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Hazard Assessment of Chemical Contaminatnts in Soil

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SUMMARY

This report describes methods for assessing hazards to man and other organisms in the environment when they are exposed to soil contaminants resulting from past waste disposal, spills, leaks and local aerial pollution, but not from more diffuse aerial deposition, such as acid rain.

Hazard assessment is based on a comparison of maximum tolerable exposure levels (MTEL) with the estimated or measured environmental exposure levels (EEL). The MTEL is derived from toxicological experiments with experimental species, taking into account an appropriate safety factor.

The potential effect of chemicals on man is estimated from animal dose-response toxicity studies, using oral, dermal and, when appropriate, inhalation exposure routes. Epidemiological studies as well as case studies can be a valuable source of additional information. The potential effects of chemicals on other organisms in the environment are estimated from dose-response toxicity tests on indicator organisms, such as mammalian species, higher plants, soil micro-organisms and earthworms. If necessary, tests can be extended to other organisms, such as birds, fish, Daphnia and bacteria.

In this report particular attention is paid to the assessment of exposure levels. The level and route of exposure of organisms in the environment (including man) depends on the distribution of the chemical between the solid, gaseous and liquid phases. The duration of the exposure depends on the mobility and rate of degradation of the chemical and the contamination characteristics. The partitioning of a chemical between the solid, liquid and gaseous phases can be estimated from the physico-chemical properties of the chemical and soil, whereas degradation rates usually have to be measured. The chemical and soil properties having most influence on exposure are described and methods for their determination are summarised.

A detailed mathematical model, which can be used to estimate total human exposure by oral, inhalation and dermal routes, is presented. Although not

fully validated, it gives an indication of the most important exposure routes and the level of exposure.

A step - wise approach to hazard assessment for man is recommended. The first step is an initial evaluation to establish whether potential exposure exists. If not, no further assessment is required. If there is a potential exposure, a preliminary assessment is carried out by comparing MTEL values with EEL values calculated using the Human Exposure to Soil Pollutants (HESP) model. The HESP model has the advantage that it calculates not only the total exposure of man to soil contaminants, but also calculates the equilibrium concentrations of the contaminants between various environmental compartments. This allows comparison of exposure levels with generally accepted ambient environmental exposure standards, e.g. air-, ground- and surface water quality guideline levels. If the calculated EEL exceeds the MTEL for a particular exposure route then EEL values should be measured. If the measured EEL exceeds the MTEL, a hazard is likely, and a risk assessment should be carried out to estimate the probability of the hazard being realised under local circumstances (this step is beyond the scope of this report).

Hazard assessment for other organisms in the environment should be conducted following the same principles as for man. MTEL values are determined using key indicator organisms, preferably those which are relevant for the contaminated site.

The exposure assessment for man is illustrated using DDT, toluene and zinc as examples. The model calculations suggest that, as expected, for highly volatile compounds the inhalation route is the most important. For water soluble substances which are poorly sorbed by soil, ingestion of residues taken up by crops can be important. For compounds which bioaccumulate, such as DDT, ingestion via meat and dairy products can be an important exposure route. For many compounds inhalation of dust and dermal sorption appear to contribute little to the total exposure.

A. INTRODUCTION

The focus of environmental interest and concern evolved from water and air pollution in the 1950s to the 1970s to soil pollution in the 1980s partly as the result of the discovery of many locations with contaminated soil. Cases like "Love Canal" in the USA in 1976 (Whelan, 1985) and Lekkerkerk in the Netherlands in 1980 (Baas et al., 1984), where houses were built on former chemical dump sites have been widely reported. Causes of local soil contamination include burial of hazardous wastes, spills and leaks of chemicals and fuels and local aerial pollution.

There has been increasing concern about possible effects of contaminated soil on human health and the environment. Making a balanced response to this concern and deciding on remedial measures has been hampered for many years by a lack of objective and systematic methods to establish whether a situation poses an unacceptable hazard to man or the environment.

Recognising the need for reliable methods to judge the hazard for man and environment of a polluted site, ECETOC established a Task Force with the following terms of reference :

- indicate exposure routes for man and other relevant organisms in the environment of chemicals in soil and their relative contribution to total exposure;

- define minimum set of data required for a hazard assessment of chemical contaminants in soil;

- propose a practical system of hazard assessment of chemicals in soil for man and other relevant organisms in the environment.

In the past, much emphasis has been given to toxicological effects of chemicals to man and other organisms in the environment. Tests methods were established by OECD (1981, 1984, 1988). The results of such tests permit the establishment of Maximum Tolerable Exposure Levels (MTELs) using appropriate safety factors.

This report pays particular attention to the assessment of exposure of man to chemical contaminants in soil.

B. BACKGROUND

Soil consists of minerals, organic matter, water, gases and biota. Soil forming processes transform the parent material (e.g. original rock or geological deposit) into soil. Important soil forming processes are dissolution and movement of inorganic and natural organic substances by infiltrating rain and fluctuating groundwater levels. Plants and other biota as well as factors such as flooding, gravity, wind, solar radiation and temperature changes also contribute to soil formation. The organic matter is derived from dead plants and animals.

Soil is teeming with life; 1 hectare of land can support more than a million earthworms and millions of other animals such as mites, centipedes, beetles and ants, along with countless microorganisms. One hectare of soil can contain 1 ton of earthworms and more than 10 tons of microorganisms. Earthworms help maintain a porous soil structure and are an important source of food for some species of wildlife. Microorganisms play an essential role in processes such as nutrient recycling and decomposition of debris. Although soil animals and microorganisms are not readily visible they, like plants, are important environmental organisms.

No completely uncontaminated soils can be found. Through air transport natural and/or man-made contaminants have been deposited in areas at large distances from their emission source. This phenomenon contributes to the background concentration of chemicals in soil. The increasing sensitivity of analytical techniques has enabled detection of chemicals at levels which were earlier undetectable. Detectability, however, is not synonymous with unacceptability. In addition to such diffuse contamination, soils can contain chemicals such as fertilisers, plant protection chemicals, etc. as a result of cultivation practices.

This report does not deal with changes in soil quality caused by more diffuse aerial deposition or cultivation practices, although these cannot be completely neglected because they may contribute to background levels. The soil in relatively uncontaminated areas such as designated nature conservation areas

therefore may contain xenobiotic compounds or higher than normal levels of natural elements which are unrelated to local soil pollution (Edelman, 1983). In particular, the natural levels of inorganic elements e.g. heavy metals, vary widely from place to place.

The complexity of the situation as described above calls for a systematic and consistent approach to the judgement of soil pollution situations. Site specific factors, variable background levels and fluctuating and sometimes widely varying environmental conditions (e.g. climate, fauna and flora etc) should always be considered.

This report deals especially with soil contamination in relatively restricted areas resulting from localised sources such as :

- accidental spills;
- leakage from pipelines and storage tanks;
- disposal of effluents via soak away;
- leaching of chemicals from landfills;
- local aerial deposition.

Pollution resulting from such localised sources is characterised by the long term presence of chemical contaminants tending to an equilibrium situation between various environmental compartments. The same approach to hazard assessment may, however, also be applied to situations where sewage sludge containing chemical contaminants is used in cultivation practices. In the latter case the concentration of chemical contaminants introduced into the soil is generally low leading to a local equilibrium in a relatively short time period.

Exposure to the human being may occur where they live near or on a landfill or close to an emission source. Human exposure may also result from the underground spread of contaminants from landfill, from existing industrial sites or from abandoned industrial sites which are reused for e.g. residential areas, playgrounds, or agricultural purposes.

Soils contaminated with chemicals may give rise to exposure of a variety of other living organisms. Attention should also be given to the direct exposure of environmental species (plant or animal).

This report will consider which data are required and how they may be used to assess the hazard of chemicals present in the soil. Emphasis is put on the determination of the exposure levels, especially in relation to man. A step-wise approach is proposed. A first step in the process is an *initial evaluation* to establish whether a potential exposure exists. If a potential exposure may occur the next step is *exposure level estimation* using a computer model (HESP) to calculate potential environmental exposure levels.

Although the same principles can be followed to assess the hazard for other organisms in the environment, this is not worked out in such detail. Only a general scheme is discussed.

The information required to carry out both hazard assessments is described in chapter C. In chapter D the hazard assessment scheme is presented. Chapter E presents a number of examples of assessment of the hazard to man of contaminants in soil. The human exposure assessment model is described in detail in Appendix 3.

The unambiguous use of some key terms is of utmost importance; the definitions of those used in this report are presented in Appendix 1.

C. DATA REQUIRED FOR HAZARD ASSESSMENT

1. *INTRODUCTION*

The many different hazard assessment schemes available are similar in that they require data on the level of exposure of target organisms and the effects of chemicals on these or relevant indicator organisms. Data can be generated in laboratory and field studies.

This chapter indicates the minimum set of data necessary for a hazard assessment. Some tests currently used to provide the required data, but not described elsewhere, are given in Appendix 2.

2. *DATA REQUIRED FOR EXPOSURE ASSESSMENT*

Target organisms can be exposed to chemicals by one or several routes. Ultimately the total exposure concentration and the exposure duration of an organism to a chemical must be known. These depend on the physico-chemical properties of the chemical, the soil properties and the fate of the chemical in the soil. The bioavailability of the chemical to man and/or other living organisms in the environment must also be assessed. Bioavailability is closely related to the concentrations of a chemical in the liquid and gaseous phases; these can be estimated from the total concentration of the chemical present and its partitioning between the solid-liquid-gaseous phases. The degradability of a chemical is also important because this has an influence on the duration of exposure in the case of discontinued input and on the equilibrium concentration in the case of continued input. Degradability may also influence the rate of recovery of wildlife and plants damaged by spillage.

The rates of movement of chemicals within the soil and into the atmosphere and ground water are closely related to the concentrations of these chemicals in the gaseous and liquid phases. The most important mechanisms

for movement are diffusion in the gaseous phase, mass transport in the liquid phase or erosion of contaminated solid matter by wind and water.

The exposures of man and of other environmental organisms to contaminants in soil will be different and are discussed separately. Nevertheless, most of the parameters required for human exposure assessment will also be needed to assess the exposure of other environmental organisms.

The model developed to assess human exposure is described in detail in Appendix 3. The model uses a small number of parameters to characterise the chemical contaminant, the soil and the site. These are the "variable parameters" described in the sections 2.1, 2.2 and 2.3. All other, "fixed", parameters used in the model (e.g. relating to housing, behaviour, food consumption, climate) are agreed beforehand and are characteristic for a certain population in a certain region and have been selected conservatively but realistically as shown in Appendix 3.

2.1. Chemicals

To characterise a contaminant the following data are required:

- Molecular Weight.

- Water solubility (S(w) in $mg.l^{-1}$). Solubility in water influences the potential distribution of a chemical in soil.

- Octanol - water partition coefficient (Koc). This gives an indication of the potential of a contaminant to bioaccumulate and sorb to soil organic matter.

- Equilibrium vapour pressure (P in Pa) is the most important property governing the tendency of a compound to volatilise.

- pKa value. The behaviour of weak acids and bases depends on the extent to which they exist as neutral or charged species. The distribution of

chemicals in the different soil compartments will be influenced by the pKa value of the chemical and the pH of the soil.

- Diffusion coefficient in air (Da in m^2/h). This presents a measure of the rate of distribution of a compound in air as a result of molecular diffusion.

2.2. Soil

Soil is a mixture of three phases: liquid and gas present in a solid matrix. Soil characteristics depend on the original rock or geological deposit from which it comes and other parameters such as the organisms living in and on it and climatological factors. With time they modify the original material, giving distinct horizons within the profile (see the podzol below). This modification results in a wide variety of soils differing in physical and chemical characteristics (EEC, 1985). Even within one soil type large variations may occur within a short distance. This section deals with the properties affecting the sorption and the movement of chemicals in soils and consequently their biological availability.

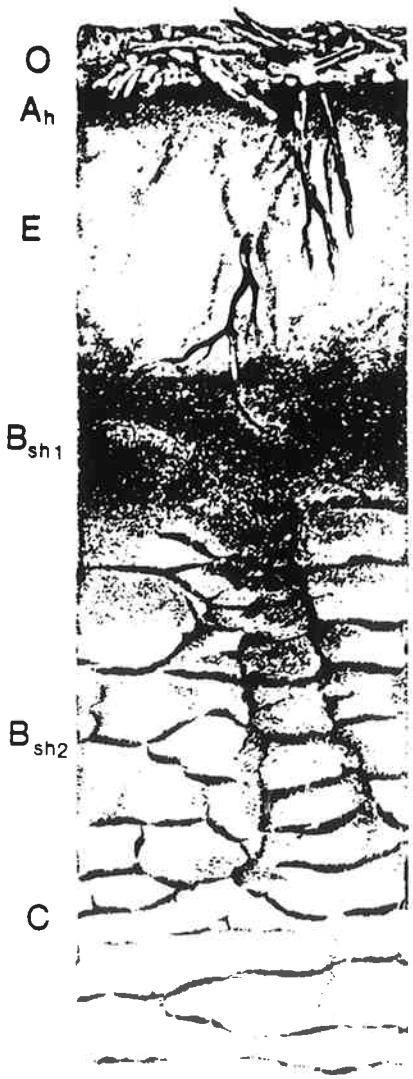
Profile of a podzol

Organic horizon formed from accumulation of organic material deposited on the surface. Accumulation of humidified organic material intimately associated with mineral fraction.

Loss of humus and sesquioxides.

Illuvial concentration of humus and sesquioxides.

Material from which the soil is presumed to have been formed from.



adapted from Mueckenhausen (1982)

2.2.1. Physical Characteristics of Soils

Physical characteristics of soil, such as porosity and permeability affect the movement of water and vapour and hence the movement of the dissolved chemicals. The particle size distribution has a major effect on porosity (cf. Appendix 3 for definitions of units).

- Porosity (SNp in $m^3.m^{-3}$). Porosity is the volume of pore space in the total volume of soil. The pore space can be occupied by air or water. In the saturated zone of the soil, below the water table, all of the pore space is occupied by the groundwater. In the unsaturated zone, above the water table, water occupies only a fraction of the pore space.

- Air and water content (SNa and SNw in $m^3.m^{-3}$). The air and water content of soil influence the mobility of the contaminant in the soil.

- Density (Sg in $g.m^{-3}$). The density is directly related to porosity. The bulk density of mineral soils normally ranges from 1 to 1.8 $g.cm^{-3}$ (Ahlrichs, 1972; Klute, 1986).

- Permeability (P in $m^2.h^{-1}$). Permeability is defined as the rate at which water passes through a given section of core, under the pressure corresponding to the height of the column of soil used for the determination. It is largely dependent on soil porosity.

- Particle size distribution. Generally, three categories of particle size are distinguished: clay, silt and sand, the last being divided sometimes into fine sand and coarse sand. The EEC (1985) defines the clay, silt and sand size fractions as <2 , 2 to 50 and 50 to 2000 μm equivalent diameter respectively. The particle size distribution determines the surface area of a soil, the finest fractions having the largest specific surface.

2.2.2. Chemical Characteristics of Soils

- Organic carbon content (F(oc)). Part of the soil originates from decomposition of plant and animal tissues and newly synthesised microbial products. These humic substances are polymers of high molecular weight composed mostly of aromatic structures with acidic functional groups. Surface soils generally have an organic carbon content varying from 1 to 10 %, but for most cultivated soils it is between 1 and 4 % (Scheffer and Schachtschabel, 1977).

- Cation Exchange Capacity (CEC, in meq.$100g^{-1}$). Clays and humic compounds are negatively charged and cations are bonded to them. The CEC is defined as the quantity of cations which can be exchanged and is a function of the organic matter content, the pH and the content and nature of the clay fraction of the solid phase. The CEC is especially important for positively charged substances and is one of the parameters determining the mobility of these in the soil compartment.

- pH. pH is usually determined in a soil/water mixture. It should be noted that the pH of such a mixture does not necessarily reflect the conditions at the surface of soil particles which often behaves as if it is around 2 pH units below the pH of the solution. Thus, the degree of dissociation of weak acids sorbed onto soil particles is less than in the solution.

- Redox Potential (Eh in mV). As a result of a restricted supply of oxygen some zones of soil become more anaerobic. The redox potential indicates the degree to which conditions are aerobic or anaerobic and thus determines the oxidation state of a compound in soil (e.g. FeII or FeIII). Well drained acid soils have redox potentials up to +800 mV whereas under anaerobic conditions this potential may reach negative values (e.g. - 300 mV). Maximum annual fluctuations up to +800 mV have been reported for soil horizons affected by different groundwater levels (Schachtschabel et al., 1984).

2.3. Other Site Specific Factors

In addition to the properties of the chemical and the soil listed above, climatic factors such as temperature, wind velocity and rainfall together with geomorphological factors influence the fate of a chemical.

If the rainfall intensity is greater than the infiltration rate, surface run-off may occur. Although surface run-off is a common phenomenon for bare soils, little run-off occurs on slopes with dense vegetation (Chorley, 1978).

Knowledge of run-off from snow pack is of increasing importance, because rapidly melting snow packs can suddenly release soil enriched with chemicals (Colbeck, 1981).

In arid areas, movement of chemicals in soil is generally very limited but evaporation can be significant, while strong winds can relocate contaminated soils and flash floods can cause much surface run-off due to poor vegetation cover.

Particularly where nature conservation areas are contaminated, it may be important to list the environmental species living on, in and near the contaminated land. This is required to establish the relevant exposure routes and the key environmental species in the contaminated area. Methods to determine species diversity and density can be found in OECD (1988).

The presence of microbes in soil is necessary for the mineralisation of organic contaminants. Quantification of the microbial biomass gives an indication of the potential for soil biodegradation of organic compounds.

2.4. Fate and Behaviour of Chemicals in Soil

The fate and behaviour of chemicals in soil is affected by a variety of degradation reactions inside the soil compartment and by transfer processes, both within the soil and to other environmental compartments (i.e. air, water and subsoil). Both phenomena determine the exposure pattern and duration. Transfer processes determine the area and targets likely to become contaminated.

2.4.1. Transformation reactions. The rate of degradation provides an indication of the extent to which an organic compound is converted to e.g. soil organic matter, carbon dioxide, nitrogen, methane and water or other decomposition products. The transformation processes can be by abiotic or biotic reactions but in most cases both occur simultaneously. Water is generally ubiquitous and can react with some chemicals. Decreasing soil moisture decreases biodegradation rates in soil as a result of reduced microbial activity.

- Abiotic reactions. The main reactions in the transformation of chemicals are: hydrolysis, redox reactions, photolysis and complex formation. Rate constants of hydrolysis reactions are generally pH dependent and many are available (e.g. Mabey and Mill, 1978). Environmentally relevant pH values range from pH 3 to 9 (more generally 4 to 8).

  Photochemical degradation of chemicals can occur in the top soil either by direct or sensitised photolysis (ECETOC, 1981). This pathway is not very important because it is restricted to the soil layer exposed to sunlight.

- Biotic reactions. Most organic chemicals are degraded in soil and eventually mineralised to inorganic material. Conversion of the parent compound to other products frequently results in a loss of biological activity but in a few cases (e.g. thiophosphates) the initial conversion products are more toxic than the original compound (Korte, 1987).

A great variety of microorganisms capable of degrading chemicals is present in soil e.g. bacteria, fungi, algae. The rate of biodegradation of organic chemicals depends on many other factors such as the inherent nature of the chemical, its concentration and toxicity, the temperature, the moisture content, the presence of nutrients, oxygen, organic carbon, clay, iron- and aluminium oxides and pH. Inorganic compounds such as heavy metals are not biodegradable while some halogenated organic chemicals degrade only slowly. Although biological activity occurs mainly near the soil surface there is evidence in the literature of biodegradation occurring at greater depths (e.g. Aldicarb, Jones, 1986).

Soil can cope with a certain load of chemicals provided the chemical is inherently biodegradable and there is sufficient time. Due to covalent bonding to soil particles, some chemicals may not be bioavailable and will not therefore biodegrade.

While reports show that many types of chemical can be degraded in soil, in many cases a well defined biotic or abiotic degradation pathway cannot be identified in isolated cultures. Pure culture studies may not reveal the true fate of chemicals in natural soils and may not be representative of <u>in situ</u> conditions.

