The Arizona Border Study

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Quality Systems and Implementation Plan for Human Exposure Assessment

The University of Arizona
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Standard Operating Procedure **SOP-IIT-A-13.0**

Title: Probabilistic Approach of Exposure Calculation of Dermal Exposure

Source: The University of Arizona

U.S. Environmental Protection Agency
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Exposure & Dose Research Branch

STANDARD OPERATING PROCEDURE FOR PROBABILISITIC APPROACH OF EXPOSURE CALCULATION OF DERMAL EXPOSURE

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.

Objectives

Calculate dermal exposure using the probabilistic approach.

Introduction to Probabilistic Approach of Exposure Calculation

Probabilistic approach refers to the use of the Monte Carlo simulation to find exposure estimates based on the deterministic exposure calculation equation.

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. Assumptions about the type of variables are:

- uncertainty: variable that are uncertain because insufficient information about a true, but unknown, value.
- variability: variable describe the variation in a population.

The simulation that uses the two types of variables is called a 2-D simulation. It will result in a family of forecast distributions. The standard error of a particular percentile of the forecast distribution can then be estimated.

More detail about the Monte Carlo simulation can be found in many literature papers.

Deterministic Exposure Calculation

The content of this section is taken from SOP#11 which explain the deterministic exposure calculation of dermal exposure.

The equation[1] used to calculate the dermal exposure for each subject is as follows:

$$E = [\sum_{s=1}^{S} C_{Ds} \times A_{ps} \times T_{ps} \times (1 - DO_{ps})] + [\sum_{s=1}^{S} C_{Ss} \times (S_{ps} \times SA_{ps} - SO_{ps}) \times M] \qquad (10\text{-}1)$$

where E is the total dermal exposure to pesticide (chlorpyrifos or diazinon), μg/day.

s is surfaces contacted per day.

C_{Ds} is concentration of dislodgeable surface residue, $\mu g/m^2$.

A_{ps} is surface area contacted by subject p, m^2/day.

T_{ps} is transfer from surface by subject p, proportion.

DO_{ps} is dislodgeable residue transferred to oral route by subject p via hands, food, and objects, proportion.

C_{Ss} is concentration of pesticides in soil, μg/g.

S_{ps} is soil covering on skin from surface s for subject p, g/m^2.

SA_{ps} is surface area of skin exposed to surface s for subject p, m^2.

SO_{ps} is soil or dust from surface s transferred to oral route by subject p, g/day.

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[1] Modified from "Research Solicitation : Human Exposure Assessment", Office of Research & Development, 1993. The variable AF_D, dermal absorption fraction, in the source equation is not included in this equation.

M is matrix effect of soil, proportion.

Assumptions and Values of Variable Used in the Deterministic Calculation

This section is taken from SOP#11 which explain the deterministic exposure calculation of dermal exposure.

Equation 10-1 being used to calculate the dermal exposure is modified from the source equation. Only variables regarding exposure, not dose, are retained. So the variable AF_D, dermal absorption fraction for the chemical, is not included in this equation. Assumptions made and/or values used for the rest of the variables are discussed below:

Surface contacted, s

There are 2 types of dislodgeable surface area in NHEXAS study. One is the floor surface area, and the other is the window sill surface. The later is assumed to be a representative of all surfaces such as furniture other than the floor in the house, and is called "non-floor surface".

As a result, there are totally 3 surfaces considered in this equation: Surface 1 is the measured concentration of residue on non-floor surface (sill), surface 2 is the measured concentration of residue on floor surface, and surface 3 is measured concentration of yard soil.

Surface area contacted, A_{ps}

For a 6-9 month old child, it is estimated[2] that he/she plays in an area of 18.6 m^2, and comes into contact with 25% of that surface. Therefore, the surface area contacted is 4.65 m^2. These 2 age groups, however, are not present in our dermal exposure calculation.

The floor surface area contacted by adults and children is assumed to be 10% and 50% of the total floor surface area in the house, respectively. The non-floor surface area is assumed to be proportional to the floor surface area, so it is assume as 30% of the total floor surface area in the house. The non-floor surface area contacted by each subject is then assumed to be equal to 50% and 70% of the non-floor surface area for adults and children, respectively. Therefore, the surface area contacted by adults and children are 15% and 21% of the total floor surface area, respectively.

Transfer from surface, T_{ps}

[2] "Insecticide absorption from indoor surfaces: Hazard assessment and regulatory requirements", Berteau Pe, et. al., ACS Symposium Series 382, Washington DC: Amer. Chem. Society, 1989.

