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The University of Arizona
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Standard Operating Procedure **SOP-IIT-A-15.0**

Title: Probabilistic Approach for Calculating Ingestion Exposure from Day 4 Composite Measurements, the Direct Method of Exposure Estimation

Source: The University of Arizona

U.S. Environmental Protection Agency
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STANDARD OPERATING PROCEDURE FOR PROBABILISTIC APPROACH FOR CALCULATING INGESTION EXPOSURE FROM DAY 4 COMPOSITE MEASUREMENTS, THE DIRECT METHOD OF EXPOSURE ESTIMATION.

This Standard Operating Procedure (SOP) uses data that have been properly coded and certified with appropriate QA/QC procedures by the University of Arizona NHEXAS team.

Objective

Calculate the ingestion exposure using composite food chemical residue values from the day of direct measurements. The calculation is based on the probabilistic approach.

Introduction to Probabilistic Approach of Exposure Calculation

The probabilistic approach refers to the use of the Monte Carlo simulation to estimate exposure levels based on deterministic exposure calculation equations.

Most real-world problems involving elements of uncertainty are too complex to be solved by strict analytical methods. There are simply too many combinations of input values to calculate every possible result. Monte Carlo simulation is an efficient technique for analyzing these types of problems. It is simple technique that requires only a random number table or a random number generator on a computer.

The software used for this approach in this SOP is Crystal Ball. When a simulation is run, Crystal Ball uses the Monte Carlo method to generate random numbers for the assumption cells that conform to real-life possibilities. Each set of random numbers effectively simulates a single "what-if" scenario of interest. As the simulation runs, the model is recalculated for each scenario and results are dynamically displayed in a forecast chart. The final forecast chart reflects the combined uncertainty of the assumption cells on the model's output.

Each variable needs an assumption regarding its distribution and characteristic. The concentration variables use the optimum fit distribution obtained from the Distributional Method explained in SOP#4. Other variables use distributions specified by using values from reference papers. Two types of variables are used:

- uncertainty variable is a variable that is uncertain because of insufficient information about its true, but unknown, value.
- variability variable is a variable that describes the variation in a population.

Simulations that use both types of variables are called 2-D simulations. A 2-D simulation will result in a family of forecast distributions. The standard error of a particular percentile of the forecast distribution can then be estimated.

Deterministic Exposure Calculation

The content of this section is taken from SOP#6 which explain the deterministic exposure calculation of ingestion exposure.

The equation used to calculate the direct ingestion exposure for each subject is as follows:

$$E_T = \frac{\left[\sum_S C_S \times W_S + \sum_L C_L \times W_L\right]}{BW} \qquad (12\text{-}1)$$

where E_T is the total ingestion exposure to all chemical residues found in the food items consumed by each subject during the day of measurement, kg/day.

C_S is the concentration of the chemical residue, chlorpyrifos or diazinon, in the composited solid food items consumed by each subject during the day of measurement, mg/kg.

W_s is the weight of composited solid food items consumed by each subject during the day of measurement, kg.

C_L is the concentration of the chemical residue, chlorpyrifos or diazinon, in the composited liquid food items consumed by each subject during the day of measurement, mg/kg.

W_L is the weight of the composited liquid food items consumed by each subject during the day of measurement, kg.
BW is the body weight of each subject, kg.

Up to 2 percent of chlorpyrifos or diazinon concentrations of in beverages and water are detectable. Therefore, we conclude that the population exposures to chlorpyrifos or diazinon from consumption of beverages and water are equivalent to zero. Only exposure to the chemicals in solid food are discussed in this SOP.

The consumption unit used in the Diet Diary questionnaire is "serving". This unit has to be converted to kilograms. The conversion is explained in SOP#8.

Probabilistic Approach of Ingestion Exposure Calculation

Without the liquid food terms, equation 12-1 becomes:

$$E_T = \frac{\left[\sum_{S} C_S \times W_S\right]}{BW} \qquad (12\text{-}2)$$

All variables in the equation are of variability type. However, using all variability type variables will not yield the 2-D results. Alternatively, the distribution parameters of any of the variability variables can be assign as uncertainty variables to enable the 2-D simulation. In this SOP, the mean and standard deviation of the body weight variable will be assign as uncertainty variables. First, the two parameters will be calculated from the NHEXAS database. Then the corresponding values will be obtained from other studies similar to NHEXAS. The IIT data analysis team will make comparisons and use their judgement to assign appropriate quantitative assumption for the uncertainty of the two values. When information about a parameter is limited, the assumptions often result in uniform or triangular distributions.

Therefore;

$$BW = f(\mu_{BW}, \sigma_{BW}) \qquad (12\text{-}3)$$

where μ_{BW} and σ_{BW} are the mean and standard deviation of body weight variable and are assumed as uncertainty variables with a uniform or triangular distribution.

Variable List

Variable	Description
HHID	household I.D.
TFDMASS	total mass of solid food consumed (kg)
BW	body weight (kg)
MEAN	mean of the body weight
SD	standard deviation of the body weight

Variable	Description
C_DT	measured concentration of chlorpyrifos in the composite of solid food with the BDL values censored using the distributional method. The unit is mg of chemical residue per kg of food, mg/kg.
D_DT	measured concentration of diazinon in the composite of solid food with the BDL values censored using the distributional method. The unit is mg of chemical residue per kg of food, mg/kg.
EC_DT	exposure to chlorpyrifos in solid food, using the concentration data with the BDL values censored using the distributional method. The unit is mg/kgBW.day.
ED_DT	exposure to diazinon in solid food, using the concentration data with the BDL values censored using the distributional method. The unit is mg/kgBW.day.

Procedure

The concentration data will be censored with the Distributional Method explained in SOP#4. The procedure explained next is for estimating unweighted exposure for the data sets. Weighted exposure estimates can be obtained by using the SUDAAN program. The unweighted exposure estimates, with corresponding sampling weights, will be used as the program's inputs. The sampling weights used will be calculated and adjusted according to the processes explained in details in SOP # 9 and 10.

The procedure for the unweighted exposure estimation in this SOP is the following:

1. In **Crystal Ball**, open **INGESTION EXPOSURE DIRECT**. Assign an assumption for each of the following variable: ***TFDMASS, BW, MEAN, SD, C_DT,*** and ***D_DT.***
2. Assign forecast for ***EC_DT,*** and ***ED_DT,*** the calculation of ingestion exposure corresponding to equation 12-2.
3. Choose the ***MEAN,*** and ***SD*** assumptions as uncertainty, and rest of them as variability. Run this model as a 2-D simulation.

Spreadsheet Format

In **INGESTION EXPOSURE DIRECT**:

Column	Variable
1	***HHID***
2	***BW***
3	***MEAN***

Column	Variable
4	***SD***
5	***TFDMASS***
6	***C_DT***
7	***D_DT***
8	***EC_DT***, calculated from (***TFDMASS*** × ***C_DT***)/***BW***
9	***ED_DT***, calculated from (***TFDMASS*** × ***D_DT***)/***BW***