As an example of biotic reactions involving metals, mercury may be mobilised under anaerobic conditions by microbial alkylation leading to volatile mercuryalkyl compounds such as $Hg(CH_3)$ or $HgCH_3Cl$. These compounds may then be transferred to other environmental compartments. Similar reactions are reported for other elements e.g. tin and arsenic (Korte, 1987).

2.4.2. <u>Transfer processes</u>. As soil has liquid, gas and solid phases, the relevant partition phenomena for chemical contaminants are the following:

i) partition between soil particles and soil water. This can be estimated from the octanol-water coefficient, charge and nature of

the solid material;

ii) partition between soil-air and soil particles. For weakly sorbed chemicals vapour pressure movement may be an important transfer mechanism;

iii) partition between soil-air and water. The vapour pressure of the substance and its water solubility are the factors determining distribution.

The transfer of chemical between its sorbed state on soil particles and the pore air is not well understood. Two types of process, which depend on the humidity of the soil should be considered (Chiou and Schoup, 1985). If the water content of the soil is very low there is a direct exchange between the sorbed and the vapour state. When the water content is high there is first an exchange between the soil particle and the surrounding water and afterwards a migration from the water to the pore air. In the case of heavily polluted sites the concentration of a chemical in the water and air phases is controlled by its solubility and vapour pressure rather than by sorption.

Of the three phases, the air and water phases are mobile and therefore determine the mobility of chemicals. This can lead to four types of transfer: diffusion, leaching, run-off and volatilisation.

i) Mobility via the aqueous phase. For chemicals with a low vapour pressure, transfer via the aqueous phase is generally the main transport process in the soil. The potential of a chemical to leach from the surface to the deeper horizons depends on the amount and direction of movement of the water in the soil, which is directly related to meteorological conditions, and on the degree of sorption. Using laboratory experiments it is possible to determine only the relative leaching potential. In the field an assessment of leaching requires a knowledge of the movement of water which is very difficult to determine especially in the zone not saturated with water.

ii) Mobility via the gaseous phase. Chemicals can move within soil or be lost from soil in the gaseous phase. These processes depend on the vapour pressure of the chemical, the degree of sorption and meteorological conditions. Loss from the soil surface depends on the rate of movement of the chemical in both water and gaseous phases to the soil surface (Jung and Otto, 1987).

2.4.3. Models

Models have been developed to estimate the fate and behaviour of chemicals in soil for specific situations. They take into account the effect of soil organic matter, soil hydraulic properties and degradation rates on the leaching of chemicals. They are widely used, especially for pesticide applications, but have not been fully validated under a range of field conditions (Jury et al., 1983; Carsel et al., 1985; Leistra, 1986; Wagenet and Hutson, 1986).

2.5. Exposure Routes

2.5.1. Introduction. Man and other environmental organisms may be exposed to contaminants present in soil via various routes. The relative importance of each depends on the characteristics of the chemical and the soil and the habitat, behavioural and morphological characteristics of the species exposed.

Only the exposure to the original chemical in the soil, and not to its degradation products, will be discussed in this report. If degradation products are formed, a separate assessment of their hazard may be required.

Persistent chemicals may require a more detailed investigation of possible exposure routes than readily degradable chemicals which may disappear before a significant exposure duration has occurred.

When assessing the exposure of organisms it is necessary to distinguish between the concentration of a chemical (as detected by extraction and

measurement) and the concentration available to exert a biological effect. This distinction is especially important for soil. The more strongly a chemical is sorbed to soil particles, the lower its bioavailability.

The significance of the different pathways of exposure to a chemical of organisms at the top of the food chain will depend on the transformation of the chemical by species lower in the food chain.

2.5.2. Exposure routes for man

In this section attention will be paid to the contribution to the total daily intake by man of contaminants via the oral, the inhalational and dermal exposure routes as far as this relates to local soil pollution. To establish total exposure, the background exposure should also be taken into account. The various routes are shown in Fig. 1 and discussed extensively in Appendix 3.

i) The oral exposure route

Exposure by the oral route can occur from:

- the daily fluid intake by man;
- direct ingestion of soil particularly by infants (playing toddlers);
- indirect uptake via food crops, raised on contaminated soil;
- indirect uptake via meat and dairy products from cattle, pigs and poultry fed with feed crops raised on contaminated soil;
- indirect uptake via fish and molluscs, caught in surface waters receiving contaminated groundwater and land run-off.

ii) The inhalational exposure route

The inhalational exposure routes are:

- inhalation of dust, originating from contaminated soil;

- inhalation of vapour released from soil;
- inhalation of air, containing chemical evaporated from the water during a shower.

iii) The dermal exposure route

The dermal exposure routes are:

- infants playing with contaminated soil;
- digging in contaminated soil by adults;
- skin sorption of contaminants via the domestic water supply (when introduced into the model of Appendix 3, this exposure route did not contribute significantly to the total uptake).

2.5.3. Exposure routes for other environmental organisms

The large number of species within each group of organism in various habitats require that specification of the pattern of exposure has to be very general. Based on a rough classification into terrestrial-, soil- and aquatic organisms, the exposure routes for such organisms are shown below and represented in Fig. 2 and 3.

- Micro-organisms may take up contaminants from soil by active or passive membrane uptake processes. Transport through the cellular membrane strongly depends on the membrane composition and the nature and molecular structure of the chemical.

- Soil organisms may be exposed by inhalation of soil air and particles (rats, mice, moles), skin contact with soil and pore water and contact with vapour (arthropods, nematodes) and/or by ingestion of inorganic soil particles, pore water and organic biomass (earthworms).

- Plants may take up contaminants by underground parts, foliar deposition and by direct uptake through leaves.

For plants growing on contaminated soil, roots will have a high potential for uptake through direct exposure. The migration of chemicals from the roots to fruits and seeds is generally low (Ryan et al., 1988). In leafy crops, for example lettuce, transport of chemical to the leaves in the transpiration stream may be important.

For compounds with a low vapour pressure and a very low solubility (e.g. DDT) the uptake through leaves may be a significant exposure route. In areas where the soil is contaminated dry deposition onto leaves of soil dust contaminated with persistent chemicals could also be a significant exposure route for crops.

- Terrestrial animals. Terrestrial animals may be exposed by inhalation of volatile organic compounds and contaminated soil particles, by skin contact with contaminated soil and/or by ingestion of contaminated soil, water and organisms. The dominant exposure routes will normally be the food chain and will be more or less comparable with the routes of human exposure.

  All animals, especially of higher order, can be indirectly exposed before and after birth by transfer of contaminant in the mothers tissue to progenies (e.g. for birds and reptiles by accumulation in eggs and for mammals through placenta and mothers milk).

- Aquatic organisms. Water bodies may receive contaminated groundwater or surface water (via run-off). The chemicals, either dissolved or sorbed to particles, may be distributed over large areas.

  Aquatic organisms may be exposed by direct uptake through the gills (fishes), by sorption through the skin (e.g. fishes, molluscs, nematodes) and/or ingestion of suspended matter, sediment and contaminated biomass (e.g. benthic fishes, arthropods, shellfish).

  Chemicals strongly bound to particles may pass into the food chain mainly by organisms living in and feeding on sediment or by filter-feeders (e.g. molluscs). For hydrophobic organic compounds like

polycyclic aromatic hydrocarbons this might be the dominant exposure route to fish. Skin and gill uptake play a more important role as exposure routes with more water soluble compounds such as HCB and methylmercury (Burton and Bennett, 1987).

When contaminants enter the aquatic environment they may be bound by the sediment. If the sediment is not subsequently covered by clean sedimentary material, they can be mobilised by microbial metabolism, bioturbation and redox processes and may constitute a long-term source of exposure to aquatic organisms.

3. *DATA REQUIRED FOR EFFECTS AND DOSE RESPONSE ASSESSMENT*

This section defines the information required to assess the potential of a contaminant to cause adverse effects to man and other environmental organisms.

3.1. Man

Human beings may be exposed via the oral, inhalation and dermal routes. Soil contaminants can enter the human body by each, and often all routes. The relative contribution of each to the total exposure is strongly dependent on the physico-chemical properties of the contaminant.

To make an assessment for man, the following data are desirable:

- the maximum daily oral dose having no adverse effect,
- the maximum daily inhaled dose having no adverse effect, and
- the maximum dermal dose causing no local and systemic effects.

If this information is not yet available it can be obtained from toxicological experiments relevant for the respective exposure route. All available toxicological knowledge is based on volunteer exposure studies, epidemiological studies and case studies.

3.2. Environmental Organisms

The ultimate environmental concern is the care of populations of species rather than individual organisms (Council of Europe, 1981). Because experimental work with populations under field conditions is time consuming and costly, most experimental work in the environmental area is carried out with relatively small numbers of organisms in the laboratory, while exposure duration is often relatively short. The tests aim to establish a dose/response relationship and, based on this, a no adverse effect concentration.

Indicator organisms include plants (monocotylodons and dicotylodons), earthworms, soil microorganisms and if necessary birds, fish and Daphnia.

The reliability of dose/response assessments from single species tests is limited because:

i) effects on few individual organisms under laboratory conditions cannot readily be extrapolated to populations or ecosystems under field conditions, and
ii) results of tests of short term duration cannot reliably be extrapolated to long-term exposure of periods lasting sometimes for several generations.

D. HAZARD ASSESSMENT OF CHEMICALS IN SOIL

1. *INTRODUCTION*

Hazard assessment in the context of this report is defined as the estimate of adverse effects which may result from substances present in soil, due to their exposure level and to their toxicity to man and/or other environmental organisms.

Because the hazard of chemicals in soil depends on the specific characteristics of the site, only a general approach to hazard assessment can be given and not a standardised procedure. These general principles should be applied on a case by case basis.

Knowledge of the intrinsic toxicological properties of a chemical and of the exposure conditions are the principal requirements for a hazard assessment. All desirable data are, however, rarely available and estimates or theoretical assumptions often have to be made. The degree of realism in these estimates determines the reliability of the final hazard assessment; this requires expert judgement.

A risk assessment might be required in some cases. Risk assessment is the estimation of the probability that a hazard occurs under site specific conditions. This report is restricted to hazard assessment but indicates when a risk assessment may be required.

Unlike many hazard assessment schemes, the approach adopted here takes into account not only the hazard to man but can also be applied to other environmental organisms.

2. *CONCEPT OF HAZARD ASSESSMENT*

The hazard assessment of chemical substances involves a comparison of the Maximum Tolerable Exposure Levels (MTEL) with estimated or measured Environmental Exposure Levels (EEL). The main parameters to be determined

are thus the MTELs for each exposure route (e.g. inhalation, oral and dermal routes) and the EELs for the same routes. The quality and availability of data, whether measured or estimated, must be considered during the hazard assessment process.

3. *MAXIMUM TOLERABLE EXPOSURE LEVEL*

The MTEL is defined as the maximum dose of chemical taken up by a target organism or the concentration to which the organism is exposed which does not lead to an adverse effect over prolonged exposure periods. The establishment of MTELs for man and other environmental organisms is discussed separately.

3.1. Man

The MTEL for each specific exposure route can be established from an estimate of the no-adverse effect dose or concentration derived from the dose/response findings in investigations involving each relevant exposure route and applying of appropriate safety factors. The safety factor should be conservative but realistic and take account of inter species differences, variations in sensitivity of the target species and the quality of the data. Often a safety factor of 100 can be used but it may be higher in cases where the adverse effects could be irreversible or where there is a high degree of uncertainty associated with the data. For carcinogenic chemicals safety factors may be inappropriate and other approaches have been used in estimating tolerable exposure.

Examples of MTEL's are the Acceptable Daily Intake (ADI) and Tolerable Daily Intake (TDI) for the oral exposure route. TLV's , MAC and MAK values and other similar workplace limits are developed to protect workers but may be useful as reference values after application of extra safety factors to account for the total population, 24 hours day and life time exposure. Before using such limits, however, the data on which they are based should be examined, particularly with regard to the type of toxic activity each is intended to control. Maximum Immission Concentration

(MIC) values can be used as MTEL's for the aerial exposure route. Where agreed limit values exist there is no need for further testing.

3.2. Other Environmental Organisms

As indicated in Chapter C 3.2, tests on such organisms suffer from a number of disadvantages. Some of the disadvantages can be overcome by selecting the right key organism(s), choosing sensitive toxicological parameters and applying a correct dose/response test. The MTEL can be established by applying a conservative but realistic safety factor to the No-Observed Effect Level (NOEL) as derived from the test.

The establishment of a no-adverse effect concentration for a small number of individuals can indicate the effect of soil pollutants on populations of species or ecosystems. Such an extrapolation is complicated because it requires the selection of parameters which allow quantification of the health state or the condition of a population or an ecosystem. Such parameters include decrease in species diversity, decrease in reproduction rate, changing standing crop biomass, changing gross or net primary energy production etc.. These parameters are not always well understood and often difficult to quantify (Schaeffer et al., 1988; Dutch Health Council, 1989).

The method of Slooff et al. (1986) correlates the lowest NOEL or lowest LC_{50} found from a set of laboratory tests on a given chemical, and the NOEL for ecosystems of the chemical determined under (semi-)field conditions. The proposed procedure also includes a description of the minimum set of acute toxicity data that are needed. The Dutch Health Council (1989) discussed different procedures including the one developed by EPA (1984) and proposed an alternative procedure. In a first step the use of three fixed test species for each specific environmental compartment is recommended. Although these approaches are attractive from a water and soil management point of view, basically they lack scientific validation.

4. *EXPOSURE ASSESSMENT*

Exposure assessment is "the process of measuring or estimating the intensity, frequency and duration of exposure to a hazardous agent" (US Nat. Res. Council, 1983, adapted).

It is essential to determine each route via which man and/or other key organisms in the environment are exposed to chemical substances present in soil. The first step is the characterisation of the contaminant source (cf Chapter C - 2).

In addition, information on the local environment, its sensitivity and uniqueness as well as its use by man (e.g. residential, agricultural, industrial) is required. This information is necessary for the selection of the relevant exposure routes and key environmental species.

The next step involves estimation of the relative contribution of each exposure route to total exposure and quantification of the exposure via each route to determine the EEL's. Finally estimation of the exposure duration and pattern is required.

4.1. Man

A step-wise approach is advocated to assess the hazard to man. The first step in the process is an *initial evaluation* to establish whether a potential exposure exists. If so, the next step is an *exposure level estimation* using a computer model to calculate potential environmental exposure levels (EELs).

This approach is based on a report by Golder Associates May 1986 (Reades and Gorber, 1986) relating to decommissioning a polluted site. A more comprehensive approach has been developed by Veerkamp and ten Berge to estimate the exposure levels of soil contaminants to man (see Appendix 3). A number of exposure routes were identified and subsequently quantified. The exposure routes are ingestion, inhalation and dermal sorption.

These main exposure routes can be subdivided on the basis of the intermediate environmental compartment involved. The following subdivision has been used throughout the programme:

- direct ingestion of soil or dust
- dermal exposure to soil or dust
- inhalation of particulate matter
- inhalation of vapours
- ingestion of crops
- ingestion of meat and dairy products
- ingestion of fish
- ingestion of drinking water
- exposure when bathing in contaminated water
- dermal exposure during bathing.

The "Human Exposure to Soil Pollutants" (HESP) model described in Appendix 3 requires a limited number of input data and a set of agreed, conservative but realistic assumptions, e.g. regarding housing, behaviour, food consumption and climate. The model uses parameters relevant to the Dutch population, but can be adapted to situations in other countries. Although during the development of the HESP model many literature references and experimental data were evaluated, the model still requires validation and should be used with caution.

If the *preliminary exposure level estimation* indicates significant exposure, a *definitive exposure assessment* should be carried out. This definitive exposure assessment should be based on measurement of the exposure concentrations and consideration of the degree of retention in the body (Bennett, 1981).

Apart from exposure resulting from contaminated soil, man can be exposed to background levels of the same contaminant. Background contaminant levels may contribute significantly to total human exposure through air, drinking water and food.

For a number of chemicals background concentrations in air, drinking water and various foods are known. These concentrations may vary from area to area, while the actual intake into the human body will vary depending on feeding habits, food choice, food availability etc.. In a number of countries data are available on the average daily uptake of contaminants from the food (Buss and Linsay, 1978; De Vos et al, 1984; Staarink and Hackenbrack, 1987; FAO/WHO, 1987).

4.2 Other Environmental Organisms

Because of the vast number of different species of environmental organisms (e.g. plants, terrestrial (including soil) animals, soil microorganisms) and their totally different morphological, physiological and behavioural properties it is extremely difficult to assess the exposure characteristics for each species involved. As part of the source characterisation, however, it is possible to select a few key plant and animal species representing various habitats and behavioural patterns at the contaminated site. For each selected key organism the exposure characteristics should be evaluated. Use of mathematical models may increase understanding and provide estimates where actual measurements are lacking. Attention must be paid to the possibility of biomagnification of contaminants in the food chain especially where environmental organisms are used as human food. The metabolism of contaminants by environmental organisms is another important factor to consider; generally, but not always, this leads to the formation of substances with significantly lower toxicity.

The duration of exposure is an important factor when assessing the exposure. It is important to know if a contaminant is transformed, and if so, what the transformation rate is and which metabolites are formed. An estimate can then be made of the period during which the contaminant is likely to be present and how its concentration will decrease with time.

5. *HAZARD ASSESSMENT*

As indicated above, the assessment of the hazards of chemicals in soil is essentially the comparison of the Maximum Tolerable Exposure Levels (MTELs) with the estimated or measured Environmental Exposure Levels (EELs). Although this may seem a simple task, in reality it is rarely simple to judge and often non-, or only partly, quantifiable parameters have to be taken in to account. For those reasons a hazard assessment of chemicals present in soil is a task for experts.

To simplify the process of Hazard Assessment, a step-wise approach is recommended (see Fig 4).

5.1. Man

5.1.1. Preliminary Hazard Assessment. If the initial evaluation has indicated a potential exposure, the next step is the comparison of the potential EELs, as calculated with the preliminary exposure assessment model, with the MTELs of the same exposure routes.

If all EELs are lower than their respective MTELs, no hazard will exist because of the conservative approach taken in their estimation. Consequently no further work is required.

If one or more EELs exceed their respective MTELs, a potential hazard may exist and a definitive hazard assessment is required.

5.1.2. Definitive Hazard Assessment. This should be based on measurement of environmental exposure levels. These measurements can be restricted to those exposure routes which, are shown by the exposure assessment model, to be relevant and significant.

When comparing the measured EELs with the MTELs two situations which may lead to a significant hazard can be distinguished:

i) An EEL exceeds the MTEL, indicating that a potentially significant hazard exists.

ii) There is more than one exposure route, and although the EEL of each does not exceed the individual MTELs the combination of routes leads to a total exposure which exceeds the potentially hazardous level. This second possibility requires expert judgement to assess whether or not a potentially hazardous level is exceeded since exposure duration, intake versus uptake and metabolic and pharmacological data have to be taken into account.

5.2. Other Environmental Organisms

Assessment of hazard to environmental organisms or populations/ecosystems follows the same principles as human hazard assessment. EELs are to be compared with MTELs. If an EEL is lower than the MTEL of the same route, the hazard is acceptably low. If more than one significant exposure route exists expert judgement is required to assess if a potentially hazardous level is exceeded. If the EEL is greater than the MTEL then further studies should be carried out, preferably under field or simulated field conditions, to determine if there is a hazard under realistic conditions. In the absence of such further data it should be presumed there is a potential hazard.

Many of the principles outlined above are also accepted and applied by DECHEMA (1989) without explicitly recommending a step-wise approach to protect man and the environment from the adverse effects of heavy metals present in soil.

The primary aim of environmental conservation is the protection of populations of species and ecosystems, rather than individual organisms (Council of Europe, 1981). A second aim may be the maintenance of soil functions in relation to the current or anticipated soil use. The acceptability of particular concentrations in soil depends on the local situation and is determined by its sensitivity, uniqueness and properties.

Small, transitory effects are considered of no ecological significance if the size and duration of the effect is less than those caused by natural processes; for example, the transitory effects of temperature changes and rainfall on soil microorganisms and earthworms.

Movement of chemicals in soil is generally slow compared to that in water and air. With localised soil contamination the area affected will be relatively small and the effect on populations of environmental species restricted. If a chemical also has a short persistence populations may quickly recover from any toxic effects by reproduction of survivors or immigration. Thus testing of the toxicity of chemicals to plants and soil organisms is generally not necessary for chemicals which rapidly degrade.

