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HAZARD ASSESSMENT OF CHEMICAL CONTAMINANTS IN SOIL
REVISED APPENDIX 3

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HESP

HUMAN EXPOSURE TO SOIL POLLUTANTS
VERSION 2.00

Technical Report No 40

Revised Appendix 3

THE CONCEPT

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PREFACE

As indicated in the ECETOC Technical Report No. 40 "Hazard Assessment of Chemical Contaminants in Soil" (1990), hazard assessment is a necessary step to evaluate the significance of the presence of contaminants in the environment. Part of the hazard assessment process is the estimation of exposure.

This Appendix 3 of the above mentioned report describes "The Concept of HESP". HESP 2.00 is a computer programme to estimate the exposure of human beings to contaminants in soil and is essentially an updated version of the original Appendix 3 of the ECETOC Technical Report No. 40. As compared to the original version of HESP, the same approach is maintained but a number of formulae and value choices are improved as a result of recent scientific publications and discussions with specialists from the RIVM (Dutch State Institute for Public Health and the Environment) and representatives of BASF, Bayer, DSM and Hoechst.

All assumptions, value choices and formulae to calculate the potential exposure of human beings in specific situations are described in this document. The "HESP User Guide", Version 1.3 by W. Veerkamp, Shell Internationale Petroleum Maatschappij (SIPM), and B.W. Laffoon, Computer Management Group, the Netherlands, describes how to run the userfriendly PC version of the computer programme to estimate human exposure as based on the assumptions and equations of this revised Appendix 3 of ECETOC Technical Report No. 40.

The HESP 2.00 model can be applied to carry out a Preliminary Exposure Assessment in an early phase of the hazard assessment process (see scheme in Fig. 1). In cases where the Preliminary Hazard Assessment indicates the possibility of significant exposure, a Definitive (site specific) Exposure Assessment (which usually includes measurement of exposure concentrations for relevant exposure routes) is required as basis for the Definitive Hazard Assessment.

Only the latter can provide a sound basis for decisions regarding possible measures.

The ECETOC Technical Report No. 40 "Hazard Assessment of Chemical Contaminants in Soil" (1990), presents the full description of the hazard assessment process and indicates the place of HESP in this process.

About this Appendix

This revised Appendix is a guide for the use of the HESP 2.00 programme. It contains the following chapters:

Section 1: Introduction, which gives some background information on the HESP model developed by SIPM and DSM in cooperation with the Dutch governmental authorities (Ministry of Housing, Physical Planning and Environment (VROM) and RIVM) and representatives of BASF, Bayer and Hoechst.

Section 2: Gives a detailed description of all equations used in the programme.

Section 3: Gives a description of the model parameters used in the calculations with a set of default values used for the Dutch situation. The scenario used is called Netherlands 1.00.

Section 4: Conains the literature used for the development of the programme.

Annex I: Alphabetic listing and description of all parameters used in the document are given.

1. INTRODUCTION

Based on a report for a specific site decommissioning by Golder Associates (Reades and Gorber, 1986) a more general approach has been developed to assess the exposure levels of soil contaminants for human beings. The initial set of equations and assumptions has been published in the ECETOC Technical Report No. 40, "Hazard Assessment of Chemical Contaminants in Soil" (ECETOC, 1990). In consultation with DSM (who provided a few modules for the HESP model) and with representatives of BASF, Bayer and Hoechst, and after discussions with representatives of the Dutch governmental authorities the model has been updated, based on the most recently published literature including e.g. the review of v.d. Berg (1991) examining exposure of human beings to soil pollution. The HESP model is directed towards estimating the exposure of man to chemicals, which are present in the environment as soil contaminants. A number of possible exposure routes were identified and subsequently quantified. The main exposure routes taken into account in this model are:

INHALATION,
INGESTION,
DERMAL ABSORPTION.

These main exposure routes can be subdivided on the basis of the intermediate environmental compartment involved. The following subdivision in exposure routes is used throughout the program:

- direct ingestion of soil or dust,
- inhalation of vapours,
- inhalation of particulate matter,
- inhalation during bathing,
- ingestion of garden produce,
- ingestion of drinking water,
- ingestion of meat and dairy products,
- ingestion of fish,
- dermal exposure to soil or dust,
- dermal exposure during bathing,

- dermal exposure during swimming.

Depending on the land use, relevant exposure routes in that particular situation can be selected and included in the calculations.

The HESP model is directed towards estimating the exposure to two types of residents: an adult and a young child. The calculated results, which may be either the total exposure or the concentration in specific compartments represent the greatest cumulative intakes for individuals living at a contaminated site (referred to as "Maximum Average Exposure"), or Predicted Environmental Concentrations (PEC), where "average" indicates the total yearly uptake presented as mg/d independent of the season.

The model assumes that a house is located in the middle of a contaminated site and concentrations of substances are assumed not to change with time.

