, with respect to geometric means and geometric standard deviations. The testing will be repeated with the current version to ensure the subsequent code or documentation modifications were done correctly.

### **8.5 Future Plans**

Based on current plans and any feedback from CARES Version 1.0 users, the CARES Technical Team will draft the remaining strategies and request future user groups to perform the Validations. These users will be drawn from industry, academia, and regulatory agencies. Users outside the CARES Technical Team will be used primarily for the last two categories, System Testing and Model Validation.

# 9. Future CARES

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# Chapter 9 – Future CARES

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## 9.1 Introduction

CARES Version 1.0 contains all the base modules and most of the capabilities originally envisioned several years ago by the development team. However, some of the more complex, database related, or time consuming modifications could not be incorporated into Version 1.0. One strength of CARES, however, lies in its ability to incorporate future enhancements without detracting from the programs current usefulness

This chapter outlines the future enhancements of CARES that the team had originally envisioned or which came to light during development. It is expected that these enhancements will increase the ease of use of the program, strengthen the program by incorporating new data or modules, and increase the functionality of CARES within existing modules.

## 9.2 CARES Modularity: Basis for Future Enhancements

Object oriented programming techniques were used in the creation of CARES so that new exposure modules and analyses or reporting methods could be written and incorporated into CARES as developing policy, advancing technology or new data were acquired. Furthermore, for more sophisticated cumulative risk assessments where the mode of action is known, it may be important for CARES to be able to accommodate the output of Physiologically Based Pharmacokinetic (PBPK) models that have a time scale of less than a day.

To take full advantage of this opportunity, a Programmer's Interface Application (PIA) needs to be written so that programmers unfamiliar with the Notitia interface could write a new module and successfully incorporate that module into CARES. This task is of the highest priority because it will ensure that CARES will continue to be enhanced by professional users that wish to take advantage of the already rich features in CARES.

## 9.3 The Reference Population

A unique feature of CARES is its use of the 1990 U.S. census as the basis for establishing the reference population. This random sample of the U.S. population was drawn from a 5 million person sub-sample, the Public Use Micro Data Sample (PUMS). Individuals in the PUMS had completed the long form of the US. Census, and as can be observed by using the Data Explorer within CARES, have provided extremely rich demographic information about themselves. This information has been used successfully within CARES to create a match between individuals in the reference population and people in the Continuing Survey of Food Intake for Individuals. In this manner it was possible to infer additional critical demographic information (e.g. food consumption habits, body weight) about the reference population from a second survey.

This strategy of matching individuals between surveys represents the best and most logically consistent approach for incorporating new data into CARES. For example, plans are underway to incorporate into CARES information on the residential use of pesticides currently being collected by the Residential Exposure Joint Venture into CARES (See Section 9.5). This enhancement to CARES will reduce uncertainty about pesticide use in US residences and improve the quality of residential exposure and risk assessment.

At some point in the future, it may be desirable to generate alternative reference populations that meet new specific objectives or even to replace the current reference population with one based upon US Census completed in the year 2000.

A practical implementation that may have immediate benefits would be to create smaller, randomly drawn, yet representative subsets of the reference population derived from the PUMS. This would allow the risk assessor to more efficiently conduct contribution, sensitivity or uncertainty analysis without so large an investment in computation time.

Finally, it is entirely feasible that the CARES platform and methods could provide the basis for risk assessments in other sectors of the US or Europe. For example, subgroups, such as the military or college age men and women may be of interest in the US as may the general population in the UK or the European Union. In order to adapt CARES for these applications, a new reference population would have to be developed along with the supporting surveys and modules for the targeted population.

## **9.4 Dietary Module**

Use of the residue data template as presently implemented in CARES is somewhat cumbersome. The CARES development team has envisioned a “smart data entry wizard” that would greatly increase the user’s ability to process and enter residue data for analyses. The data entry wizard would be able to accommodate data entry required by other CARES modules as well.

Future versions of CARES may include a “toolbox” to more effectively work with residue values. Depending on the goal of the exposure analysis, the user may select the option of calculating a mean (needed when doing a chronic dietary analysis or analyzing blended commodities) from the residue distribution for a given food, or using individual values or a distribution of food residues. In some cases it may be necessary to create mathematical distributions representing possible residue values. At present these residue data distributions must be created outside of the CARES instead of creating them using a toolbox within CARES.

Residue Imputation programs have been written to create individual single-serving residue distributions from composite sample data such as that commonly reported in USDA’s Pesticide Data Program. These routines could be incorporated into CARES as objects that could be selected by the risk assessor.

Pesticide residue data often contain many non-detected/non-quantified values. EPA has established a policy for assigning values to these in Human Health Food Exposure Assessments (EPA, 1992). A simpler way to enter these LOD/LOQ data using these rules should be developed rather than being required to entering these values individually. Alternatively, CARES could incorporate



distribution-fitting routines that would predict and substitute a range of values below the LOD instead of simply replacing non-detects with a value at one half the LOD. Such procedures would retain variability that certainly must exist within the residue data below the LOD.