Hazard assessment must take into account that some chemicals, for example heavy metals, are naturally present in the environment. The environment has sometimes adapted to high localised concentrations and particular plant and animal associations have developed. Such areas are sometimes protected and ecologically regarded as valuable. On the other hand if the chemicals are introduced to other locations they may exert an adverse effect.

E. EXAMPLES OF HUMAN HAZARD ASSESSMENT

1. *EXAMPLES PUBLISHED IN THE LITERATURE*

Exposure route assessment and comparisons of EELs with MTELs, calculated according to the AERIS model, have been carried out to determine safe levels for soil pollutants at two former refinery sites in Canada (CCREM, 1988 - a, b). Results from exposure route models in this study indicate that the total exposure estimates are generally dominated by one or two routes. For highly volatile substances such as benzene, the inhalation of vapour is the major route; the exposure duration generally decreases rapidly with time due to the evaporation of the substance. For water soluble substances, poorly sorbed by soils, the ingestion of crops dominates over other routes because this group of substances is relatively easily translocated from ground water into plants via root uptake. The direct ingestion of soil and indoor dust accounts for the largest portions of the exposure estimates of relatively persistent and lipophilic substances. Inhalation of total suspended particulate matter and dermal sorption generally seem to contribute little to the total intake for all types of substances.

Another important result from this study is that exposure route analyses frequently reveals that the infant is the dominant receptor of soil contaminants. Direct consumption of soil is particularly important for small children in the age group between 2 and 6 years. Most young children tend to ingest relatively large amounts of soil and indoor dust. This phenomenon has been found also by various other authors (Kimbrough et al., 1984; Van Wijnen and Stijkel, 1988).

2. *EXAMPLES OF HAZARD ASSESSMENT USING THE HESP MODEL*

Three examples of hazard assessment for contaminants in soil will be discussed in this section. The three soil contaminants chosen are DDT, toluene and zinc. The results of the calculations presented and discussed below are based on data taken from Tables 1-4 and derived from the Human

Exposure to Soil Pollutants (HESP) Model described in Appendix 3. The calculations are based on assumptions described and explained in that Appendix.

The model uses the variable parameters listed in Table 1 and assumes that (1) the contaminated area is 300 m long and 100 m broad, and that the contaminants (2) are present in the top 1.5 m of the soil, (3) uniformly distributed and (4) present at a constant concentration at the levels indicated in the respective Tables. It must be emphasised that especially condition (4) may not be realistic and therefore will lead to an overestimation of the exposure as compared with a real situation.

The Tables 2, 3 and 4 show the estimated human exposure to the three soil contaminants. The concentration of the contaminant in soil, which forms the basis for the calculations, is indicated at the top of the table. The calculated exposure to the soil contaminant (at the indicated soil concentration) via the various exposure routes and the total exposure is then presented. The calculations are made for both an adult and a child. The exposure, expressed in $mg.kg^{-1}.day^{-1}$ sorbed, makes a direct comparison with the ADI possible. Finally the calculated concentrations of the contaminant in various environmental compartments is given. The resulting data make a comparison with established criteria possible.

It must be emphasised that the results of the model calculations should be treated with care. Although the assumptions are "conservative but realistic" and where possible based on empirical data and validated literature publications, the results are nevertheless no more than an approximation to reality.

2.1. DDT

The Acceptable Daily Intake (ADI) for DDT was set at 0.02 $mg/kgbw^{-1}$ (FAO/WHO, 1986).

By far the major background uptake of DDT is derived from food. The total dietary intake in the USA in 1970 was 0.0004 $mg.kgbw^{-1}.d^{-1}$ for the sum of

DDT, DDE and TDE which was half the uptake of 5 years before (IARC, 1973). Now 20 years later with DDT phased out in many countries, the background uptake is considered not to contribute significantly to total exposure.

The calculations listed in Table 2 show the exposure of adults and children to a concentration of 5 $mg.kg^{-1}$ DDT in soil. It is evident that vegetables and meat/dairy products are the most significant exposure routes for DDT. Other exposure routes are one or more orders of magnitude less important. For children, exposure to soil and dust, either by ingestion or dermal contact, cannot be completely disregarded although these routes together contribute only about 5% to total exposure. Exposure of children to DDT is about 5 times higher than exposure of adults when expressed in $mg.kgbw^{-1}.d^{-1}$.

Using the HESP model, it is possible to calculate the total exposure of adults and children to DDT resulting from increasing concentrations of DDT in soil. It can be seen from Fig. 5 that the ADI for DDT will only be exceeded for adults at extremely high concentrations of DDT in soil. For children the ADI will be exceeded when the DDT concentration in soil is higher than about 100 $mg.kg^{-1}.d^{-1}$.

The bend in both uptake curves is caused by the limited water solubility of DDT which in turn is the limiting factor for uptake in vegetables and grass, the food for cattle. After the bend in the curve the uptake is strongly determined by ingestion and dermal uptake of soil and dust.

From the lower part of Table 2 it can be seen that the concentration of DDT in drinking water will not exceed the EEC drinking water standard at a soil concentration of 5 $mg.kg^{-1}$. Nevertheless, at that concentration in soil the calculated concentration of DDT in roots of vegetables and in milk does exceed the residue limits (0.1 $mg.kg^{-1}$ vegetable and 0.05 $mg.kg^{-1}$ milk) set in The Netherlands. This result requires actual measurement of the DDT concentration in these foodstuffs. The residue limits for above ground parts of vegetables and for meat are not exceeded (Bestrijdingsmiddelenwet, 1962).

2.2. Toluene

No Acceptable Daily Intake figure exists for toluene. Ambient background levels in food and drinking water are not available. Thus comparison of the total sorbed dose with a maximum tolerable exposure level of toluene is not possible.

The data given in Table 3 indicates that the three most important exposure routes for toluene are inhalation of vapour, ingestion of vegetables and consumption of drinking water. The last assumes permeation of toluene through polyethylene drinking water pipelines present in contaminated soil. It appears that the exposure of children to toluene present in soil is about 2.5 times higher than of adults per unit body weight.

By changing the hypothetical concentration of toluene in the soil Figure 6 shows that for both adult and child the total sorbed dose levels off at a concentration of about 2000 $mg.(kgbw.d)^{-1}$. This is caused by the limited water solubility and the vapour pressure of toluene.

The only reference values for toluene available which may be used as maximum tolerable exposure levels (MTEL) for comparison with the calculated environmental exposure levels (EEL) are concentrations in air. Usable reference values are the TLV-TWA and the WHO Lowest Observed Effect Level which are both set at 375 $mg.m^{-3}$ (ACGIH, 1988-89) and the WHO ambient Air Guideline level which is set at 7.5 $mg.m^{-3}$ (WHO, 1987).

Air monitoring data suggest that 0.75 $\mu g.m^{-3}$ could be regarded as an upper-bound background level to which all populations are exposed (WHO, 1987). The ambient air guideline level for toluene proposed by the WHO will not be exceeded no matter what the toluene level in soil (Figure 7). This is due particularly to the limited volatility of toluene. It should be stressed here that the higher concentrations of toluene in the soil as indicated in Fig. 7 are hypothetical and unrealistically high. Nevertheless these concentrations do not exceed the WHO ambient air guideline level.

2.3. Zinc

Zinc is an essential element and normally present in food and water. The daily zinc requirement for children is 6 mg and for adults 7.5 to 18 mg. Long-term consumption of 200 mg zinc per day causes no adverse health effects (WHO, 1973). Natural levels of zinc in soil in The Netherlands range from 6 mg/kg^{-1} in sand to 190 mg/kg^{-1} in loam (Edelman, 1983).

The ADI range for zinc is (provisionally) set at 0.3-1.0 $mg.kgbw^{-1}.d^{-1}$ (JECFA, 1982).

The most important human exposure routes for zinc in soil are ingestion of vegetables and ingestion and dermal sorption of soil and dust (cf Table 4). The latter two routes are particularly relevant for children. Drinking water causes no exposure because zinc does not permeate through drinking water pipes. Exposure of children to zinc present in soil is about 4 times higher than in adults per unit body weight.

The total sorbed zinc dose for adults and children in $mg.kgbw^{-1}.d^{-1}$ by all exposure routes as a function of the zinc concentration in soil is shown in Figure 8. From this figure it appears that the lower limit of the ADI is exceeded for a child at a zinc soil concentration of about 2,000 mg/kg^{-1}. The upper limit for a child will be exceeded only at zinc concentrations in excess of 20,000 $mg.kg^{-1}$. For an adult even the lower limit will not be surpassed. Accepting that the higher limit of the ADI should not be exceeded, according to the HESP model zinc concentrations in soil below about 20,000 $mg.kg^{-1}$ are not hazardous for man. When the zinc concentration in soil exceeds 2,000 $mg.kg^{-1}$ it may be necessary to carry out a definitive hazard assessment but only when families with small children consume significant quantities of vegetables grown in their own garden and the children play often on bare contaminated soil.

At a soil concentration of 300 $mg.kg^{-1}$, the concentration in ground water will reach a level of 5 $mg.l^{-1}$, being the EEC drinking water guide level. This level however is not health related but based on the organoleptic properties of zinc (EEC, 1980). Treatment of the ground water will

normally be required when it is to be used for the preparation of drinking water and contains more than 5 $mg.l^{-1}$.

2.4. Conclusions

The results from the exposure assessment model indicate the following trends:

i) children generally receive a higher exposure per unit body weight of soil contaminants compared with adults. Soil/dust ingestion by small children is important.

ii) in the total exposure estimates generally one or two routes dominate.

iii) for highly volatile compounds the inhalation route is important.

iv) the uptake of soil contaminants via crops is the most significant exposure route with all three examples. For a persistent and lipophilic compound like DDT, the ingestion of meat and dairy products is an important exposure route.

v) inhalation of dust and dermal sorption seem to contribute little to total exposure for all three substances.

F. CONCLUSIONS AND RECOMMENDATIONS

Hazard assessment of chemicals in soil for man and environmental species is possible by the approach outlined in this report.

For human hazard assessment a step-wise approach is recommended. If an initial evaluation indicates a potential exposure, the following steps are advocated:

Step 1 - Preliminary Hazard Assessment: comparison of Maximum Tolerable Exposure Levels (MTEL) derived from experimental data with the Environmental Exposure Level (EEL) calculated using the Human Exposure to Soil Pollutants model (HESP, see Appendix 3). As the HESP model uses conservative but realistic assumptions, it can be concluded when the EEL is lower than the MTEL, no hazard exists. Where the EEL is higher than the MTEL it is generally necessary to proceed to step 2.

Step 2 - Definitive Hazard Assessment: comparison of MTELs with measured EELs, but only of those exposure routes which, according to the HESP model, significantly contribute to total exposure. If the measured EELs are lower than the MTELs, no hazard will exist. In the opposite situation a potential hazard exists and a risk assessment is generally required.

Step 3 - Risk Assessment: this step involves the assessment of the probability that the potential hazard is realised under the local circumstances. This step is beyond the remit of the present Task Force.

For calculations using the HESP model data only a limited number of variables are required. These data include chemical properties of the contaminant, soil characteristics and contaminant concentrations at various soil depths. In addition the model requires a large number of fixed parameters relating to the climate, housing, human behaviour and food consumption which vary in different countries/regions or cultural groups and should be established beforehand.

The HESP model has the advantage that it calculates not only the total exposure of man to soil contaminants but also the equilibrium concentrations of

the contaminants between various environmental compartments. This allows comparison of exposure levels with generally accepted ambient environmental exposure standards, e.g. air-, ground- and surface water quality guideline levels.

When using the HESP model and carrying out hazard assessments the following data were often lacking: background exposure levels and natural exposure levels, average dietary intake levels for contaminants and the amount of food consumed from gardens. It would be useful if such data could be estimated and/or determined.

Hazard assessment for other organisms in the environment exposed to contaminants present in soil is yet in its infancy. In many cases MTELs are not available and exposure routes not known or quantifiable. The Task Force recommends that this matter is addressed systematically for key environmental species.

Although most of the general conclusions of CCREM (CCREM, 1988 a,b) are parallelled by the results of the exposure calculated by the HESP model, further investigations are required to verify whether the estimated exposures are realistic. Although during the development of the HESP model many literature references and experimental data were evaluated, the model still requires validation and should be used with caution.

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TABLE 1

VARIABLE INPUT PARAMETERS FOR THE EXPOSURE ASSESSMENT MODEL

PARAMETER	SYMBOL	UNITS	DDT	TOLUENE	ZINC
CHEMICAL CHARACTERISTICS					
MOLECULAR WEIGHT	MW	–	354	92	65
LOG OCTANOL/WATER PART. COEF.	LOG K_{ow}	–	6.19	2,69	–
SORPTION PARTITION COEFF.	K_d	ml/g	–	–	60
WATER SOLUBILITY	S_w	mg/l	$3,2X10^{-3}$	515	60*
EQUILIBRIUM VAPOUR PRESSURE	P	Pa	$2,5X10^{-5}$	$2,9X10^{3}$	$1X10^{-3}$
AIR DIFFUSION COEFFICIENT	D_a	m^2/h	$8,2X10^{-6}$	$8,2X10^{-6}$	$8,2X10^{-6}$
SITE CHARACTERISTICS					
CONTAMINANT CONCENTRATION AT 0 – –1,5 meter		mg/kg	5	10	3000
SOIL CHARACTERISTICS					
ORGANIC CARBON CONTENT	F_{oc}	–		0,02	
POROSITY	SN_p	m^3/m^3		0,5	
AIR CONTENT	SN_a	m^3/m^3		0,3	
SOIL BULK DENSITY	Sg	g/cm^3		1,50	
SOIL ACIDITY	pH			6	

* FOR ZINC, THE WATER SOLUBILITY OF ZINC SULPHATE IS USED

TABLE 2

ESTIMATED HUMAN EXPOSURE BY SOIL CONTAMINANTS

COMPOUND : DDT
SOIL CONC. : 5.0 MG/KG dry weight

PATHWAY	ABSORBED DOSE MG/KG.D	
	ADULT	CHILD
INHALATION		
– VAPOUR	5.05E–09	8.68E–09
– DUST	3.45E–08	5.20E–08
– SHOWER	2.11E–09	3.22E–09
INGESTION		
– SOIL/DUST	2.57E–06	7.98E–05
– VEGETABLES	1.90E–04	6.99E–04
– WATER	5.47E–07	1.91E–06
– MEAT/DAIRY	1.92E–04	1.28E–03
– FISH	2.56E–07	8.16E–07
DERMAL		
– SOIL/DUST	2.29E–06	3.45E–05
TOTALS	**3.87E-04**	**2.09E-03**

IMPORTANT CALCULATED ENVIRONMENTAL CONCENTRATIONS

CONC. IN GROUNDWATER	1.91E–04	(mg/l)
CONC. IN SURFACE WATER	2.74E–06	(mg/l)
CONC. IN DRINKING WATER	1.91E–05	(mg/l)
CONC. IN VEGETABLES ROOT	6.94E–01	(mg/kg fr weight)
CONC. IN VEGETABLES STEM	4.93E–03	(mg/kg fr weight)
CONC. IN MEAT	5.88E–01	(mg/kg fr weight)
CONC. IN MILK	1.73E–01	(mg/kg fr weight)
CONC. IN FISH	8.16E–02	(mg/kg fr weight)
CONC. IN OUTDOOR AIR	1.67E–11	(g/m3)
CONC. IN INDOOR AIR	1.67E–11	(g/m3)
CONC. IN BASEMENT AIR	3.01E–11	(g/m3)

TABLE 3

ESTIMATED HUMAN EXPOSURE BY SOIL CONTAMINANTS

COMPOUND : TOLUENE
SOIL CONC. : 10.0 MG/KG dry weight

PATHWAY	ABSORBED DOSE MG/KG.D	
	ADULT	CHILD
INHALATION		
– VAPOUR	6.03E–03	1.04E–02
– DUST	6.89E–08	1.04E–07
– SHOWER	2.70E–04	4.10E–04
INGESTION		
– SOIL/DUST	5.13E–06	1.60E–04
– VEGETABLES	4.48E–03	1.65E–02
– WATER	3.46E–03	1.21E–02
– MEAT/DAIRY	8.02E–06	6.66E–05
– FISH	2.46E–06	7.82E–06
DERMAL		
– SOIL/DUST	4.59E–06	6.90E–05
TOTALS	**1.43E-02**	**3.97E-02**

IMPORTANT CALCULATED ENVIRONMENTAL CONCENTRATIONS

CONC. IN GROUNDWATER	1.21E+00	(mg/l)
CONC. IN SURFACE WATER	1.20E–02	(mg/l)
CONC. IN DRINKING WATER	1.21E–01	(mg/l)
CONC. IN VEGETABLES ROOT	1.09E+01	(mg/kg fr weight)
CONC. IN VEGETABLES STEM	5.60E+00	(mg/kg fr weight)
CONC. IN MEAT	1.66E–02	(mg/kg fr weight)
CONC. IN MILK	1.10E–02	(mg/kg fr weight)
CONC. IN FISH	7.82E–01	(mg/kg fr weight)
CONC. IN OUTDOOR AIR	2.00E–05	(g/m3)
CONC. IN INDOOR AIR	2.00E–05	(g/m3)
CONC. IN BASEMENT AIR	3.59E–05	(g/m3)

TABLE 4

ESTIMATED HUMAN EXPOSURE BY SOIL CONTAMINANTS

COMPOUND : ZINC
SOIL CONC. : 3000.0 MG/KG dry weight

PATHWAY	ABSORBED DOSE MG/KG.D ADULT	CHILD
INHALATION		
– VAPOUR	2.53E−07	4.35E−07
– DUST	2.07E−05	3.12E−05
– SHOWER	0.00E+00	0.00E+00
INGESTION		
– SOIL/DUST	1.54E−03	4.79E−02
– VEGETABLES	9.27E−02	3.42E−01
– WATER	0.00E+00	0.00E+00
– MEAT/DAIRY	1.58E−06	1.49E−05
– FISH	4.47E−07	1.42E−06
DERMAL		
– SOIL/DUST	1.38−03	2.07E−02
TOTALS	**9.57E-02**	**4.10E-01**

IMPORTANT CALCULATED ENVIRONMENTAL CONCENTRATIONS

CONC. IN GROUNDWATER	2.43E+01	(mg/l)
CONC. IN SURFACE WATER	2.41E−01	(mg/l)
CONC. IN DRINKING WATER	0.00E+00	(mg/l)
CONC. IN VEGETABLES ROOT	1.70E+02	(mg/kg fr weight)
CONC. IN VEGETABLES STEM	1.72E+02	(mg/kg fr weight)
CONC. IN MEAT	2.16E−03	(mg/kg fr weight)
CONC. IN MILK	2.68E−03	(mg/kg fr weight)
CONC. IN FISH	1.42E−01	(mg/kg fr weight)
CONC. IN OUTDOOR AIR	8.39E−10	(g/m3)
CONC. IN INDOOR AIR	8.39E−10	(g/m3)
CONC. IN BASEMENT AIR	1.51E−09	(g/m3)