The programme screens and input are given in the HESP User Guide Version 1.3 by Veerkamp and Laffoon (1992).

2. THE EQUATIONS

2.1. Quantification of direct ingestion

The following equations are used to calculate uptake of a chemical as a result of the direct ingestion of either soil or dust:

$$DU = (\Sigma\ DU_{x,n}) * C_s / W \qquad \text{(eq. 1)}$$

where $DU_{x,n}$ = uptake resulting from direct ingestion of soil or dust per unit body weight per season (mg soil/d),
n = dust or soil,
x = summer or winter,
W = receptor's weight,
C_s = C_t (concentration in the soil top layer).

$$DU_{x,dust} = AID * f_{a,ing} * f_{rs,i} * N_i \qquad \text{(eq. 2)}$$

$$DU_{x,soil} = AID * f_{a,ing} * N_o \qquad \text{(eq. 3)}$$

where AID = amount of soil ingested daily by man (mg/d), based on the average amount ingested on a yearly basis,
$f_{a,ing}$ = fraction of uptake/intake for ingestion,
$f_{rs,i}$ = soil fraction in dust indoors,
N_y = fraction of time spent annually indoor; outdoor; sleeping or absent from location (= $N_{s,y}$ + $N_{w,y}$).

$$N_{x,y} = \Sigma\ tx1_y/24 * (tx2_y/7) * f_x \qquad \text{(eq. 4)}$$

where $tx1_y$ = time spent indoor, outdoor, sleeping or absent from the location in a season in hours per day,

$tx2_y$ = time spent indoor, outdoor, sleeping or absent from the location in a season in days per week,

f_x = fraction of the season,

$N_{x,y}$ = fraction of time spent (indoors, outdoors, sleeping or absent) in season.

2.2. Quantification of dermal absorption

The following equations are used to calculate the dermal absorption of chemicals through skin contact with either contaminated soil or dust:

$$DA = (\Sigma\ DA_{x,n}) * C_s / W \qquad \text{(eq. 5)}$$

where $DA_{x,n}$ = dermal absorption equivalent for soil or dust per day in a season (kg soil/d),

C_s = C_t (concentration in the top soil layer),

$$DA_{x,dust} = A_{exp} * DAE_i * DAR * f_m * f_{rs,i} * N_i * 24 \qquad \text{(eq. 6)}$$

$$DA_{x,soil} = A_{exp} * DAE_o * DAR * f_m * N_o * 24 \qquad \text{(eq. 7)}$$

where A_{exp} = surface of exposed part of the body,

DAE = amount of soil or dust on the skin,

DAR = dermal absorption rate,

f_m = matrix factor,

Outdoors

$$A_{exp} = A_{fh} \quad \text{(adult)} \qquad \text{(eq. 8)}$$

$$A_{exp} = A_{ah} + A_{lf} \quad \text{(child)} \qquad \text{(eq. 9)}$$

Indoors

$$A_{exp} = A_h \quad \text{(adult)} \qquad \text{(eq.10)}$$

$$A_{exp} = 0.5 * A_{ah} \quad \text{(child)} \qquad \text{(eq.11)}$$

where A_{ah} = surface area of the arm and hands,
A_{lf} = surface area of the legs and feet,
A_{fh} = surface area of forearm and hands,
A_h = surface area of the hands.

2.3. Quantification of the inhalation of particulate matter

The following equations are used to calculate the inhalation of particulate matter both indoors and outdoors:

$$IP = (\Sigma\ IP_{y,x}) * C_s / W \qquad \text{(eq.12)}$$

where IP = inhaled chemical via dust,
$IP_{y,x}$ = inhaled particulate matter per season in soil equivalents (mg soil/d),
y = indoors, outdoors, sleeping or absent,
C_s = C_t (concentration in the top soil layer),

$$IP_{y,x} = VA * TSP_y * f_{rs,y} * f_r * f_{a,inh} * N_y \qquad \text{(eq.13)}$$

where f_r = fraction retained in the lung,
VA = volume of air breathed,
TSP_y = total suspended particulates outdoors or indoors,
$f_{a,inh}$ = fraction uptake/intake for the lung,
N_y = $N_{sleep} + N_{indoor}$.

$$TSP_i = 0.75 * TSP_o \qquad \text{(eq.14)}$$

where TSP_i = local suspended particulates indoors,
TSP_o = local suspended particulates outdoors.