Matching of individual food consumption records with residue data has traditionally been time consuming within existing dietary exposure assessment programs. This could be simplified within CARES by adding an additional “layer” of selection to the FCID food- form breakdown.

## **9.5 Residential Module**

The residential module could be greatly strengthened by incorporating temporal use/usage data to better predict actual use patterns and co-occurrence of use of residential pesticides. Some of these databases are currently under development such as the Residential Exposure Joint Venture (REJV) survey. As described in Section 9.3, it is envisioned that this database can be brought into CARES using the population matching procedures developed for the dietary module.

The CARES technical team has already developed prototype utilities for characterizing data using a wide range of distributions. These options need to be integrated into CARES in the form of a readily accessible tool that can be used to specify the characteristics of input data distributions. Such a tool should include the ability to also characterize residue decay over time.

Finally, future versions of the CARES residential model will allow the user to create custom scenarios using user-defined algorithms. In addition, it may be necessary for some cases to be able to resolve exposure and risk on a time scale of less than one day. In such situations it may be necessary for CARES to incorporate output from PBPK models that describe delivered dose at a target within the body on a short time scale.

## **9.6 Water Module**

The water module currently incorporated exists in a simplified form of the module initially envisioned by the CARES technical team (see Water Module White Paper - Appendix E.). The module has been developed as a prototype within CARES but a tutorial illustrating its use has not been provided at this time. The essential features of the Water Module in CARES Version 1.0 are summarized below:

### **Creation of the 365-Day Residue Profile**

The CARES Water Module has the ability to randomly select one year from a multi-year array of 365-day residue profiles and assign a profile to each individual within the reference population. These profiles, which can be derived from modeling or monitoring data, capture true day to day variability while retaining temporal and spatial consistency.

### **Defining the Degree of Granularity**

The degree of spatial granularity currently represented within CARES is at the level of the State. In the future, it may be important for the risk assessor to have

other options for spatial resolution such as US Farm Resource Regions, Crop Growing Regions, or the 8-digit Hydrological Unit.

### **Spatial Surrogation**

Recognizing that there is often a paucity of data on pesticide residues in drinking water, procedures should be developed to allow the risk assessor to assign data from one location to another location. These geographic locations then should be able to be linked and randomly assigned to individuals in the reference population who live in like locals.

### **Types of Water**

In some cases it may be necessary for CARES to be able to account for the different forms in which water is consumed. For example the residue profile in tap water at home may be different from the profile in tap water away from home. Residues in indirect water in food and beverages at home may be different from residues in indirect water in food or beverages away from home or in bottled water. The risk assessor may wish to evaluate the impact of these differences. Therefore, procedures should be available that would make it possible to fully incorporate a rich database if it were available.

### **Water Treatment and Residue Decay Over Time**

It may be important for the risk assessor to be able to adjust residues profiles based on studies on the effect of water treatment or other methods that may cause pesticide residues in drinking water to decline over time or assume different levels in finished water vs. raw water.

## **9.7 Aggregation and Cumulation**

Enhancements that will allow the user to compare exposure estimates with benchmark doses determined over consistent time intervals will be considered. This could include providing a tool for matching the duration of exposure with the duration of the toxicity study used to establish the benchmark dose and for filtering exposure and dose time series using a moving average or other type of filters. (see Chatfield, 1996 or Diggle, 1991).

Aggregation and cumulation methods for internal doses, doses predicted by PBPK models, or doses that have their effect on a time scale of less than one day may also be considered.

## **9.8 Contribution/Sensitivity/Uncertainty Analyses**

As in the water module, the currently incorporated CSU module was developed to a greater extent in a prototype than is currently implemented in CARES Version 1.0. These features have been discussed in Chapter 7 and include:

- Deep drill-down capability
- The ability to summarize exposure and risk at different percentiles (e.g. 95th 99th or 99.9th) for individuals, sub-populations or the entire population.

- The ability to compare exposure or risk distributions for 2 or more sub-populations and to be able to compare the results from multiple simulations as required by sensitivity or uncertainty analyses.

## **9.9 Documentation of CARES Simulations**

A systematic approach needs to be developed to fully document the assumptions and data used in a simulation so that it can be exactly reproduced.

An archive needs to be developed so that past simulations may be saved using a logical file structure and so that user-specific files can be easily located and reincorporated into subsequent assessments.

## **9.10 Validation and Testing**

Again time constraints severely limited the planned validation and testing efforts for CARES Version 1.0. These detailed plans are laid out in Chapter 8 and Appendix E.

Based on user feedback and validation, other, suggested enhancements will be evaluated as they are received.

## **9.11 Evergreen CARES – A Business Model**

The CARES administrative team is in the process of developing a business model for CARES. The intent of this activity is to place the continued development and oversight of CARES on a more permanent footing. This will permit CARES to be enhanced and expanded to meet the needs of the risk assessment community.

## **9.12 References**

Chatfield, C. 1996. *The Analysis of Time Series*, Chapman and Hall.

Diggle, P.J. 1991. *Time series: A Biostatistical Introduction*, Oxford Statistical Science Series, Clarendon Press, Oxford.