FIGURE 1

Some important exposure routes of man to soil contaminants

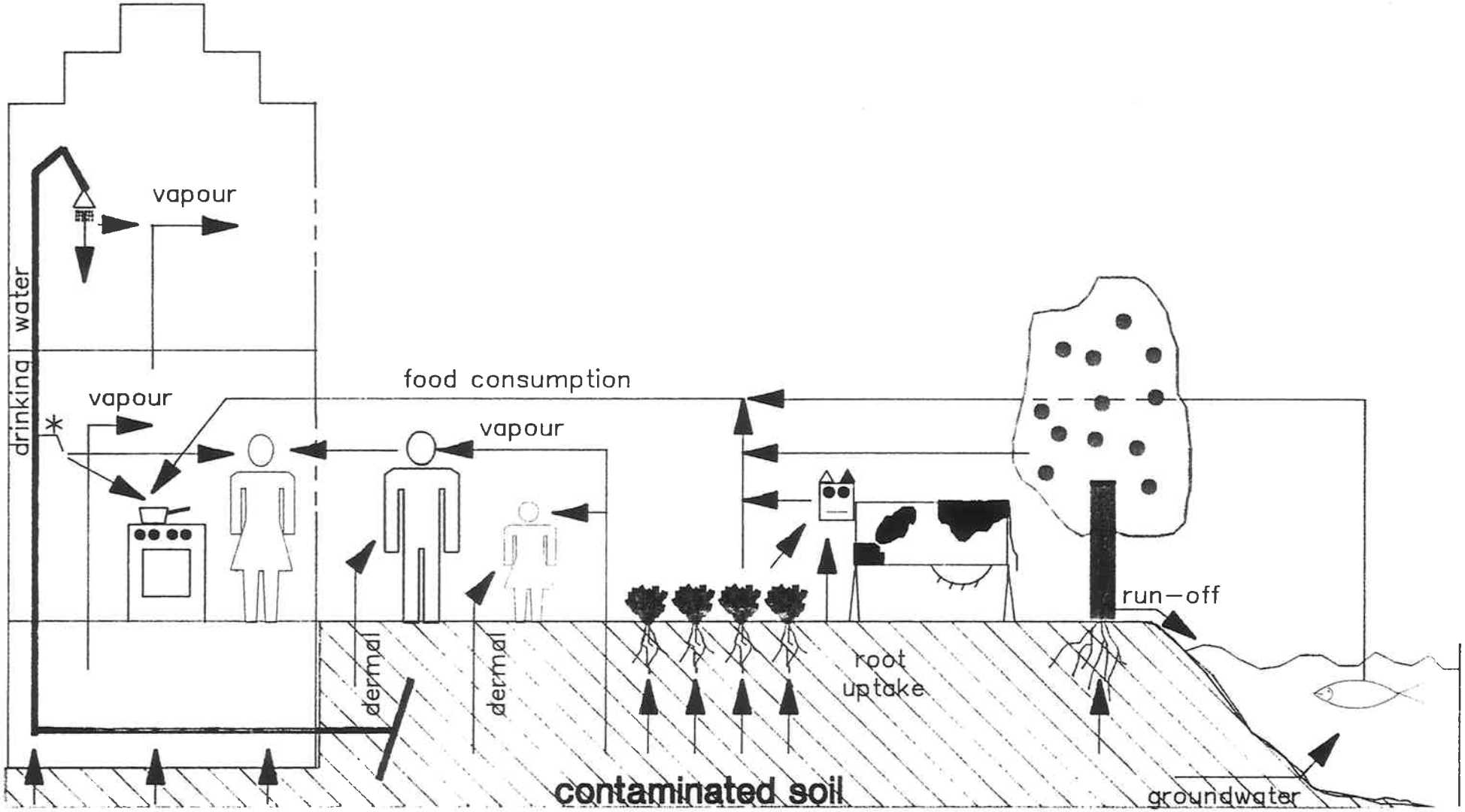


FIGURE 2

Some important exposure routes of environmental organisms to soil contaminants

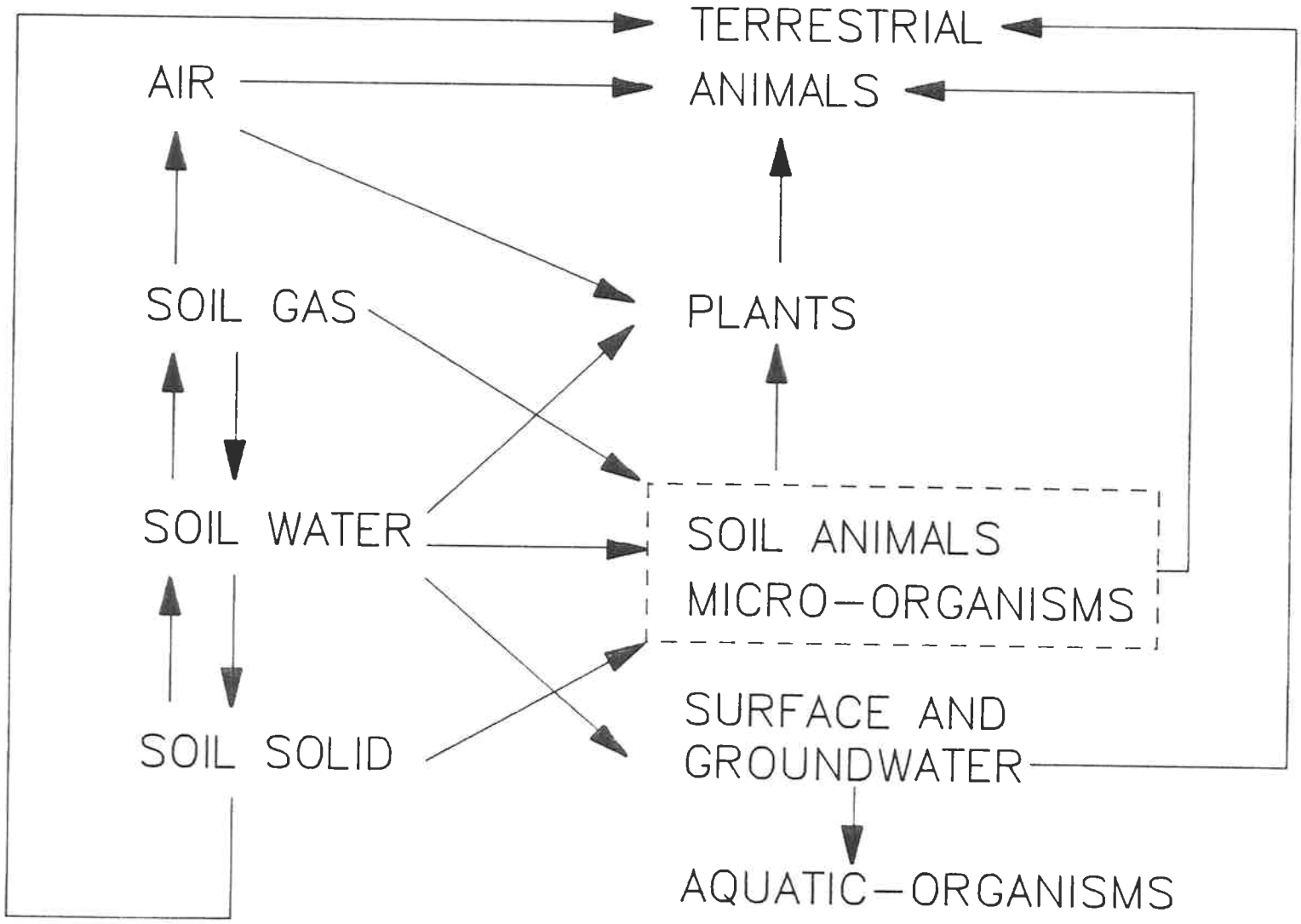


FIGURE 3

Some important groups of environmental organisms exposed to contaminated soil

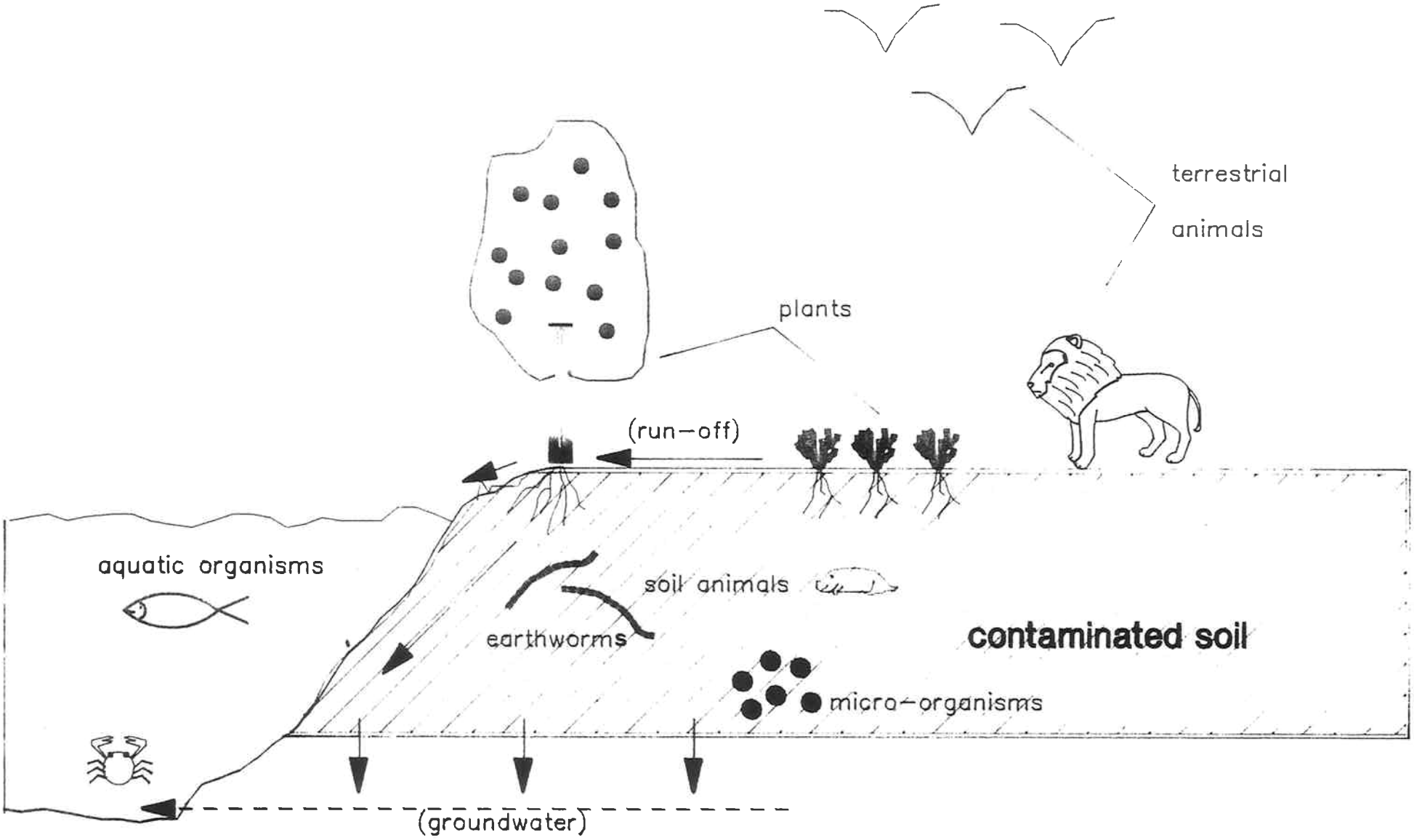


Figure 4

HAZARD ASSESSMENT OF CHEMICAL CONTAMINANTS IN SOIL (stepwise approach)

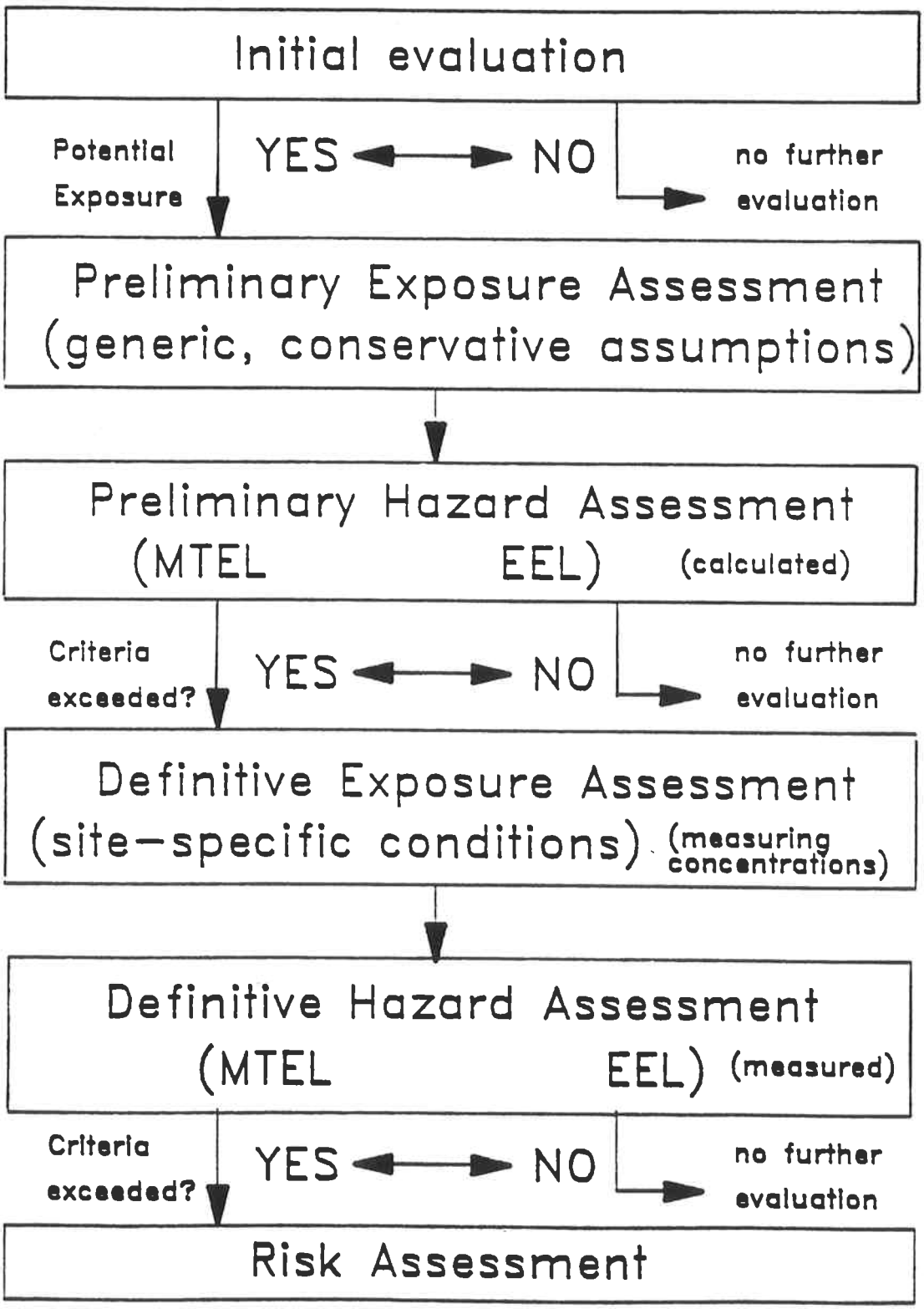


FIGURE 5

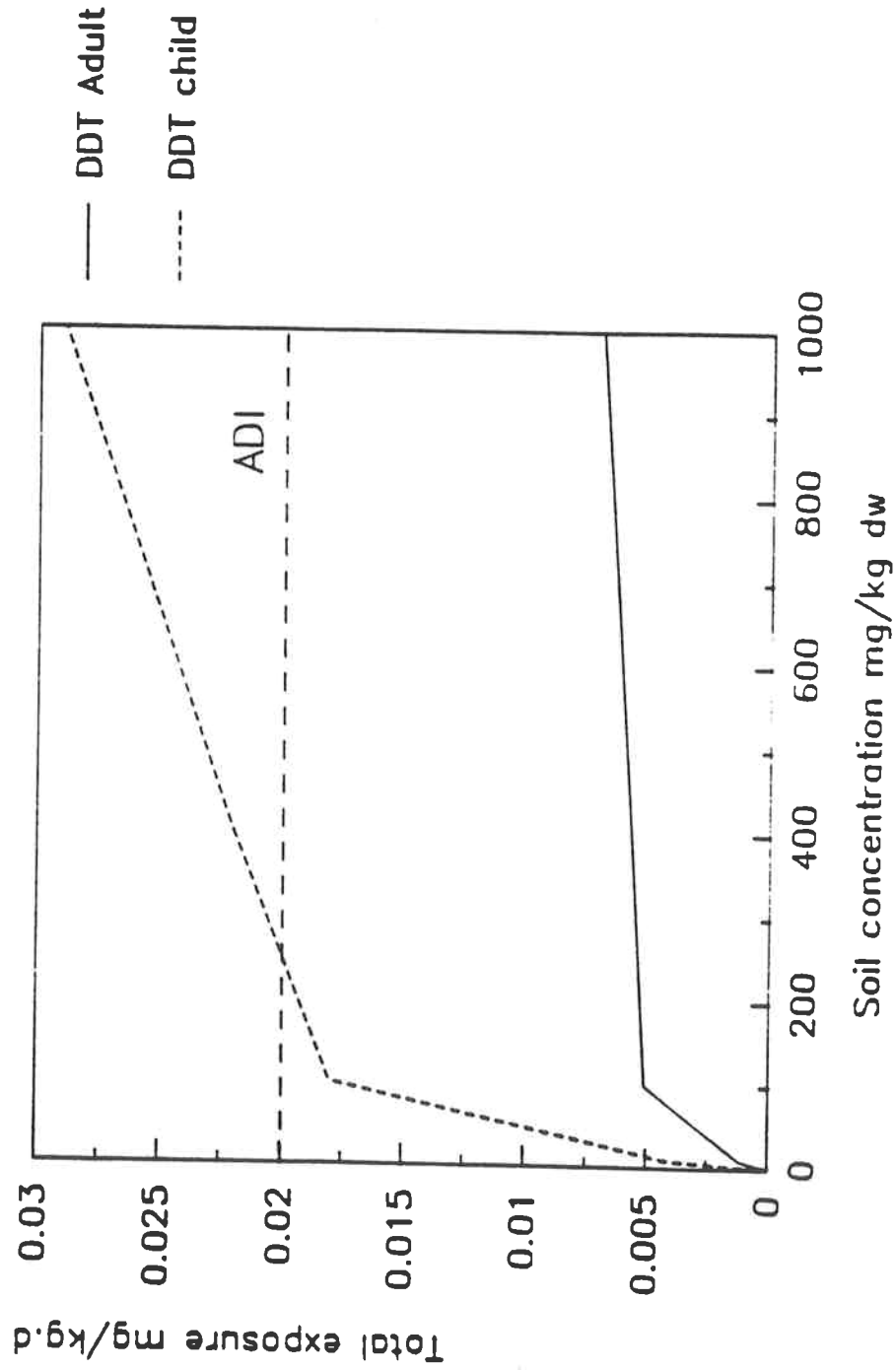

Human Exposure to Soil Pollutants
DDT
DDT Adult
DDT child
ADI
Total exposure mg/kg.d
0.03
0.025
0.02
0.015
0.01
0.005
0
0
200
400
600
800
1000
Soil concentration mg/kg dw

FIGURE 6

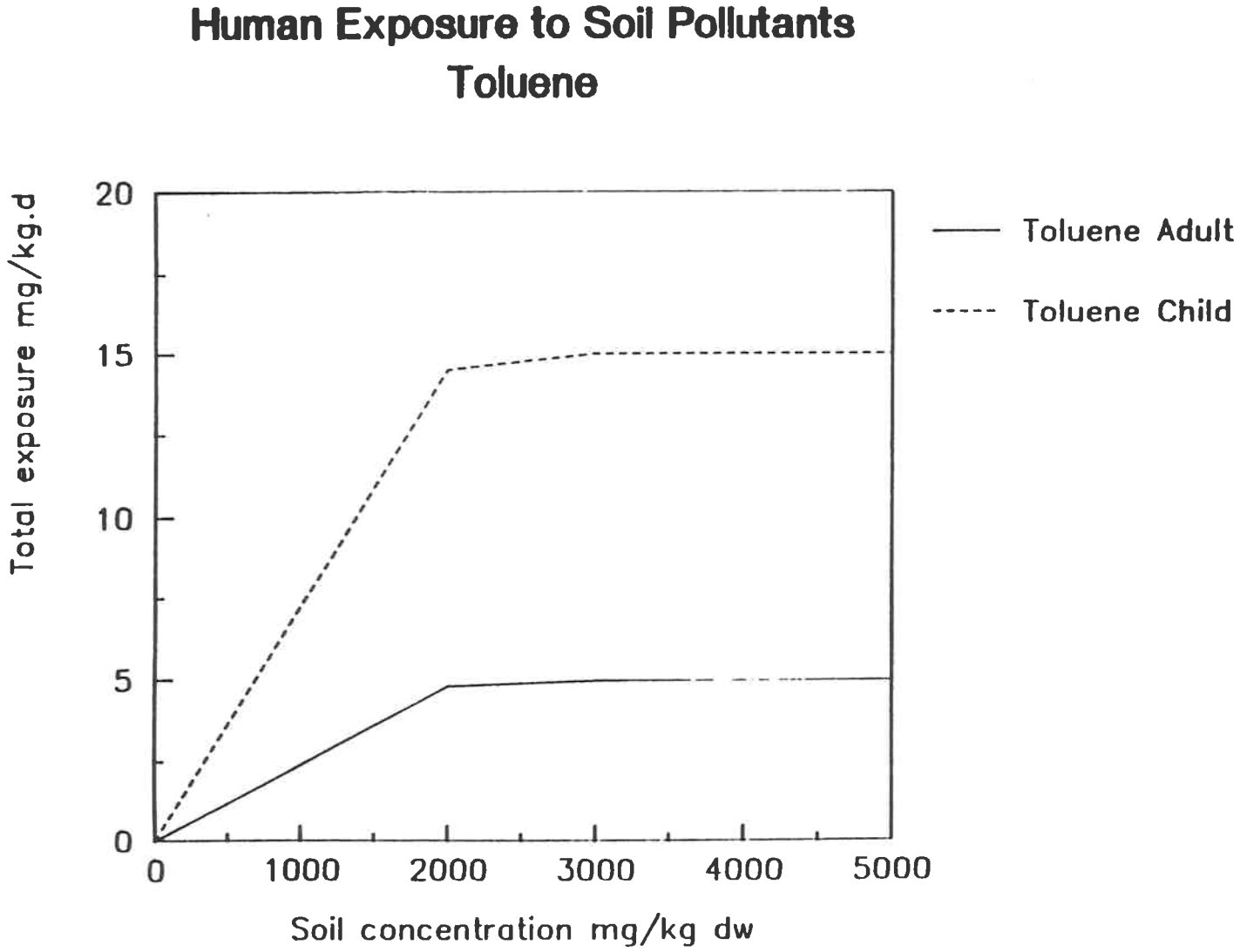

Human Exposure to Soil Pollutants
Toluene
Total exposure mg/kg.d
20
15
10
5
0
0
1000
2000
3000
4000
5000
Soil concentration mg/kg dw
Toluene Adult
Toluene Child