2.4. Quantification of the inhalation of vapours

2.4.1. *Calculation of the fugacity*

The following equations are used to calculate the contaminant partition within the soil:

$$Z_a = 1 / (R * T_{soil}) \quad \text{(eq. 15)}$$

$$Z_w = S / P \quad \text{(eq. 16)}$$

where P = vapour pressure at T_{soil},
S_w = solubility in water at T_{soil},
S = solubility in water at T_{soil}
$S = S_w/M$,
Z_a = fugacity capacity constant air,
Z_w = fugacity capacity constant water,
R = gas constant (8.3143),
T_{soil} = temperature of the soil,

OR $Z_w = 1 / H_s$ (eq. 17)

WITH $\ln H_s = \ln H_T + 0.024 (T_{soil} - T)$ (eq. 18)

AND $H_T = P / S(T)$ (eq. 19)

where $P(T)$ = vapour pressure at T,
$S(T)$ = solubility in water at T,
T = temperature related to $P(T)$ and $S(T)$,
H_T = Henry's law constant for temperature T,
H_s = Henry's law constant for T_{soil}.

$Z_s = K_d * SG * Z_w / SN_s$ (eq. 20)

where Z_s = fugacity capacity constant soil,
K_d = partition coefficient soil-water,
SG = specific gravity,
SN_s = volume phase of solid phase.

For organic contaminants:

$K_d = K_{oc} * f_{oc}$ (eq. 21)

$K_{oc} = 0.411 * K_{ow}$ (eq. 22)

$f_{oc} = f_{om} / 1.724$ (eq. 23)

where K_d = partition coefficient soil/water,
K_{oc} = partition coefficient for octanol-water corrected for organic carbon,
f_{oc} = fraction organic carbon,
f_{om} = fraction of organic matter,
K_{ow} = partition coefficient octanol-water.

For inorganic contaminants:

K_d is an input parameter.

$Pa = (Z_a * SN_a) / (Z_a * SN_a + Z_w * SN_w + Z_s * SN_s)$ (eq. 24)

$Pw = (Z_w * SN_w) / (Z_a * SN_a + Z_w * SN_w + Z_s * SN_s)$ (eq. 25)

$Ps = (Z_s * SN_s) / (Z_a * SN_a + Z_w * SN_w + Z_s * SN_s)$ (eq. 26)

where Pa = mass fraction in soil gas phase,
Pw = mass fraction in soil liquid phase (water),
Ps = mass fraction in soil solid phase (absorbed to soil minerals),
SN_a = volume phase of gas fraction (air),
SN_w = volume phase of liquid phase (water),
SN_s = volume phase of solid phase (soil).
$SN_s = 1 - SN_a - SN_w$

2.4.2. *Soil concentration to be used in the calculations*

Outdoors:

IF $C_d \geq C_m$

IF $C_d > C_t$

THEN $C_{s,o} = 0.1 * C_t + 0.5 * C_m + 0.4 * C_d$ (eq. 27)

ELSE $C_{s,o} = C_t$ (eq.27a)

ELSE IF $C_m \geq C_t$

THEN $C_{s,o} = 0.17 * C_t + 0.83 * C_m$ (eq. 28)

ELSE $C_{s,o} = C_t$ (eq.28a)

Where L_c = length of the diffusive path in the soil

Basement:

Construction with an open (direct earth) floor

IF $C_d \geq C_m$

IF $C_d > 0.1 * C_t$

THEN $C_{s,bo} = 0.5 * C_m + 0.5 * C_d$ (eq. 29)

ELSE $C_{s,bo} = C_t$ (eq.29a)

ELSE IF $C_m \geq 0.01 * C_t$

THEN $C_{s,bo} = C_m$

ELSE $C_{s,bo} = C_t$
(In the case C_t is used, the calculations are performed using eq. 40)

Where L_c = length of the diffusive path in the soil,
$C_{s,bo}$ = average soil concentration used in the calculation for the basement air concentration (open).

Construction with a concrete floor

$$C_{s,bc} = 0.068 * C_t + 0.340 * C_m + 0.592 * C_d \quad \text{(eq. 30)}$$

Where L_c = length of the diffusive path in the soil,
$C_{s,bc}$ = average soil concentration used in the calculation for the basement air concentration (concrete).

2.4.3. *Calculation of the maximum soil concentration*

In those situations, where transport of the chemical from the soil compartment to other compartments is calculated via the porous water, the concentration of the porous water cannot exceed the water solubility. Therefore $C_s = C_{s,max}$

$$C_{pw} = C_s * SG * Pw / SN_w \quad \text{(eq. 31)}$$

When $C_{pw} > S_w$ then $C_{pw} = S_w$ will be used for the calculations and hence C_s becomes:

$$C_{s,max} = S_w * SN_w / SG * P_w \qquad \text{(eq. 32)}$$

$$C_{sa} = C_{s,max} * SG * Pa / SN_a \qquad \text{(eq. 33)}$$

where C_s = C_t, C_m or C_d,
C_{sa} = soil air concentration of contaminant,
C_{pw} = soil water concentration of contaminant,
calculation of C_{sa} and C_{pw} depend on the concentrations of the soil compartment (t=top, m=middle and d=deeper layer).