The transfer from the two dislodgeable surfaces is estimated by the ratio of the measured concentration from dermal wipe (hands wipe) to the concentration of residue on the dislodgeable floor and soil surface.

Dislodgeable residue transferred to oral route, DO_{ps}

The dislodgeable residue transferred to oral route is calculated by[3]:

$$DO_{ps} = SA_{ph} / SA_{ps} \qquad (10\text{-}2)$$

where

SA_{ph} is surface area of skin on the hands that is used to transfer material to mouth or food, m^2. This is assumed to be 25% of the hands area[4].

SA_{ps} is the surface area of skin exposed to surface s, m^2.

Soil covering on skin, S_{ps}

The values used for soil covering on skin are 8 and 11.1g/m^2 for children and adults, respectively[5].

Surface area of skin exposed to surface, SA_{ps}

The total surface area of the skin is calculated from the following equation[6]:

$$SA = 0.0239\, H^{0.417}\, W^{0.517} \qquad (10\text{-}3)$$

where H is height of subject, cm.; and W is body weight of subject, kg.

The surface area of skin exposed to surface for a subject is assumed to be the area of hands, feet, legs and arms of the body for children; and hands and feet for adults. The percentage of total body surface area by part[7] is used to get the surface area of skin exposed for children and adults, respectively. For adults, the percentage of total body surface by part used is as follows :

Gender	Hands	Feet
Male	5.2	7.0
Female	5.1	6.5

[3] "Research Solicitation : Human Exposure Assessment", Office of Research & Development, 1993.
[4] "Research Solicitation : Human Exposure Assessment", Office of Research & Development, 1993.
[5] Exposure Factor Handbook, 1997.
[6] Exposure Factor Handbook, 1997.
[7] Exposure Factor Handbook, 1997, Table 6-6 and 6-8.

Children are categorized into 7 age groups, and are not distinguished by gender. The percentage of total body surface area by part of each age group for children is as follows:

Age	Hands	Feet	Legs	Arms
<1	5.30	6.54	20.60	13.70
1-2	5.43	6.63	23.30	12.83
3-5	5.89	7.25	27.30	14.20
6-8	4.71	6.90	27.10	13.10
9-11	5.30	7.58	28.70	12.30
12-14	5.25	7.53	31.25	12.90
15-17	5.41	7.11	32.20	15.30

Soil transferred to oral route, SO_{ps}

The information on the soil from surface transferred to oral route is not available from literature papers, so it is assumed to be zero.

Matrix effect of soil, M

The matrix effect of soil is assumed[8] to be 0.15.

Probabilistic Approach of Dermal Exposure Calculation

From the equation 10-1:

$$E = [\sum_{s=1}^{S} C_{Dsi} \times A_{psi} \times T_{psi} \times (1 - DO_{ps})] + [\sum_{s=1}^{S} C_{Ss} \times (S_{ps} \times SA_{ps} - SO_{ps}) \times M] \qquad (10\text{-}1)$$

Area of *i* surface contacted per day can be written as:

$$A_{psi} = C_{i1p} \times C_{i2p} \times SA \qquad (10\text{-}4)$$

where: C_{i1p} is the non-floor surface area
C_{i2p} is the non-floor surface area contacted by each subject
SA:is the calculated total surface area of skin of respondent
i is 1,2
1: Sill surface
2: Floor surface

[8] "Research Solicitation : Human Exposure Assessment", Office of Research & Development, 1993.

Constants	Children	Adult
C_{11}	0.3	0.3
C_{12}	0.7	0.5
C_{21}	0.7	0.7
C_{22}	0.5	0.1

And, transfer from *i* surface can be writen as:

$$T_{psi}=DWP/CDs_i \quad (10\text{-}5)$$

where:DWP is measured concentration of pesticide residue on the hands, $\mu g/m^2$
CDs_i is measured concentration of dislodgeable surface residue on surface *i*
i is 1,2
1: Sill surface
2: Floor surface

The exposure calculation formula becomes:

$$E=[\sum_{s=1}^{S} C_{Dsi}\times(C_{i1p}\times C_{i2p}\times SA)\times(DWP/CDs_i)\times(1-DO_{ps})]+[\sum_{s=1}^{S} C_{Ss}\times(S_{ps}\times SA_{ps})\times 0.15] \quad (10\text{-}6)$$

C_{i1p} and C_{i2p} assumptions are considered as a uncertainty, and the others are variability.