FIGURE 7

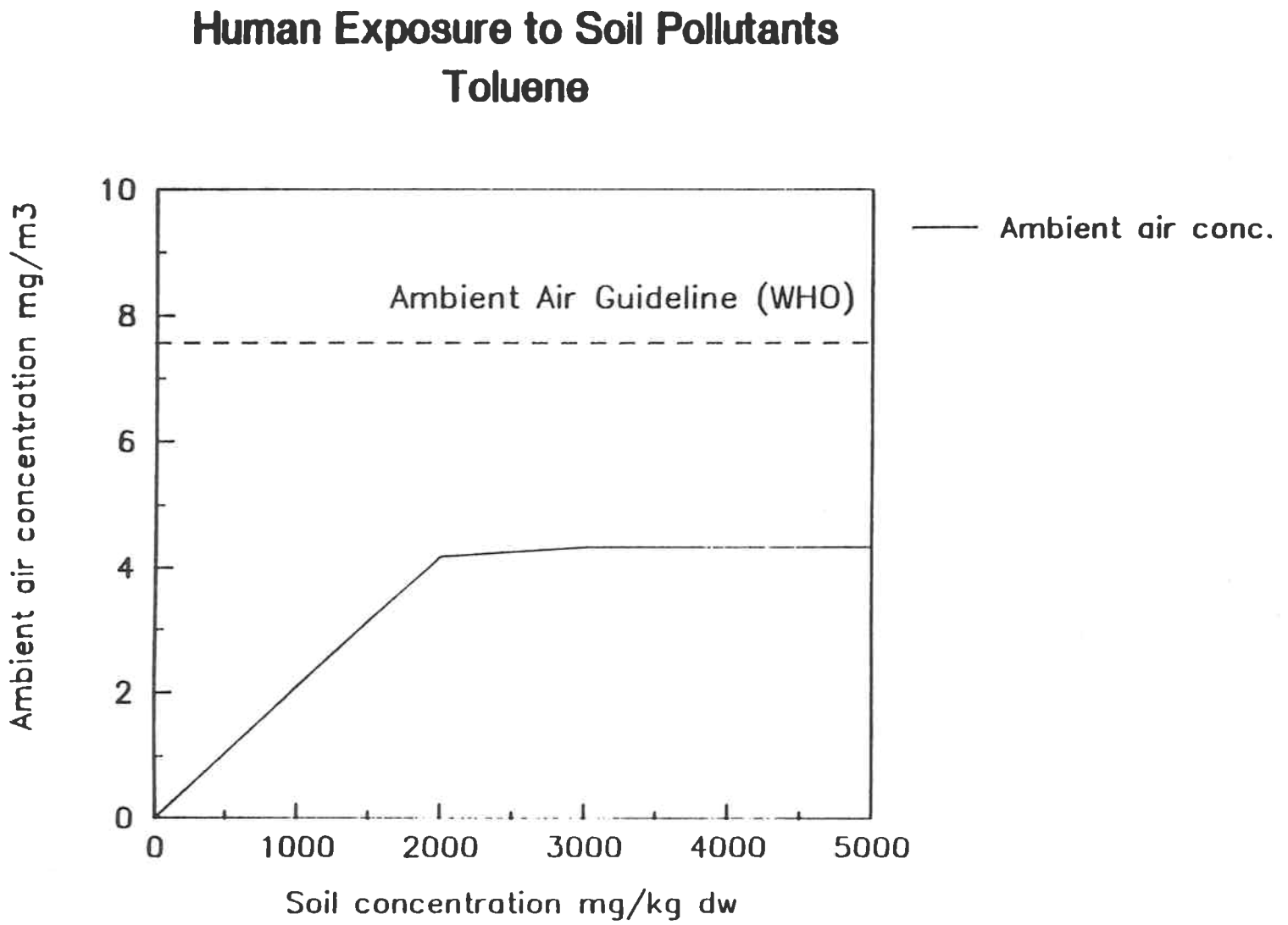
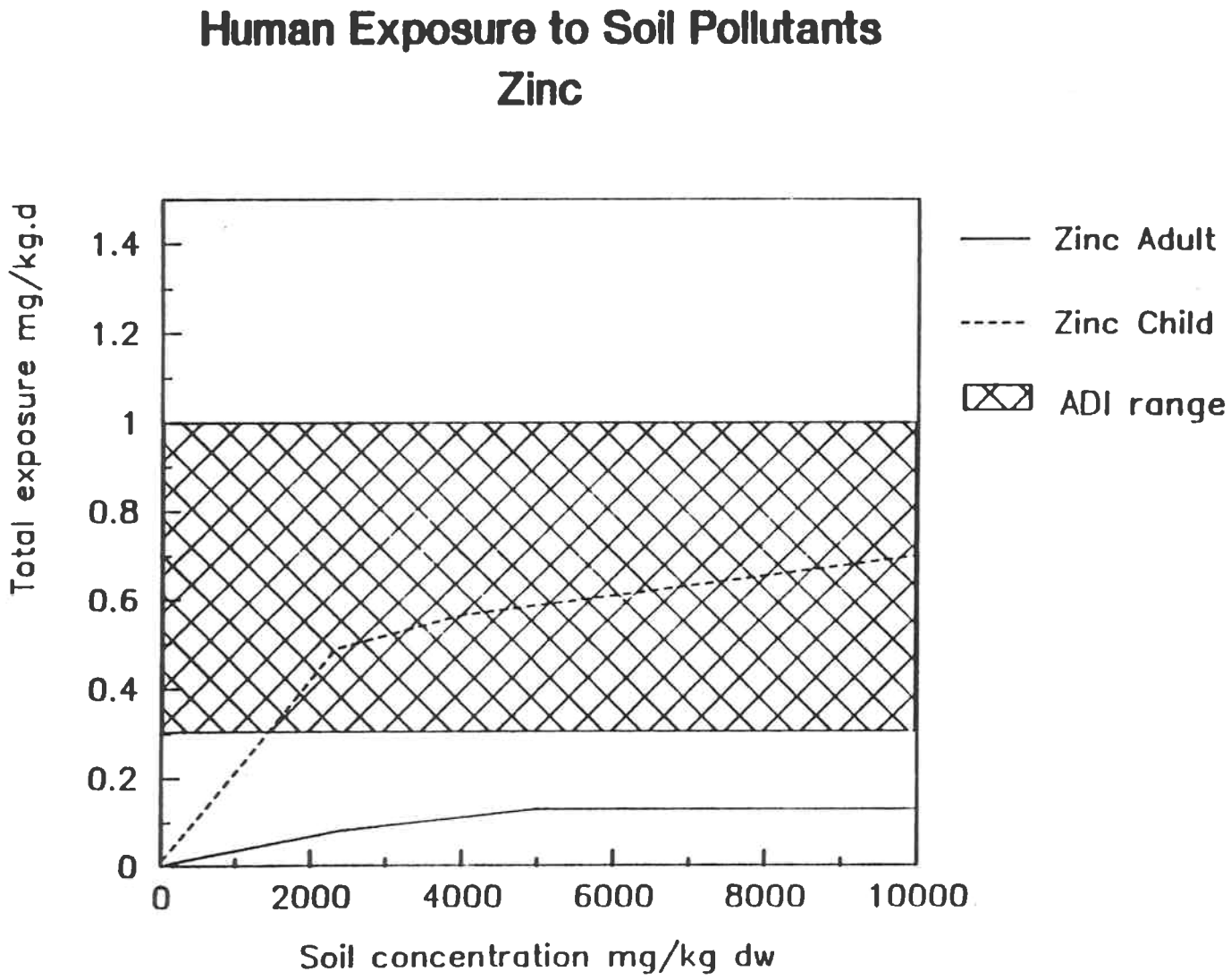

Human Exposure to Soil Pollutants
Toluene
Ambient air concentration mg/m3
10
8
6
4
2
0
Ambient Air Guideline (WHO)
Ambient air conc.
0
1000
2000
3000
4000
5000
Soil concentration mg/kg dw

FIGURE 8


Human Exposure to Soil Pollutants
Zinc
Total exposure mg/kg.d
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
2000
4000
6000
8000
10000
Soil concentration mg/kg dw
Zinc Adult
Zinc Child
ADI range

APPENDICES

APPENDIX I

GLOSSARY OF TERMS

Acceptable Daily Intake (ADI): an estimate of the amount of a chemical substance, expressed on a body weight basis, that can be taken in daily over a life time without appreciable health risk (JECFA, 1982, adapted).

Dose/response assessment: the characterisation of the relationship between the dose of a substance and the occurrence of an adverse effect.

Environmental Exposure Level (EEL): the actual level of a substance to which an organism is exposed.

Exposure assessment: the process of measuring or estimating the level, duration and frequency of exposure to a substance.

Hazard assessment: the estimate of adverse effects which may result from site specific exposure to toxic substances present in soil.

Maximum Acceptable Concentration (MAC): the concentration of a substance in the air of the work place which, as based on current knowledge, at repeated exposure up to a working life period in general does not lead to adverse health effects on the workers. (Nationale MAC-lijst, 1978-1979, Arbeids inspectie, Nederland).

Maximale Arbeitsplatzkonzentration (MAK): similar to MAC but established by the Deutsche Forschungsgemeinschaft.

Maximum Immission Concentration (MIC): maximum acceptable concentration of substances at ground level in ambient air for lifetime exposure to man (Interprovinciaal Documentatie Centrum, The Hague, The Netherlands).

Maximum Tolerable Exposure Level (MTEL): the amount (or concentration) of a chemical substance which, when taken up into (or exposed to) the target organism, does not lead to an adverse effect after prolonged exposure periods.

No Observed Effect Level (NOEL): the highest test concentration of a substance at which no effect can be observed in a test organism.

Risk assessment: the estimation of the probability that the hazard of a substance in soil occurs under site specific conditions.

Threshold limit values (TLV): the concentration of a substance in air in conditions under which it is believed that nearly all workers may be repeatedly exposed day after day without adverse effect (ACGIH, 1988-89).

Tolerable Daily Intake (TDI): is identical to the ADI but is established by the EEC -Scientific Committee for Food.

Toxicity: the intrinsic property of a chemical substance to cause adverse effects to living organisms.

APPENDIX 2

TEST METHODS TO CHARACTERISE CONTAMINANTS, SOILS, FATE OF CONTAMINANTS IN SOIL AND EXPOSURE LEVELS

1. SAMPLING PROCEDURES

1.1. Sampling of Soil

The sampling techniques must be carefully chosen to take into account both:

- the type of measurements to be performed on the samples, e.g. chemical, physical or biological;

- the nature of the site e.g. the natural heterogeneity of soil and the distribution of pollutants.

Details of the theoretical and practical aspects of sampling soils to determine soil characteristics are given in soil text books from Page et al. (1982) and Klute (1986). Examples of methods used to sample polluted soil are presented by Assink and van der Brink (1986), Barth and l'Hermite (1987), Perket (1986) and BSI (1988). The main principles are summarised below. For each investigation a detailed description of the sampling technique should be given to allow a proper assessment of the test results.

- Collection of samples for soil characterisation. The organic matter content, particle size distribution, pH and cation exchange capacity of soils are normally determined on samples collected using cores or hand held augers, typically about 2 cm in diameter. To allow for the variability of soils at least 20 cores are collected randomly from the area to be sampled and bulked together for analysis. If there are obvious major differences in soil properties across a site it is necessary to sample the different areas separately (minimum 20

cores/area). Soil properties, such as organic matter content, normally vary with depth; therefore it is sometimes necessary to separate samples from different depths. The soil is then passed through a 2 mm diameter sieve and carefully subsampled for analysis. Stones greater than 2 mm diameter are weighed and then discarded.

The porosity and permeability of soils must be measured on undisturbed cores taking care to avoid compaction during sampling. If accurate values are required then it is necessary to take large numbers of cores e.g. 20 and to analyse each one separately.

Surface soils contain a diverse range of organisms and the micro-organisms play a particularly important role in the degradation of contaminants as well as plant and animal residues. Therefore samples for use in laboratory studies on the degradation of contaminants and microbial biomass determinations must be processed and stored in such a way as to minimise harm to the microflora. Soils stored for short periods, preferably not more than one month, should be maintained under oxic conditions (unless anaerobic when sampled), in a moist condition at 4°C .

- Collection of samples for contaminant analysis. If the distribution of a pollutant is relatively uniform e.g. following aerial deposition or settling in a lagoon, then the same soil sampling techniques can be used as for determination of organic matter content etc.. Experience shows that the distribution of pollutants is often very heterogeneous e.g. on old industrial sites. If very little is known about the site then samples should be taken systematically on a grid pattern and analysed separately. A careful review of old records on the distribution of waste dumps, storage areas, buildings etc. plus a visual examination of the site can greatly improve the design of the sampling pattern and the cost effectiveness of the investigation. Surface samples can be collected using a trowel or scoop; samples down to 1-2 m using cores or hand held augers or from holes and trenches dug with a mechanical digger. When deeper samples have to be taken

drilling equipment should be used which is expensive and requires special measures to avoid contamination of the samples.

1.2. Sampling for the Characterisation and Concentration Measurement of Contaminants in Air and Surface Waters

During sampling, particularly of the water and gaseous phases great care is needed to avoid loss of chemicals e.g. by sorption onto the sampling containers. If samples cannot be analysed immediately storage conditions must be chosen to minimise loss of the chemicals e.g. storage at -20 °C to prevent microbial degradation.

In most instances samples have to be conserved in the field to avoid loss of contaminants during storage and transport prior to analysis in the laboratory.

- Sampling of air. Some volatile pollutants are also present in the gaseous phase, including those produced in situ, such as methane produced during the degradation of organic wastes under anaerobic conditions. They can be sampled by introducing hollow tube and sampling using syringes or pumps connected to a collection device.

  The sampling time should be at least 6 to 24 hours. In addition, it may be required that the samples are taken at different seasons, during different weather conditions and at sampling locations spread over the contaminated area. Because of the generally low concentration in air large volumes have to be sampled and concentrated. A complete description of the air sampling technique is given by NIOSH (1984).

- Sampling of surface and groundwaters. Surface and ground waters should be sampled at different depth. For surface waters the depth depends on stratification parameters while for ground water the depth depends on the presence of more than one aquifers. Groundwater flow direction has to be taken into account in choosing the appropriate sampling locations. Water samples often require conservation to prevent sample deterioration prior to analysis.

Samples of surface water are collected using a bailer and samples from wells using pumps. It might be necessary to sample groundwater outside the area originally contaminated, using a knowledge of the geology/hydrology of the area to decide on the best sampling locations.

2. *CHARACTERISATION OF CONTAMINANTS*

The OECD (1981) published a set of test guidelines which permit the physico-chemical characterisation of chemicals.

The diffusion coefficients in air can reliably be calculated according to Fuller et al. (1966).

3. *SOIL CHARACTERISATION*

There are no internationally agreed methods for the determination of soil properties. Currently ISO (International Standards Organisation) has several committees working on standardisation of soil testing methods. A range of techniques are described in standard soils text books, such as Klute (1986). Methods used should always be stated because the results depend on the method. Some of the more generally accepted techniques are briefly described below. Results are expressed on a dry weight basis (dried to constant weight at 105^{o}C).

- Porosity. The porosity must be determined on undisturbed cores because it should present the maximum amount of water that a soil can contain under natural conditions when it is saturated with water. Porosity can be determined by saturating the core sample with water and the determination of loss of water after drying.

- Air/water content. A certain volume of soil is dried at a temperature of 105 ^{o}C until constant weight. The difference in soil mass before and after drying is a measure of the water content. If the soil density is known, the air content can be calculated.

- Dry bulk density. The bulk density of a soil sample can be determined by measuring the mass of dry soil and the volume of its solid phase.

- Permeability. The permeability of soil to water or air can be measured by their rate of flux under carefully controlled conditions. For example water permeability can be measured by percolating water through a column of soil under constant pressure and measuring the volume collected in a certain time.

- Particle size distribution. The sample is pretreated with hydrogen peroxide to remove organic matter and if necessary with dilute acid to remove carbonates. The soil aggregates are then dispersed using an agent such as sodium hexametaphosphate. The sand fractions are determined by putting the dispersed sample through appropriate sieves and drying the material collected. Afterwards, the clay and silt fractions are determined by using the rate of sedimentation based on Stokes law. Following set periods the quantity of silt and/or clay remaining in suspension is measured gravimetrically or by the use of a hydrometer.

- Organic Carbon Content. Soil samples are digested with a chromic-sulphuric acid mixture and the excess of chromic acid, not reduced by the organic matter, is titrated with a standard ferrous salt. The organic matter content of soils containing more than about 10% of organic matter can be roughly determined by measurement of weight loss on ignition at about 600^{o}C. It is necessary to make a correction for any carbonates present. The procedure is not suitable for soils with less than 10% organic matter due to errors caused by the loss of structural water from the clay minerals.

- Cation Exchange Capacity. This can be determined by summing the amounts of exchangeable cations in soil, including exchangeable hydrogen. An alternative procedure is to replace all exchangeable cations with a single cation by equilibrating with a salt solution at a defined pH. The excess salt solution is then washed off, the exchangeable cation displaced with a second salt solution and the displaced cation quantified e.g. by flame photometry.

- pH. Soil pH is usually determined on a 1:1 soil water slurry. Instead of pure water, a salt solution such as KCl is sometimes used; values obtained are lower but more stable. The pH is measured using a glass - calomel electrode pH meter.

- Redox potential. The redox potential of soil can be measured between a platinum electrode pressed in the soil in a bore hole and a calomel electrode in the upper soil layer. For the unsaturated soil zone it is difficult to measure the redox potential of the soil because of the non-homogeneity of the soil. The interpretation of the redox potential is difficult. Expert assessment is required to obtain valuable information from the redox potential measurement.

- Microbial biomass. There is no universally accepted procedure for quantifying the numbers or weight of microorganisms in soil due to their small size and metabolic diversity. A relatively simple and rapid technique, which is gaining wider acceptance, is the Anderson - Domsch technique which measures the initial response to added glucose (Anderson and Domsch, 1978). This technique is however restricted to microorganisms capable of respiring aerobically with glucose.

4. *EFFECTS AND DOSE RESPONSE ASSESSMENT*

4.1. Man

OECD (1981) published a set of test guidelines for the detection of toxic properties of chemicals in animals. These guidelines are recommended to assess possible toxic effects in man. The tests are set up such that a proper dose/response assessment can be carried out. This dose/response assessment forms the basis for the determination of a no adverse effect concentration.