2.4.4. *Vapour flux calculation*

The following equations are used to calculate the upward flux of vapours.

$$D_{sa} = SN_a^{(10/3)} * D_a / (1 - SN_s)^2 \qquad \text{(eq. 34)}$$

$$D_{sac} = CN_a^{(10/3)} * D_a / (1 - CN_s)^2 \qquad \text{(eq. 35)}$$

$$D_{sw} = SN_w^{(10/3)} * D_w / (1 - SN_s)^2 \qquad \text{(eq. 36)}$$

$$D_{ef} = (Pa * D_{sa} / SN_a) + (Pw * D_{sw} / SN_w) \qquad \text{(eq. 37)}$$

With

$$D_a = 0.036 * \surd (76 / M) \qquad \text{(eq. 38)}$$

$$D_w = 3.6 * 10^{-6} * \surd (76 / M) \qquad \text{(eq. 39)}$$

where D_{sa} = diffusion coefficient in the gas phase in soil,
D_{sac} = diffusion coefficient in the gas phase in concrete,
D_{sw} = diffusion coefficient in the water phase

in soil,
D_a = diffusion coefficient in free air,
D_w = diffusion coefficient in free water,
D_{ef} = diffusion coefficient in soil,
CN_a = volume phase of gas fraction in concrete,
CN_w = volume phase of liquid phase in concrete,
CN_s = volume phase of solid phase in concrete.

$$J1 = ((D_{sa} / L_c) * (D_{sac} / d_c)/((D_{sa} / L_c) + (D_{sac} / d_c)))* (C_{sa} - C^{o}_{ba}) \quad \text{(eq. 40)}$$

$$J2 = D_a * (C_{sa} - C^{o}_{ya}) / X_a \quad \text{(eq. 41)}$$

$$J3 = C_{pw} * Ev / 24 \quad \text{(eq. 42)}$$

$$J4 = (D_{ef} / L_c) * ((C_{sa} - C^{o}_{ya}) * SN_a / Pa) \quad \text{(eq. 43)}$$

IF $J3 + J4 < J2$ THEN $J = J3 + J4$ (eq. 44)
ELSE $J = J2$ (eq. 45)

$J < 0$ THEN $J = 0$

Outdoors: $J_{oa} = J$

Basement:

\# Open floor $J_{ba} = J$ OR $J_{ba} = J1$

\# Concrete floor $J_{ba} = J1$

where J1 = concrete flux,
J2 = boundary layer flux,
J3 = water evaporation flux,
J4 = diffusion flux water-soil,

Ev = flux of evaporating water,
X_a = height boundary layer,
L_c = length of the diffusion path,
J = total soil flux,
J_{oa} = total flux outdoor air,
J_{ba} = total flux basement air,
C^o_{ya} = initial background indoor or outdoor concentration (y = b (basement) or o (outdoor)),
d_c = thickness of the concrete in basement wall.

2.4.5. *Dilution calculation*

The following equations are used to calculate the dilution of outdoor air:

$$Vf = Vg * Sz / L \qquad \text{(eq. 46)}$$

where Vf = dilution velocity,
Vg = mean wind velocity,
Sz = Pasquill dispersion coefficient in vertical direction, weather stability class D, (m)
L = length of contaminated area, (m)

$$Vg = (V_Y + V^*) / 2 \qquad \text{(eq. 47)}$$

V_Y = wind velocity at a height Y,
V^* = friction velocity,

$$V_Y = \ln (Y / sr) * V^* / k \qquad \text{(eq. 48)}$$

IF sr > Y THEN $V_Y = 0$

where Y = breathing height,
sr = surface roughness,
k = Karman constant (0.4),

$$V^* = k * V_h / \ln (h / sr) \qquad \text{(eq. 49)}$$

where V_h = wind velocity at a height of h,
h = height (10 m),

$$Sz = Co * 0.2 * L^{0.76} \qquad \text{(eq. 50)}$$

$$Co = (10 * sr)^{(0.53 * L^{-0.22})} \qquad \text{(eq. 51)}$$

where Co = correction factor for roughness length.

2.4.6. *Calculation of contaminant concentration in air*

The following equations are used to calculate the concentration of contaminants in outdoor air, indoor air and basement air:

$$C_{oa} = \overset{o}{C}_{oa} + J_{oa} / Vf \qquad \text{(eq. 52)}$$

where C_{oa} = contaminant concentration in outdoor air, (outdoor air concentration should not exceed the soil air concentration, unless the initial concentration is already exceeding the soil air concentration)

$$C_{ba} = \overset{o}{C}_{ba} + J_{ba} * A_t / (Vb * R_a) \qquad \text{(eq. 53)}$$

where C_{ba} = contaminant concentration in basement,
R_a = ventilation rate

Open floor:
$A_t = 1 * w$
$A_t = 2 * 0.25 * (1 + w)$