Variable List

Variable	Description
HHID	Household I.D.
C_{Ds1}	Measured concentration of dislodgeable surface residue on the sill surface, $\mu g/m^2$.
C_{Ds2}	Measured concentration of dislodgeable surface residue on the floor surface, $\mu g/m^2$.
A_{PS1}	Area of sill surface contacted per day, m^2/day.
A_{PS2}	Area of floor surface contacted per day, m^2/day.
DWP	Measured concentration of pesticide residue on the hands, $\mu g/m^2$.
T_{PS1}	Transfer from sill surface (proportion).
T_{PS2}	Transfer from floor surface (proportion).
DO_{PS}	Dislodgeable residue transferred to oral route via hands, food, and objects (proportion).
ED_{S1}	Dermal exposure to pesticide (chlorpyrifos or diazinon) via sill surface,

Variable	Description
	µg/day.
ED_{S2}	Dermal exposure to pesticide (chlorpyrifos or diazinon) via floor surface, µg/day.
ED	dermal exposure to pesticide (chlorpyrifos or diazinon) via both dislodgeable surfaces (sill and floor), µg/day.
C_{Ss}	measured concentration of pesticide (chlorpyrifos or diazinon) in soil, µg/g.
S_{PS}	soil covering on skin, g/m^2.
SA_{PS}	surface area of skin exposed to the soil surface, m^2.
SA_{PH}	surface area of skin on the hands that is used to transfer material to mouth or food, m^2.
SO_{PS}	soil transferred to oral route, g/day.
M	matrix effect of soil (proportion).
ES	dermal exposure to pesticide (chlorpyrifos or diazinon) via soil surface, µg/day.
DE	total dermal exposure to pesticide (chlorpyrifos or diazinon), µg/day.
HT	height of respondents, cm.
BW	body weight of respondents, kg.
SA	calculated total surface area of skin of respondent, m^2.
C_{DS1P}	Assumption of C_{DS1}
C_{DS2P}	Assumption of C_{DS2}
SAP	Assumption of SA
C_{11P}	Assumption of C_{11}
C_{12P}	Assumption of C_{12}
C_{21P}	Assumption of C_{21}
C_{22P}	Assumption of C_{22}
$DWPP$	Assumption of DWP
SA_{PSP}	Assumption of SA_{PS}
DO_{PSP}	Assumption of DO_{PS}
C_{SSP}	Assumption of C_{SS}
S_{PSP}	Assumption of S_{PS}
MP	Assumption of M
DEP	Forecast of DE, Dermal exposure

Procedure

The concentration data in each media 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 **Dermal Expo Chlorpyrifos.xls** or **Dermal Expo Diazinon.xls** file. Add variables C_{Ds1P}, C_{Ds2P}, $TFSAP$, C_{11P}, C_{12P}, C_{21P}, C_{22P}, $DWPP$, SA_{PSP}, DO_{PSP}, C_{SSP}, S_{PSP}, MP, DEP.
2. Assign an assumption for each variable. Assign a forecast for DEP, the calculation of dermal exposure.
3. Run this model as a 2-D simulation. Choose the C_{11}, C_{12}, C_{21P}, C_{22P} assumptions as uncertainty, and rest of them as variability.

Spreadsheet Format

In **DERMAL EXPO CHLORPYRIFOS** or **DERMAL EXPO DIAZINON**:

Column	Variable
1	$HHID$
2	C_{Ds1}
3	C_{Ds2}
4	$TFSA$
5	A_{PS1}
6	A_{PS2}
7	DWP
8	T_{PS1}
9	T_{PS2}
10	SA_{PS}
11	SA_{PH}
12	DO_{PS}, calculated from SA_{PH} / SA_{PS}
13	ED_{S1}, calculated from $C_{Ds1} \times A_{PS1} \times T_{PS1} \times (1 - DO_{PS})$
14	ED_{S2}, calculated from $C_{Ds2} \times A_{PS2} \times T_{PS2} \times (1 - DO_{PS})$
15	ED, calculated from $ED_{S1} + ED_{S2}$
16	C_{SS}
17	S_{PS}
18	SO_{PS}
19	M
20	ES, calculated from $C_{SS} \times ((S_{PS} \times SA_{PS}) - SO_{PS}) \times M$

Column	Variable
21	DE
22	C_{DS1P}
23	C_{DS2P}
24	$TFSAP$
25	C_{11P}
26	C_{12P}
27	C_{21P}
28	C_{22P}
29	$DWPP$
30	SA_{PSP}
31	DO_{PSP}
32	C_{SSP}
33	S_{PSP}
34	MP
35	DEP