4.2. Other Environmental Organisms

Test strategies to determine toxic effects of contaminants in soil should be relevant for the populations of environmental species to be protected. In contrast with tests to predict toxic effects in man, it cannot be determined in advance which tests are to be carried out. As a general approach to environmental testing, it is required that the test methods are standardised, representative and predictive for the field situation. It is necessary to carry out tests in a soil medium because soil strongly influences the bioavailability of contaminants.

An extensive list of tests, either available or under development, relevant for the terrestrial environment is produced by OECD (1988). Some of the more widely accepted tests relevant for this report are summarised below.

- Microorganisms. Various laboratory tests procedures have been developed to determine the toxic effect of pesticides on soil micro-organisms (Anderson, 1985). These are based on assessing the effects of chemicals on important functions carried out by soil microorganisms, particularly soil respiration (degradation of organic matter to CO_2) and nitrogen transformations, such as ammonification (release of ammonium from organic matter) and nitrification (oxidation of ammonium to nitrite and nitrate).

- Soil Animals. The earthworm Eisenia foetida can be used as an appropriate soil animal test organism for which OECD has developed a test guideline (OECD, 1984-a). The LC_{50} is determined after 7 and 14 days.

- Higher Plants. OECD (1984-b) has developed a test guideline for higher plants and this has been adopted by the European Commission. LC_{50} (concentration at which the rate of emergence is 50 per cent of that of the control) and EC_{50} (concentration at which the change in growth is 50 per cent of that of the control) values are determined. Normally 2 or 3 test species are used, including a monocoteledenous and a dicote-

ledenous species.

This method can also be used to bioassay contaminated soil collected from outdoor sites, provided it is possible to collect a sample of a similar soil which is uncontaminated, as a control.

- Other Terrestrial Organisms. Populations of organisms such as birds and mammals are not normally at risk due to the localised nature of soil pollution. If the area is an important habitat for endangered species then toxicity data may be required. Mammalian toxicity data are normally available because the tests are done to assess potential effects to man. There are well developed methods for measuring toxicity to birds (OECD, 1984-c).

- Aquatic Organisms. These organisms can be exposed to chemicals which were originally present in soil but which were removed from that compartment via underground water (leaching) or by direct run-off. Adequate test guidelines assessing the toxicity of chemicals to aquatic organisms (e.g. fish and Daphnia) were published by the OECD (1981).

5. *CHARACTERISATION OF THE FATE OF CONTAMINANTS IN SOIL*

5.1 Transformation Reactions

The main transformation reactions to which contaminants in soil are subjected are described below.

- Hydrolysis. Measurement of the rate of hydrolysis should be carried out in the absence of light using pure water or buffer solutions at pH values normally found in the environment (pH 4-9). The concentration of the buffer solution should be low in order to avoid salt effects which can lead to an acceleration or deceleration of the reaction. Sterile solutions and glassware should be used to avoid side-reactions which might affect the hydrolytic rate constants.

A detailed procedure for testing substances for hydrolysis is given by OECD (1981). A comparison of the OECD and EPA stability is given by Grayson (1986).

- Photolysis. Compared with the extensive studies of organics in the vapour state or dissolved in water, little is known about the processes that affect the photolytic fate of chemicals at the soil surface. Although several systems have been used for measuring photolysis of chemicals at the soil surface, the apparatus used by Burkhard and Guth (1981) is recommended. Soil samples are sprayed with the test chemical and photodegradation is studied in the Hanau-Suntest apparatus. The fate of some chemicals present on environmental surfaces is reviewed by Miller et al. (1987).

- Biodegradation. Mineralisation rates in soil i.e. the complete conversion of organic compounds to inorganic products, can only be determined accurately with radiolabelled compounds. Other experimental approaches, designed to study the disappearance of parent chemicals in soil, are based on either soil perfusion systems, soil biometers, gas flow-through systems, or integrated systems (Guth, 1981). For pesticides a large data base is available on their persistence in soil. In most cases these data are only valid for normal application concentrations for agricultural use.

  For industrial chemicals biodegradation data in aquatic systems are often the only ones available. One can assume that when a chemical biodegrades in the aqueous environment, it will also biodegrade in soil. Methods for assessing aquatic biodegradation are described in detail by OECD (1981). A critical evaluation of these OECD methods was given by ECETOC (1985, 1986-a, -b). Studies in aquatic systems can give a guide to degradation rates in soil but close correlations are not expected because of differences in levels of microbial activity and other factors such as sorption on soil and diffusion into biomass. It should be emphasised that negative results obtained with these aquatic tests are not a definite proof that those chemicals will not biodegrade under field conditions. It is well known that microorganisms may

acclimatise to chemicals and degrade them only after a certain lag time.

For screening purposes and for well defined families of chemicals, biodegradability can be predicted using a quantitative structure-activity relationship technique (Dearden and Nicholson, 1986).

5.2. Sorption-Desorption phenomena

The batch sorption or batch desorption technique has often been used in laboratory studies to assess the soil sorption potential. The technique consists of mixing an aqueous solution of the chemical of known concentration with a given quantity of soil until an equilibrium is reached. The amount of sorbate removed from the solution at equilibrium is assumed to be sorbed. Details of the test method can be found in OECD (1981).

Beside this experimental approach to determine K values, numerous studies have shown that the sorption of non-ionic compounds expressed on the basis of organic carbon (Koc), can be correlated with molecular properties like their solubility or octanol-water coefficient (Kow).

Many of the (Koc) values reported are based on empirical equations that relate to the solubility (S), such as the expression given by Karickoff et al. (1979):

$$\text{Log Koc} = 0.44 - 0.54 \times \text{Log S (in mole fraction/L)},$$

or to the Kow like in the relationship given by Chiou et al (1983):

$$\text{Log Koc} = 0.904 \text{ Log Kow} - 0.542 \ .$$

Often used experimental methods to determine the octanol/water partition coefficient are the shake-flask method and reverse phase HPLC (ECETOC, 1983). Calculation methods, like the calculation of the molecular

connectivity, may be more time saving (ECETOC, 1983). Connectivity tables are reported in the literature (Gerstl and Helling, 1987).

5.3 Mobility

With respect to mobility, a distinction should be made between tests measuring the mobility in the aqueous phase, i.e. by leaching, or via the gaseous phase e.g. by volatilisation.

- Via aqueous phase. The measurement of the mobility of a chemical in soil is based on chromatographic principles. Lysimeter trials (Jarczyk, 1983; Jung and Otto, 1987) are the closest to real environmental conditions. As these tests run for more than one year, they are costly and not suitable for routine trials.

  Laboratory tests use soil columns (BBA, 1986; EPA, 1985) or soil thin or thick layer tests (Helling and Turner, 1968; Gerber et al., 1970; Gerber and Guth, 1973; EPA, 1982-a; Guth, 1983). In these tests the leaching of a given compound is expressed in relation to the leaching of a reference substance. To obtain comparable relative values, "relative mobility factors or RMF's" (Guth, 1983) and "relative leaching indices" (Helling and Turner, 1968) are proposed.

  It has been shown that the octanol/water partition coefficient (Kow) correlates strongly with the RMF values, except for ionic chemicals (Briggs, 1981; Guth, 1983). As the partition coefficients can be calculated (cf. 5.2 above) the necessity to perform leaching tests is less.

- Via gas phase. Volatilisation losses are measured by sorption of the chemical from the atmosphere onto horizontally mounted filter traps placed at varying heights above the soil surface (Caro and Taylor, 1971) or by air sampling in a suitable solvent (Caro and Lemon, 1971).

  The influence of air flow, temperature, concentration, and soil organic matter content on the rate of volatilisation of a contaminant from soil

can be determined in laboratory tests. In a typical experiment the chemical is incorporated uniformly in the soil sample at a specified concentration and nitrogen, at varying relative humidities, is passed over the soil. The evaporated chemicals are trapped in a suitable solvent and then analysed. To keep the soil moist, water is available at the base of the soil column (Spencer and Cliath, 1973).

It has been shown that the ratio between the equilibrium vapour pressure and the water solubility is a good indicator of the volatilisation rate of a chemical of weakly sorbed chemicals from soil. Calculation of this constant will be sufficient and often render further testing superfluous.

A model for the evaporation of chemicals from soil to air is given in Appendix 3. Mathematical models were also developed which consider the movement of the chemical to the soil surface for subsequent volatilisation (Jury et al., 1980).

6. *ANALYTICAL DETERMINATION OF EXPOSURE LEVELS*

The model described in Appendix 3 indicates which exposure routes are significant.

6.1. Metals

Critical for trace metal analysis are sampling, sample preparation and sample storage. Water samples must be stabilised through acidification immediately after sampling (Valenta et al., 1977). Samples should be transported and stored at -20° C. For analysis of trace metals in soil, biota or particulates, the samples are destructed with a mixture of nitric and hydrochloric acid, hydrofluoric acid or perchloric acid at high temperatures under pressure (Eller, 1985).

Trace metals in water samples may be analysed directly or after destruction of the organic matrix by UV-irradiation or by strong acids.

Extraction with organic solvents containing complexing agents (e.g. ammoniumpyrolidine, dithiocarbamate in methylisobutylketone) allows the concentration of the trace metals, which are back extracted into diluted nitric acid. The water solutions are analysed using atomic sorption spectroscopy (AAS) or inductive coupled plasma emission spectroscopy (ICP). With these spectroscopic methods the total amount of trace metals and not the biologically available fraction is determined. A better value for the bioavailable trace metals (free ion or weak complex) is obtained by analysing the water samples without any pretreatment by differential pulse polarography or anodic stripping voltametry.

6.2. Organic contaminants

Samples should be stored at -20°C. To diminish degradation processes, water samples should be stored at 5°C (EPA, 1982-b). For the analysis of organic contaminants in sorbents containing air or water contaminants, plants, animal tissues, soil and water an extraction with a suitable organic solvent is performed. Other extracted materials may interfere thus a further fractionation is often required and may involve:

- acid, base and neutral fractionation by partitioning between organic solvents and acidic, neutral and basic aqueous solutions;
- column chromatography on alumina, silicagel, florisil or reversed phase chromatography;
- separation on polarity by liquid/liquid partitioning with acetonitrile, dimethylsulphoxide or other solvents.

For gas chromatographic analysis highly polar compounds present in the sample (e.g. carboxylic acids, phenols, amines), have to be converted to into more volatile derivatives (e.g. by silylation). For high performance liquid chromatography (HPLC), derivatives are prepared which show a strong UV sorption. At present the most reliable analytical method is GC-MS (gas chromatography - mass spectroscopy). Volatile contaminants can be identified by high resolution GC-MS and comparison with existing mass spectra libraries (Keith, 1980).

The detection limit of an analytical method is a function of the sampling method, the sample preparation and the analytical technique. The concentration levels of the contaminants in environmental samples can be in the range of the detection limit of the analytical technique even after concentrative steps. As a consequence, the variation in the results between different laboratories increases when the concentration level of the contaminants decreases. Dependent on the method the % standard deviation can reach 50 % at the ppb level and 20 % at the ppm level (Asshauer, 1989). Analytical variability is normally less than the variability of the sampling in the field (Frehse and Timme, 1980). The interpretation of low levels of contaminants should always be carried out carefully.

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APPENDIX 3

HESP

HUMAN EXPOSURE TO SOIL POLLUTANTS

Model for exposure assessment of humans resulting from soil contaminants

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CONTENTS

1. *EXPOSURE ASSESSMENT OF MAN TO ORGANIC AND INORGANIC CHEMICAL CONTAMINANTS IN SOIL*

Based on a report for a specific site decommissioning by Golder Associates May 1986 (Reades and Gorber, 1986) a more comprehensive approach has been developed to estimate the exposure levels of soil contaminants for man. A number of exposure routes were identified and subsequently quantified. The exposure routes are:

Inhalation
Ingestion
Dermal Absorption

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

- direct ingestion of soil or dust
- dermal exposure to soil or dust
- inhalation of particulate matter
- inhalation of vapours
- ingestion of crops
- ingestion of meat and dairy products
- ingestion of fish
- ingestion of drinking water
- exposure when bathing in contaminated water
- dermal exposure during bathing.

Depending on the land use it can be determined beforehand which exposure routes to man may exist. Only the relevant route is included in the calculation.

2. *QUANTIFICATION OF THE DIRECT INGESTION*

The following equations are used to calculate the direct ingestion of either soil or dust.

$$DI = (\Sigma\ DI_{x,n}) * C_s \qquad \text{(eq. 1)}$$

where $DI_{x,n}$ = direct ingestion of soil or dust per unit body weight per season (mg soil/kg-bw.d)
n = dust or soil
x = summer or winter
C_s = total concentration in soil

$$DI_{x,dust} = AID_x * f_a * f_{rs} * N_i / W \qquad \text{(eq. 2)}$$

$$DI_{x,soil} = AID_x * f_a * N_o / W \qquad \text{(eq. 3)}$$

where AID_x = amount ingested daily per season (mg/kg-bw.d)
f_a = fraction absorbed
f_{rs} = soil fraction in dust
N_o = fraction of days outside
N_i = fraction of days inside
W = receptor's weight

$$AID_x = A_{hi} * d_l * SG * (1 - f_{voids}) * f_t * k_{us} \qquad \text{(eq. 4)}$$

where A_{hi} = surface area of the inside of the hands
d_l = thickness of the dust or soil layer
SG = density of dust or soil
f_{voids} = fraction of empty volume between particles
f_t = fraction of hours daily this occurs;
for dust: $(16 - txl_o)/16$
for soil: $(txl_o/8)$
txl_o = time spent outside per day in season

k_{us} = number of times the total amount covering the skin surface is ingested per active period

$$N_o = (tx2_o/7) * f_x \qquad \text{(eq. 5)}$$

$$N_i = (7 - tx2_o)/7 * f_x \qquad \text{(eq. 6)}$$

where N_o = fraction of days outside
N_i = fraction of days inside
$tx2_o$ = time spent outside per week in season
f_x = fraction of the year per season

3. *QUANTIFICATION OF THE DERMAL ABSORPTION*

The following equations are used to calculate the dermal sorption of chemicals through contact with either contaminated soil or dust.

$$DA = (\Sigma\ DA_{x,n}) * C_s \qquad \text{(eq. 7)}$$

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

$$DA_{x,dust} = AED_{x,dust} * f_m * f_{rs} * N_i / W \qquad \text{(eq. 8)}$$

$$DA_{x,soil} = AED_{x,soil} * f_m * N_o / W \qquad \text{(eq. 9)}$$

where $AED_{x,n}$ = amount exposed to daily by dust or soil
f_m = matrix factor

$$AED_{x,dust} = A_h * d_1 * SG * (1 - f_{voids}) * (12\text{-}tx1_o) * DAR/100 \qquad \text{(eq. 10)}$$

$$AED_{x,soil} = A_{fh} * d_l * SG * (1 - f_{voids}) * txl_o * DAR/100 \quad \text{(eq. 11)}$$

where A_h = surface area of the hands
A_{fh} = surface area of forearm and hands
DAR = dermal absorption rate

4. *QUANTIFICATION OF THE INHALATION OF PARTICULATE MATTER*

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

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

where $IP_{y,x}$ = inhaled particulate matter per season in soil equivalents (mg soil/kg.d)
y = indoor or outdoor (dust)
x = summer or winter

$$IP_{y,x} = ITSP_{y,x} * f_r * f_a * N_y / W \quad \text{(eq. 13)}$$

where $ITSP_{y,x}$ = inhaled total suspended particulate matter per season
f_r = fraction retained in the lung
f_a = absorbed fraction
N_y = fraction of days spent inside or outside

$$ITSP_o = VA * (tsl_o/24) * TSP_o * f_{rs} \quad \text{(eq. 14)}$$

$$ITSP_i = VA * ((24-tsl_o)/24) * TSP_i * f_{rs} \quad \text{(eq. 15)}$$

where $ITSP_y$ = inhaled total suspended particulate matter inside or outside
VA = volume of air breathed

TSP_o = total suspended particulates outside
TSP_i = total suspended particulates inside

5. *QUANTIFICATION OF THE INHALATION OF VAPOURS*

5.1. Calculation of the outdoor air concentration

The following equations are used to calculate the concentration of contaminants in the outdoor air.

$$N_{oa} = K_{os} (C_{sa} - C_{oa}) \qquad \text{(eq. 16)}$$

where N_{oa} = diffusive flux to the outdoor (o) air (a)
K_{os} = overall soil phase mass transfer coefficient
C_{sa} = concentration in soil-air
C_{oa} = concentration in the outdoor air

$$C_{sa} = (C_s * H) / (K_d * R * T) \qquad \text{(eq. 17)}$$

where C_{sa} = concentration in soil air
C_s = concentration in the soil
H = Henry's Law Constant
K_d = sorption partition coefficient
R = universal gas constant
T = temperature of the soil surface

$$K_d = K_{oc} * f_{oc} \qquad \text{(eq. 18)}$$

where K_{oc} = organic carbon partition coefficient
f_{oc} = fraction of organic carbon in soil

$$1 / K_{os} = 1 / K_s + 1 / K_g \qquad \text{(eq. 19)}$$

where K_s = the soil-air phase mass transfer coefficient
K_g = the gas phase mass transfer coefficient

$$K_s = D_{ef} / L_s \quad \text{(eq. 20)}$$

where D_{ef} = the effective molecular diffusibility of the chemical within the soil pore spaces
L_s = length of the diffusive path in soil

$$L_s = L_{cmax} / 2 \quad \text{(eq. 21)}$$

where L_{cmax} = depth of contamination in the soil

$$D_{ef} = D_a * (SN_a^{10/3}) / SN_p^2 \quad \text{(eq. 22)}$$

where D_a = diffusion coefficient through air
SN_a = air content of soil
SN_p = porosity of soil

$$K_g = 0.029 * V_{10}^{0.78} * L^{(-0.11)} * Sc^{(-0.67)} \quad \text{(eq. 23)}$$

where V_{10} = the wind velocity at a height of 10 m
Sc = the solute gas phase Schmidt number
L = the length of evaporation surface

$$Sc = u / (p * D_a) \quad \text{(eq. 24)}$$

where u = viscosity of air
p = density of air

$$N_{oa} = K_s * (C_{sa} - C_{si}) \quad \text{(eq. 25)}$$

where C_{si} = the concentration at the interface

$$N_{oa} = K_{gs} * (C_{si} - C_{up}) \quad \text{(eq. 26)}$$

where K_{gs} = mass transfer coefficient for diffusive sublayers

C_{up} = concentration at the upper edge of the diffusive sublayer

$$K_{gs} = D_a / X_a \quad \text{(eq. 27)}$$

where X_a = the thickness of the air sublayer

$$X_a = 26 * V_1 / V^* * Sc^{1/3} \quad \text{(eq. 28)}$$

where V_1 = the kinetic viscosity of air

V^* = the friction velocity

$$V^* = (V_{10} * k) / \ln((h + sr)/sr)) \quad \text{(eq. 29)}$$

where k = Karman constant

h = height (wind velocity)

sr = surface roughness

$$C_{oa} = C_{up} - (N_{oa} / Prc * V^*) * \ln(Y / X_a) \quad \text{(eq. 30)}$$

where Y = the distance the breathing zone is above the air-soil interface

Prc = Prandtl constant

5.2. Calculation of the indoor (basement and living room) air concentration

$$N_{ba} = K_{os} * (C_{sa} - C_{ba}) \qquad \text{(eq. 31)}$$

where N_{ba} = diffusive flux to the basement air
C_{ba} = concentration in basement-air

$$1 / K_{os} = 1 / K_s + 1 / K_b \qquad \text{(eq. 32)}$$

where K_b = the concrete-air phase mass transfer coefficient

$$K_b = D_{efc} / d_c \qquad \text{(eq. 33)}$$

where D_{efc} = the effective molecular diffusibility of the chemical within the pores of the concrete
d_c = thickness of the concrete

$$D_{efc} = D_a * (CN_a^{10/3}) / CN_p^2 \qquad \text{(eq. 34)}$$

where CN_a = air content of concrete
CN_p = porosity of concrete

$$C_{ba} = N_{ba} * A_t / (V_b * R_a) \qquad \text{(eq. 35)}$$

where A_t = total area of basement walls and floor
R_a = rate of air exchange per hour
V_b = volume of the basement

$$C_{la} = 0.1 * C_{ba} \qquad \text{(eq. 36)}$$

or if $C_{1a} < C_{oa}$ then

$$C_{1a} = C_{oa} \qquad \text{(eq. 37)}$$

where C_{1a} = concentration in living room air

5.3. Calculation of the Amount of Inhaled Vapours (IV)

The following equations are used to calculate the amount of chemicals inhaled as vapours in and outdoors.

$$IV = \Sigma\ IV_{y,x} \qquad \text{(eq. 38)}$$

where $\Sigma\ IV_{y,x}$ = total inhaled vapour

$$IV_{o,x} = VA * (txo_1 / 24) * C_{oa} * f_a * N_o/W \qquad \text{(eq. 39)}$$

$$IV_{i,x} = VA * ((24-txo_1) / 24) * C_{1a} * f_a * N_i/W \qquad \text{(eq. 40)}$$

6. *QUANTIFICATION OF THE EXPOSURE THROUGH CONSUMPTION OF GARDEN PRODUCES, MEAT, FISH, MILK AND DAIRY PRODUCTS*

The concentration in plant tissues is in this model dependent on two processes, namely uptake through the roots with subsequent internal transport and deposition of dust on the leaves with subsequent uptake. Both processes have been separately described below. The total concentration in the plant is supposed to be the addition of the result of both processes.

The intake by cattle is determined in a similar way as for man, taking into account inhalation of vapour and dust, plant consumption, water consumption and soil ingestion. The concentration of contaminants in meat and milk is

calculated using a distribution coefficient according to data published by Travis and Arms (1988).

The concentration in fish is calculated using a bioconcentration factor according to Bysshe published in the Handbook of chemicals property estimation methods (1982).

6.1. Calculation of the concentration in plants due to root uptake

6.1.1. Inorganic substances. Based on experimental data a relationship between K_d and BCF (relation between the concentration in tissue of the above ground parts of plants and an environmental compartment) has been proposed by Baes.

$$\ln K_d = A + B * \ln BCF_{plant} \qquad \text{(eq. 41)}$$

where A = constant (3.02)
B = constant (-0.85)
r^2 = 0.68 for this relationship

Based on data presented by Dijkshoorn et al. (1981, 1983a, 1983b) a pH and organic carbon content depending K_d value according to the following equation is proposed for the model.

$$K_d = K_d^* * 10^{0.25 * (pH - 8) * (1.5 * f_{oc} * 100 + 0.5 * f_{clay} * 100) / 27} \qquad \text{(eq. 42)}$$

where K_d^* = K_d for a standard soil with f_{oc} = 0.10 and f_{clay} = 0.25.

$$C_{pl} = BCF * C_s \quad \text{(based on dry weight)} \qquad \text{(eq. 43)}$$

6.1.2. Organic substances. Based on data presented by Ryan et al. (1988) a relationship between BCF_{plant} and K_{ow} has been established.

6.1.2.1. Concentration in the stem

$$BCF_{stem} = (SG / (SG * K_{oc} * f_{oc} + SN_w)) * ((10^{(0.95 * \log K_{ow} - 2.05)} + 0.82) * (0.784 * 10^{-0.434((\log K_{ow} - 1.78) / 2.44)^2})) \quad \text{(eq. 44)}$$

where SG = soil bulk density
SN_w = soil water content

$$C_{pl} = BCF_{stem} * C_s \text{ (based on fresh weight)} \quad \text{(eq. 45)}$$

where C_{pl} = the concentration in the stem of the plant.
C_s = total concentration in soil (including water phase)

6.1.2.2. Concentration in the root

$$\log (BCF_{root} - 0.82) = 0.77 \log K_{ow} - 1.52 \quad \text{(eq. 46)}$$

$$C_{pl} = BCF_{root} * C_{pw} \text{ (based on fresh weight)} \quad \text{(eq. 47)}$$

where C_{pw} = concentration in porous water.

6.2. Calculation of the concentration in plants due to deposition

$$C_{pl} = (f_{in} / Y_v * f_{Ei}) * (1 - (1 - e^{-f_{Ei} * t_e}) / (f_{Ei} * t_e)) * DR_o * f_{rs} * C_s \text{ (based on dry weight)} \quad \text{(eq. 48)}$$

where f_{in} = initial fraction of interception.
Y_v = vegetative productivity
f_{Ei} = weathering constant
t_e = crop growth period
DR_o = deposition rate outside
C_s = concentration in the soil

6.3. Calculation of the uptake through consumption of crops

$$VI = C_{pt} * Q_{fv} * fh_{max} * f_a / W \qquad \text{(eq. 49)}$$

where VI = Vegetable and fruit equivalent uptake in mg/kg-bw.d
Q_{fv} = Fruit and Vegetable consumption per day
fh_{max} = maximum fraction of consumption of home grown produce

$$C_{pt} = (C_{pl}(up) + C_{pl}(dep)) * 0.5 + C_{pl}(root) * 0.5 \qquad \text{(eq. 50)}$$

where C_{pt} = average concentration in consumed garden produce

6.4. Calculation of the intake of chemicals by cattle

$$DI_C = C_s * AID_C * (txo_C / 24) * f_{ac} * N \qquad \text{(eq. 51)}$$

where DI_C = direct ingestion of contaminant through soil ingestion per unit body weight per season
AID_C = amount of soil ingested daily by cattle
txo_C = time spent outside per day by cattle
f_{ac} = absorbed fraction by cattle
N = fraction of days annually this occurs

$$IP_c = C_s * VA_c * (txo_c / 24) * TSP_o * f_{rs} * f_{rc} * f_{ac} * N \quad \text{(eq. 52)}$$

where IP_c = Inhaled contaminant through particulate matter
VA_c = volume of air breathed by cattle per day
f_{rc} = fraction retained in the lung

$$IV_c = VA_c * C_{oa} * (txo_c / 24) * f_{ac} * N \quad \text{(eq. 53)}$$

where IV_c = Inhaled vapours by cattle

$$VI_c = C_{pl} * Q_{pc} * f_{ac} \quad \text{(eq. 54)}$$

where VI_c = Vegetation intake equivalent
Q_{pc} = plant consumption

$$DI_{cw} = (C_t * (1 - f_g - f_s) + C_{gw} * f_g + C_{sw} * f_s) * Q_{wc} \quad \text{(eq. 55)}$$

where DI_{cw} = direct ingestion through drinking water
C_t = concentration of the contaminant in the service pipe after t days of stagnancy
f_g = fraction of ground water used as drinking water
f_s = fraction of surface water used as drinking water
C_{gw} = concentration in ground water
C_{sw} = concentration in surface water
Q_{wc} = water consumption

$$TI_c = DI_c + IP_c + VI_c + DI_{cw} \quad \text{(eq. 56)}$$

where TI_c = Total intake of contaminants for cattle

6.5. Calculation of the concentration in meat, milk and fat

$$\log K_{me} = - 6.880 + 0.832 * \log K_{ow} \qquad \text{(eq. 57)}$$

$$\log K_{mi} = - 6.786 + 0.731 * \log K_{ow} \qquad \text{(eq. 58)}$$

$$\log K_{fa} = - 3.457 + 0.500 * \log K_{ow} \qquad \text{(eq. 59)}$$

where K_{me} = meat/diet partition coefficient
K_{mi} = milk/diet partition coefficient
K_{fa} = fat/diet partition coefficient

$$C_z = TI_c * K_z \qquad \text{(eq. 60)}$$

where C_z = concentration in the products
z = index indicating meat, milk or fat

6.6. Calculation of the uptake through consumption of meat, milk and dairy products

$$MI = (\Sigma (C_z * Q_z * f_z)) * f_a / W \qquad \text{(eq. 61)}$$

where MI = Equivalent uptake of meat, milk and dairy products
Q_z = product consumption
f_z = fraction of cattle product from the location

6.7. Calculation of the concentration in fresh water organisms

$$\log BCF_m = C * \log K_{ow} - D \qquad \text{(eq. 62)}$$

where BCF_m = bioconcentration factor for aquatic organisms
m = index indicating the aquatic organism
C = constant
D = constant

$$C_m = C_{sw} * BCF_m \qquad \text{(eq. 63)}$$

where C_m = concentration in aquatic organism

$$FI = \Sigma\, C_m * Q_m * f_z * f_a / W \qquad \text{(eq. 64)}$$

where FI = Equivalent uptake through consumption of aquatic organisms
Q_m = aquatic organism consumption
f_z = fraction of Q_m from the vicinity of the location

7. *QUANTIFICATION OF THE EXPOSURE THOUGH DRINKING WATER*

7.1. Calculation of the permeation through plastic service-pipes

$$C_t = (2 * D_{pe} * C_{pw} * \delta t)/ r * d_e \qquad \text{(eq. 65)}$$

where C_t = concentration of the contaminant in the service pipe after t days of stagnancy
C_{pw} = concentration of the contaminant in the soil water phase outside the service pipe
δt = number of days that the water is stagnant
D_{pe} = permeation coefficient
r = internal radius of the pipe
d_e = thickness of the pipe wall

7.2. Calculation of the extent of evaporation during showering

$$k_{wa} = (((H/RT) * kL * kG)/((H/RT) * kG + kL)) * (Ad/Vd) * t_f \quad \text{(eq. 66)}$$

where k_{wa} = extent of evaporation
kG = gas mass transfer coefficient
kL = liquid mass transfer coefficient
A_d = surface area of the droplet
V_d = volume of the droplet
t_f = falling time of the droplet

$$kG = K_g / 3600 * \sqrt{18/M} \quad \text{(eq. 67)}$$

$$kL = K_l / 3600 * \sqrt{44/M} \quad \text{(eq. 68)}$$

where M = molecular weight
K_l = liquid phase exchange rate (CO_2)

7.3. Calculation of the inhaled vapour during showering

$$IV_w = ((k_{wa} * V_w * C_t / V_{bath}) /2) * VA * t_s * N_s / W \quad \text{(eq. 69)}$$

where IV_w = inhaled vapour during showering
V_w = volume of water used
V_{bath} = volume of the bathroom
t_s = duration of showering
N_s = fraction of days showering occurs

7.4. Calculation of dermal uptake during bathing

$$DA_w = C_t * DAR_w * A_{tot} * t_b * N_b / W \quad \text{(eq. 70)}$$

where DA_w = dermal absorption per kg body weight
DAR_w = dermal absorption rate for exposure in water
A_{tot} = surface area of the skin exposed to water during bathing
t_b = bathing time
N_b = fraction of days bathing occurs

7.5. Calculation of the intake via drinking water

$$DI_w = (C_t * (1 - f_g) + C_{gw} * f_g) * Q_w / W \qquad \text{(eq. 71)}$$

where DI_w = direct ingestion through drinking water
Q_w = water consumption

7.6. Calculation of soil/ground water concentration

$$C_{smax} = S_w * K_d \qquad \text{(eq. 72)}$$

where C_{smax} = the concentration in the soil which corresponds with the solubility
S_w = water solubility

if $C_s \leq C_{smax}$ then

$$C_{sm} = C_s \quad \text{else} \qquad \text{(eq. 73)}$$

$$C_{sm} = C_{smax} \qquad \text{(eq. 74)}$$

where C_{sm} = the concentration in the soil with a maximum related to the solubility

$$C_{pw} = C_{sm} / K_d \qquad \text{(eq. 75)}$$

where C_{pw} = the concentration in pore water

$$C_{gw} = C_{pw} * L * q_{inf} / (K * d * I + L * q_{inf}) \qquad \text{(eq. 76)}$$

where q_{inf} = infiltration rate
K = hydraulic conductivity of the aquifer
d = thickness of the mixing zone in the aquifer
I = hydraulic gradient

$$q_{inf} = q_{re} / SN_p \qquad \text{(eq. 77)}$$

where q_{re} = recharge rate

7.7. Calculation of surface water concentration

$$C_{sw} = (R_o * C_s + Q_{di} * C_{gw}) / (R_o * K_d + Q_{sw}) \qquad \text{(eq. 78)}$$

where R_o = run-off of soil
Q_{di} = discharge from the aquifer in surface water
Q_{sw} = mass flow of surface water

$$R_o = SL * L * L_{ws} * SG * (1 - f_c) \qquad \text{(eq. 79)}$$

where SL = soil loss (m/h)
L_{ws} = width of the soil loss zone
f_c = fraction of area covered by housing and or growth

$$Q_{di} = K * d * I * L_w \qquad \text{(eq. 80)}$$

$$Q_{sw} = Q^{o}_{sw} + Q_{di} - Q_{ev} \qquad \text{(eq. 81)}$$

where Q^{o}_{sw} = initial mass flow of surface water

Q_{ev} = amount of water evaporated

8. *MODEL PARAMETERS*

8.1. General

This model is directed towards estimating the exposures to two types of residents: an adult and a young child. In this model they represent the greatest cumulative intakes for individuals living at a contaminated site (referred to as "Maximum average exposure"). Where average indicates the average year value calculated per day independent of seasonal changes.

The house is located in the middle of a contaminated site. Concentrations of substances are assumed to be constant horizontally and not to change with time.

8.2. Receptor characteristics

Table 1. Receptor characteristics

Description		Adult	Child	Child
Age	(y)	30	3	0-10
W	(kg)	70	10	17
VA	(m^3/d)	23	5	10
A_{tot}	(m^2)	1.8		
A_{ah}	(m^2)	0.34	0.1	
A_{fh}	(m^2)	0.17	-	
A_h	(m^2)	0.09	0.03	
A_{hi}	(m^2)	0.01	-	
A_{lf}	(m^2)	-	0.18	
Q_{fv}	(kg/d)	0.6	0.3	0.6
Q_v	(kg/d)	0.17	-	
		0.2		
Q_{pot}	(kg/d)	0.21		
Q_{fr}	(kg/d)	0.13		
Q_w	(l/d)	2.0	1.0	0.7
Q_{md}	(kg/d)	0.3		0.5
Q_{milk}	(l/d)	0.44		
Q_{mp}	(kg/d)	0.3		0.1
Q_m	(kg/d)	0.16		
Q_f	(kg/d)	0.0065		0.002

(US - FDA, 1970; ICRP, 1975; Nutrition Canada, 1977; Anonymous, 1980; Hawley, 1985; McKone and Layton, 1986)

W = weight; VA = volume of air breathed; A_{ah} = surface area of the arms and hands; A_{fh} = surface area of the forearms and hands; A_h = surface area of the hands; A_{hi} = surface area of the inside of the hands; A_{lf} = surface area of the legs and feet; Q_{fv} = fruit and vegetables consumption; Q_v = vegetables consumption; Q_w = water consumption; Q_{md} = milk/diary consumption; Q_{mp}; meat/poultry consumption; Q_f = fish consumption (fresh and estuarial).

Estimation of A_{tot} for child can be done according to:

$$A_{tot}(\text{Child}) = (W_{\text{Child}}/W_{\text{Adult}})^{0.33} * A_{tot}(\text{Adult})$$

8.3. Climate

The parameters describing climatic conditions should be adjusted to local circumstances. In this case parameters are adjusted to the Dutch situation.
The year has been divided into two seasons, summer and winter, each lasting six months. Average temperatures are 20°C in summer and 0°C in winter.
The wind velocity is assumed to be on average 7.5 $m.s^{-1}$ at 10 m above ground level in the Dutch situation.

In this model f_s = 0.5 is used.

In this model V_{10} = 7.5 $m.s^{-1}$ is used.

8.4. Equation parameters

eq. 2;
f_a = absorbed fraction
In a conservative approach used by Hawley (1985), it is assumed that 50 to 100 % of any organic or inorganic compound in the ingested soil or dust is sorbed.
Values of 10 - 30 % have been used for the gastro-intestinal tract by Hwang (1985) and Paustenbach et al. (1986).

In this model f_a = 1 is used.

f_{rs} = soil fraction in dust.
For the indoor situation this value may vary from 0.7 to 0.85 (Roberts et al., 1974). For the outdoor situation 0.5 has been used (Hawley, 1985; Paustenbach et al., 1986).

In this model f_{rs} = 0.5 is used for outdoor.

In this model f_{rs} = 0.75 is used for indoor.

eq. 4;

d_l = thickness of the dust or soil layer on the skin

Values for layer thickness varied from 6.7 -50 μm (Reades and Gorber, 1986; Lepow et al., 1975; Roels et al., 1980; McKone and Layton, 1986). Based on the reported soil concentration on the hands, the fraction of voids and the soil bulk density values are 7 -15 μm (Schaum, 1983).

In this model d_l = 20 μm is used.

SG = density of soil or dust.

In this model SG_{soil} = 1.5 and SG_{dust} = 0.7 g/cm^3 are used.

f_{voids} = fraction of empty volume between particles on the skin surface.

In this model f_{voids} = 0.5 is used.

k_{us} = rate of uptake of soil from the skin surface

As calculations based on soil coverage of the skin do not give values for the actual uptake of soil due to behavioural factors it seemed appropriate to introduce a behavioural parameter indicating the fraction of soil or dust on the skin that was actually ingested per active period. The values chosen in this model correlate with the total amount of soil ingested by adults and children being ≈ 100 mg soil/day (Lepow et al, 1975; Roels et al., 1980; McKone and Layton, 1986). The value of 100 mg/day has also been adopted by EPA (Schaum, 1983). Other values that are mentioned in literature range from 25 - 250 mg of soil under normal conditions (e.g. excluding extreme cases of pica) (van Wijnen, 1987; Binder et al., 1986; LaGoy, 1987, Paustenbach et al., 1986).

In this model k_{us} = 0.5 (Adult) and 5.0 (Child) d^{-1} is used.

(This results in a soil uptake for the child of ≈ 250 mg soil.d^{-1} and for the adult of ≈ 100 mg soil.d^{-1} during an "active" outdoor spent day.)

$t\ xy_z$ = time spent per day

Where x = summer (s) or winter (w)

y = hours/day (1) or days/week (2)

z = indoors (i) or outdoors (o)

In this model the following assumptions are used (Reades and Gorber, 1986):

- the adult spends $8 h.d^{-1}$ during $2\ d.w^{-1}$ outdoors in summer and all other time indoors
- the adult spends all time indoor in winter
- the child spends $8\ h.d^{-1}$ during $5\ d.w^{-1}$ outdoor in summer and all other time indoors.
- the child spends all time indoors in winter.

eq. 8;

f_m = matrix factor

Sorption of organic substances mixed in soil or dust is inhibited by physical-chemical bonding to the soil matrix and because only a portion of the substance present is in direct contact with the skin. The factor has been used in an other study (Hawley, 1985). In relation to the value of the DAR (eq. 10) the f_m is supposed to be 1.

In this model f_m = 1 is used.

eq. 10;

DAR = dermal absorption rate

Although rates of sorption vary according to substance, an average has been recommended as a simplification (Hawley, 1985). For the dermal sorption of TCDD 15% /24h has been reported (Poiger and Schlatter, 1980).

In this model for organic compounds DAR = 0.5% (adult) and 1% (child) h^{-1} and for inorganic compounds DAR = 0% is used.

eq. 13;

f_r = fraction retained in the lung

It is assumed (Reades and Gorber, 1986) that 75% of the inhaled suspended matter is retained in the lung and that all organic substance associated with inhaled soil or dust is sorbed; no matrix factor is introduced for the lung. The actual uptake may involve partly the gastro intestinal tract. It has been described that 50% of the inhaled particles are swallowed instead of inhaled (Paustenbach et al., 1986). For simplification of the equation the total uptake is supposed to take place via the lung tissue. Both f_a for lung and gastro-intestinal tract are 1.

In this model f_r = 0.75 is used.

eq. 14;

TSP = total suspended particulate matter

The value of TSP is based on levels measured in the Toronto area. The ratio of TSP indoor to outdoor have been reported in the range of 0.7 to 0.85 (Hawley, 1985; Roberts et al., 1974). Values may vary between 50 and 100 $\mu g/m^3$ for non urban areas and 100 - 175 $\mu g/m^3$ in urban areas (21) on average 70 $\mu g/m^3$ has been proposed of which 30 - 50% is respirable according to the EPA (Schaum, 1983).

In this model TSP = 50 (outdoors) and 37.5 $\mu g.m^{-3}$ (indoors) are used.

eq. 16;

C_{oa} = concentration in the outdoor air

The initial concentration is supposed to be negligible in comparison with the ultimately calculated outdoor air concentration.

In this model C_{oa} = 0 (initially) is used.

eq. 17;

K_d = sorption partition coefficient (C_s/C_w)

The K_d for organic compounds is based on the K_{oc} and hence on the K_{ow}. For inorganic compounds the K_d that can be used are summarised by Baes (1982) (see Table 2 p 19).

H = Henry's Law Constant

Henry's Law Constant is calculated according $H = P / S_w$.

eq. 18;
K_{oc} = organic carbon partition coefficient
The K_{oc} is calculated according to Karickoff (1981).
$\log K_{oc} = \log K_{ow} - 0.317$

eq. 21;
L_s length of the diffusive path
Calculation via this equation may give an overestimation of the length of the diffusive path.

eq. 22;
D_a = diffusion coefficient through air
A general coefficient for organic compounds has been postulated by Jury et al. (1983) of 0.018 m^2/h, and by McKone and Layton (1986) of 0.024 m^2/h. When available compound specific values should be used.

In this model 0.0295 $m^2.h^{-1}$ is used as default value (this is the actual value for benzene).

SN_p = porosity of the soil
SN_a = air content of the soil ($SN_p - SN_w$)
SN_w = water content of the soil
The porosity of the soil can be assumed depending on the characteristics of the soil (sand, peat, clay), whereas the water content generally is determined gravimetrically.

In this model SN_p = 0.5 and SN_a = 0.3 are used (supposing a sand type soil).

eq. 23;
L = length of evaporation surface

In this model L = 300 m is used as a default.

eq. 24;
u = viscosity of air

In this model u = 65.80 g.(m.h)$^{-1}$ is used.

p = density of air

In this model p = 1280 g.m^{-3} is used.

eq. 28;
X_a = the thickness of the air sublayer
A value of 1cm has been proposed by McKone and Layton (1986). In this model equation 28 has been used to calculate X_a.

V_1 = kinetic viscosity of air

In this model V_1 = 0.05137 m^2.h^{-1} is used.

eq. 29;
k = Karman constant

In this model Karman = 0.4 is used.

sr = surface roughness

In this model sr = 0.28 m is used.

eq. 30;
Y = height of the breathing zone above ground level

In this model Y = 1.5 m is used.

Prc = Prandtl constant

In this model Prc = 0.4 is used.

eq. 34;

CN_p = porosity of the concrete

CN_a = air content of the concrete

These values are assumed based on comparison with porosity and air content of soil. The porosity may vary from 1 to 2 %.

In this model CN_p = 0.02 and CN_a = 0.01 $m^3.m^{-3}$ are used.

eq. 35;

Dimensions of the basement

The dimensions of the basement are length (l), width (b), height (h) and thickness of the walls and floor (d_c).

In this model l = 10, b = 10, h = 2 and d_c = 0.1 m are used.

R_a = rate of air exchange in the basement

In this model R_a = 2 h^{-1} is used.

eq. 36;

Is based on the assumption that the concentration on the living floor is 10 % of the basement air concentration (ten Berge, 1985). Values of unto 50 % are also used in models (CCREM, 1988-a, -b).

In this model 10 % is used.

eq. 37;

Is based on the assumption that the air quality of the living room will be equal to or poorer then the ambient air quality.

eq. 41;

This equation is based on a publication by Baes (1982) on the relationship between K_d and BCF for metals.

Table 2 Relationship BCF and Kd

Metal	BCF	Kd
Chromium	0.03 ± 0.006	5000 ± 1000
Cobalt	0.06 ± 0.02	60 ± 10
Lead	0.04 ± 0.01	400 ± 200
Cadmium	0.55 ± 0.1	6 ± 1

In this model the reported K_d values are used.

The uptake of plants is specific for both plant species and individual metals. In Table 3 an overview is given for a number of plants (Sauerbeck, 1988). A range of BCF is given for a number of metals in Table 4 (Sauerbeck, 1988).

Table 3 Plant uptake of heavy metals.

high	moderate	low	very low
lettuce	onion	corn	beans
spinach	mustard	cauliflower	peas
carrot	potato	asparagus	melon
endive	radish	selery	tomatoes
cress		berries	fruit
beet			paprika
leaves(beet)			

Table 4 BCF for a number of metals.

metal	BCF
As	0.01 - 0.1
Cr	0.01 - 0.1
Hg	0.01 - 0.1
Pb	0.01 - 0.1
Cu	0.1 - 1.0
Ni	0.1 - 1.0
Cd	1.0 - 10.0
Tl	1.0 - 10.0
Zn	1.0 - 10.0
Co	0.01 - 0.1
F	0.01 - 0.1
V	0.1 - 1.0
Mo	0.1 - 10.0
Se	0.1 - 10.0
B	1.0 - 10.0

eq. 44 to 47;
These equations are based on data presented by Ryan et al (1988). In the equations C_s is the total concentration in the soil (wet weight). In this model C_s is the soil concentration based on dry weight. Therefore the equation used in this model uses 1 / K_d in stead of the correction for bulk density and water content.

eq. 48;
This equation is based on the "Users Manual for TOX-Screen" which is described in an EPA report (Hetrick and McDowell-Boyer, 1984).
f_{in} = initial fraction of interception.

In this model f_{in} = 0.4 is used.

Y_v = vegetative production.
A number of values based on fresh weight given in literature are (water content of vegetables is 80%):

Table 5 Yield of different types of crop

CROP	Y_v
cabbage	4.09
cauliflower	2.09
lettuce	2.20
mixed grain	0.30
leafy vegetables	1.90
non-leafy veg.	0.57
root	2.60
fruit	0.31
mixed crop	1.40

(Environ. Corporation, 1986; CSA, 1986)

In this model Y_v = 0.28 kg/m^2 (dry weight) is used.

f_{Ei} = weathering constant.
Suggested values are 0.033 to 0.05 d^{-1} correlating with half-live values of resp. 21 and 15 days.

In this model 0.033 d^{-1} is used.

t_e = crop growth period.
Suggested values are 150 to 180 days (length of the summer).

In this model 180 d is used.

DR_o = deposition rate outside.
The value used by AERIS is 230 mg/m^2.d (Reades and Gorber, 1986). Based on Olie et al. (1983) the deposition rate would be 43.2 mg/m^2.d (deposition 1 cm/s).

In this model 230 mg/m^2.d is used.

eq. 49;
fh_{max} = maximum fraction of consumption of home grown produce.

It was originally suggested to use 0.2 by Golder (1), but in the development of AERIS 0.05 has been proposed (CCREM, 1988a; CCREM, 1988b). For the Dutch situation 0.1 has been proposed (de Nijs et al., 1988).

In this model 0.1 is used.

eq. 50;
It is assumed that 50% of the consumed plant products are root type products and 50% are stem type products. The concentration of the above soil parts of plants is the sum of uptake/translocation and dusting.

eq. 51 - 56;
These equations are the equivalent of the calculations for human intake of chemicals through the different exposure routes. The characteristics of cattle are given in Table 6.

Table 6. Characteristics of cattle.

Description	Value	Unit
AID	0.72	kg/d
	0.25 - 0.5	kg/d
VA	130	m3/d
Q_{pc}	16.5	kg/d
Q_w	55	l/d

(Rosenblatt et al., 1983; McKone and Layton, 1986)

AID = amount of soil ingested; VA = volume of air breathed; Q_{pc} = plant consumption; Q_w = water consumption.

In this model the following assumptions are used (McKone and Layton, 1986):

- **the cattle spends 24 h/d outside during 7d/w in summer and half of the winter period.**
- **the fractions sorbed are 1.**

- the fraction retained in the lung is 0.75.
- the fraction of ground water used for drinking water 0.5.
- the fraction of surface water used for drinking water 0.5.

eq 57/58;
These equations are based on data published by Travis and Arms (1988). Linear regression was applied to develop the equations used in this model through Lotus 1,2,3.
Regression output:

	log Bme	log Kmi
Constant	- 6.88019	-6.78555
Std Err of Y	0.936826	0.806744
R squared	0.649704	0.543491
Coefficient	0.831647	0.730947
Std Err of X	0.104727	0.131379

eq 59;
This equation is based on data presented by Kenaga (1980).

eq. 62;
The constants C and D are based on published data relating log BCF and log K_{ow}.

Table 7 Relation log BCF and log K_{ow}

Species	C	D
fish mussel	0.76 0.858	0.23 0.808

(Geyer et al., 1982; McKone and Layton, 1986)

eq. 65;
This equation is based on an article by Vonk (1985) concerning permeation of organic compounds through pipes for drinking water supply.
δt = number of days that the water is stagnant.

In this study δt = 8 h is used.

P = permeation coefficient.
The permeation coefficient for a group of organic chemicals varied from 4.8 E-7 to 35 E-7 m^2/d. No permeation has been described for metals.

In this study 35 * 10^{-7} m^2/d is used.

Dimensions of the drinking water pipe.

In this study LDPE pipe with outside diameter 0.032 m and thickness of the wall of 0.0035 m are used.

eq. 66;
This equation is based on an article by Hushon et al. (1983) on environmental exposure analyses.
T = temperature of the water.

In this study T = 313 K is used.

Dimension of the droplet.

In this study the droplet is assumed to be a sphere with a radius of r = 1 mm.

t_f = falling time of the droplet.

In this study t_f = 1 s is used.

eq. 67;
K_g = the gas phase mass transfer coefficient.

In this study 29.88 $m.h^{-1}$ is used for a droplet.

eq. 68;
K_l = liquid phase exchange rate.

In this study 0.2 $m.h^{-1}$ is used.

eq. 69;
This equation is based on information given by W. ten Berge and an article by Andelman (1985).
V_w = volume of water used during showering.

In this study V_w = 150 l is used.

V_{bath} = volume of the bathroom.

In this study V_{bath} = 25 m^3 is used.

t_s = duration of showering.

In this study 0.5 h is used.

eq. 70;
DAR_w = dermal absorption rate for exposure in water.

In this study DAR_w = 1 $\mu g.cm^{-2}.(mg.l^{-1}).h$ is used (41).

eq. 71;
Q_w = water consumption.

In this study Q_w = 1 (child) and 2 (adult) l are used.

f_g = fraction of ground water used for drinking water.

In this study f_g = 0 is used for humans.

eq. 72 - 75;
These equations are used in calculating the maximum soil concentration to be used in the mass transfer and equilibrium equations (based on the limitation of the maximum water solubility).

eq. 76;
This equation is based on a mass balance for an underlying compartment of soil in the saturated zone. The dimensions of the compartment are L, length of the location; L_w, width of the location and d, thickness of the mixing zone.

IN	OUT
$q_{inf} * L * L_w * C_{pw}$	$q_{inf} * L * L_w * C_{gw}$
$K * d * I * L_w * C^o_{gw}$	$K * d * I * L_w * C_{gw}$

The mass balance is valid when dC/dt = 0.

It is assumed that $C^o_{gw} \ll C_{gw}$, therefore $C^o_{gw} = 0$ is used in the model.

eq. 77;
q_{re} = recharge rate
In the Dutch situation it is supposed that the total infiltration is on average 1 mm.d^{-1}.

In this study 1 mm.d^{-1} is used.

eq. 78;
This equation is based on a mass balance for an adjacent body of water fed by run-off soil, ground water and flow though of surface water. The run-off can either be calculated assuming loss of soil or by calculating the loss of soil using the Soil Conservation Service (SCS) method (Soil Conservation Service USDA, 1971).

IN	OUT
$Q^o_{sw} * C^o_{sw}$	$(Q^o_{sw} - Q_{ev}) * C_{sw}$
$Q_{di} * C_{gw}$	$Q_{di} * C_{sw}$
$R_o * C_s$	$R_o * C_{sw} * K_d$

The mass balance is valid when dC/dt = 0.

It is assumed that $C^o_{sw} \ll C_{sw}$, therefore C^o_{sw} = 0 is used in the model.

Diffusion coefficient in water 0.23 10^{-5} $m2.h^{-1}$ (McKone and Layton, 1986).

eq. 79;
LS = run-off of soil.
A number of run-off experimental tests have been described, but only in a few cases total erosion of soil on a yearly basis have been reported (Wauchope, 1987; Baker et al., 1978). The average loss of soil being 3 - 30 $ton.ha^{-1}$ on an annual basis (Donigian and Carsel, 1987; Haith, 1987).

In this model LS = 2 $mm.y^{-1}$ is used.

L_{ws} = width of the soil loss area.

In this model L_{ws} = 10 m is used.

f_c = fraction of the area covered with housing and or growth.

In this model f_c = 0.9 is used for urban areas.

Run-off and soil loss can also be estimated using the methods described by Mockus and Ogrosky and Wischmeier and Smith (Haith, 1980).

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ANNEX I PARAMETERS

Parameter	Description	Unit
A	constant K_d - BCF_{plant} relationship	-
A_{ah}	surface area of arms and hands	m2
A_d	surface area of the droplet	m2
A_{fh}	surface area of forearms and hands	m2
A_h	surface area of hands	m2
A_{hi}	surface area of the inside of the hands	m2
A_{lf}	surface area of legs and feet	m2
A_t	surface area of basement walls and floor	m2
A_{tot}	total surface area of the skin	m2
AED	amount exposed to daily by dust or soil	mg/kg-bw.d
AID	amount ingested daily	mg/kg-bw.d
B	constant K_d - BCF_{plant} relationship	-
BCF	bioconcentration factor for plants or aquatic organisms	-
C	constant K_{ow} - BCF_m relationship	-
c	index indicating cattle	-
C_{ba}	concentration in basement-air	g/m3
C_{dw}	concentration in the drinking water	mg/l
C_{gw}	concentration in the ground water	µg/l
C_{la}	concentration in living room air	g/m3
C_m	concentration in aquatic organisms	mg/kg-dm
C_{oa}	concentration in the outdoor air	g/m3
C_{pl}	concentration in part of the plant	mg/kg-dm
C_{pt}	average consumption in crops	mg/kg-dm
C_{pw}	concentration in external solution.	mg/l
C_s	total concentration in soil (including water phase)	mg/kg
C_{sa}	concentration in soil-air	g/m3
C_{si}	concentration at the interface (soil/air)	g/m3
C_{sm}	concentration in the soil with a maximum of C_{smax}	mg/kg-dm

C_{smax}	maximum concentration in soil which corresponds with the water solubility	mg/kg-dm
C_{sw}	concentration in surface water	mg/l
C_t	concentration of the contaminant in the service pipe after t days of stagnancy	mg/l
C_{up}	concentration at the upper edge of the diffusive sublayer	g/m3
CN_a	air content of concrete	m3/m3
CN_p	porosity of concrete	m3/m3
D	constant K_{ow} - BCF_m relationship	-
d	thickness of the mixing zone in the aquifer	m
D_a	diffusion coefficient through air	m2/h
d_c	thickness of the concrete	m
d_e	thickness of the pipe wall	mm
D_{ef}	the effective molecular diffusibility of the chemical within the soil pore spaces	m2/h
D_{efc}	the effective molecular diffusibility of the chemical within the pores of the concrete	m2/h
D_{pe}	permeation coefficient (HDPE-pipe)	m2/d
$DA_{n,x}$	dermal absorption through soil or dust per unit body weight per season	mg/kg-bw.d
DA_w	dermal absorption through water contact	mg/kg-bw.d
DAR	dermal absorption rate through soil or dust	1/h
DAR_w	dermal absorption rate for exposure in water	m/h
$DI_{n,x}$	direct ingestion of soil or dust per unit body weight per season	mg/kg-bw.d
DI_w	direct ingestion through drinking water	mg/kg-bw.d
d_l	thickness of the dust or soil layer	µm
d_o	outside diameter of a pipe	m
DR_y	deposition rate of dust	mg/m2/d
d_u	thickness of the unsaturated zone	m
f_a	fraction absorbed	-
f_c	fraction of area covered by housing or growth	-
f_{gw}	fraction of ground water used for consumption	-
f_{hmax}	maximum fraction of consumption of home grown	

	produce	-
f_{hmin}	minimum fraction of consumption of home grown produce	-
f_{in}	fraction initially intercepted	-
f_m	matrix factor	-
f_{oc}	fraction of organic carbon in soil	-
f_r	fraction retained in the lung	-
f_{rs}	fraction of soil in dust	-
f_{sw}	fraction of surface water used for consumption	-
f_t	fraction of hours daily this occurs	-
f_{voids}	fraction of empty volume between particles	-
f_x	fraction of the year per season	-
f_z	fraction of food products from the vicinity of the location (fish, dairy, milk or meat)	-
f_{Ei}	weathering constant	1/d
H	Henry's Law Constant	Pa.m3/mol
h	height (wind velocity)	m
I	hydraulic gradient	m/m
$IP_{y,x}$	inhaled particulate matter per season as soil	mg/kg-bw.d
ITSP	inhaled total suspended particulate matter	mg/kg-bw.d
IV_w	inhaled vapour during showering	mg/kg-bw.d
$IV_{y,x}$	total inhaled vapour	mg/kg-bw.d
K	hydraulic conductivity of the aquifer	m/h
k	Karman constant	-
K_b	the concrete-air phase mass transfer coefficient	m/h
K_d	sorption partition coefficient	m3/g
kG	gas mass transfer coefficient	m/h
K_{fa}	partition coefficient fat/diet	(mg/kg)/(mg/d)
K_g	the gas phase mass transfer coefficient	m/h
K_{gs}	mass transfer coefficient for diffusive sublayers	m/h
		m/h
kL	liquid mass transfer coefficient	m/h
K_l	liquid phase exchange rate (CO_2)	m/h
K_{me}	partition coefficient meat/diet	(mg/kg)/(mg/d)

K_{mi}	partition coefficient milk/diet	(mg/kg)/(mg/d)
K_{oc}	organic carbon partition coefficient	cm3/g
K_{os}	overall soil phase mass transfer coefficient	m/h
K_{ow}	octanol/water partition coefficient	g/g
K_s	the soil-air phase mass transfer coefficient	m/h
k_{us}	number of times the total amount covering the skin surface is ingested per active period equivalents	1/d
k_{wa}	extent of evaporation	-
L	the length of evaporation surface	m
L_{cmax}	depth of contamination in the soil	m
L_s	length of the diffusive path in soil	m
L_w	width of the location	m
L_{ws}	width of the soil loss zone	m
M	molecular weight	g/mol
m	index indicating aquatic organisms	-
MI	equivalent uptake through meat, milk and dairy products	mg/kg-bw.d
n	index indicating dust or soil	-
N	fraction of days annually this occurs (subscript o = outside; subscript i = inside)	-
N_b	fraction of days bathing occurs	-
N_{ba}	diffusive flux to the basement air	g/m2.h
N_{dc}	dust cleaning rate	1/w
N_{oa}	diffusive flux to the outdoor air	g/m2.h
N_s	fraction of days showering occurs	-
N_y	fraction of days spent inside or outside	-
p	density of air	g/m3
P	vapour pressure	Pa
Prc	Prandtl constant	-
Q_{di}	amount discharged from the aquifer to surface water	m3/d
Q_{ev}	amount of evaporation	m3/d
Q_{fv}	consumption of fruit and vegetables	kg/d
q_{inf}	infiltration rate	m/d

Q_m	consumption of aquatic organisms	kg/d
Q_{pc}	consumption of plants by cattle	kg/d
q_{re}	recharge rate	m/d
Q_{sw}	mass flow of surface water	m3/d
Q_w	water consumption	dm3/d
Q_z	consumption of meat, fat or dairy products	kg/d
r	internal radius of the pipe	m
R	universal gas constant	Pa.m3/mol
R_a	rate of air exchange per hour	1/h
R_o	run-off of soil	mm/y
S_w	water solubility at 10 °C	mg/l
Sc	the solute gas phase Schmidt number	-
SG	bulk density of dust or soil	g/cm3
SN_a	air content of soil	m3/m3
SN_p	porosity of soil	m3/m3
SN_w	water content of soil	m3/m3
sr	surface roughness	m
T_{soil}	temperature of the soil surface	°C
δt	number of days that the water is stagnant	d
t_b	duration of bathing	h
t_e	crop growth period	d
t_f	falling time of the droplet	s
t_s	duration of showering	h
TI	total intake of contaminants by cattle	mg/d
TSP_y	total suspended particulates	µg/m3
T_x	ambient air temperature	°C
txl_y	time spent in hours per day in season	h/d
$tx2_y$	time spent in days per week in season	d/w
u	viscosity of air	g/m.h
V^*	the friction velocity	m/h
V_1	the kinetic viscosity of air	m2/h
V_{10}	the wind velocity at a height of 10 m	m/h
Vb	volume of the basement	m3
V_{bath}	volume of the bathroom	m3
V_d	volume of the droplet	m3

V_W	volume of water used	m3
VA	volume of air breathed	m3/d
VI	uptake via fruit and vegetables	mg/kg-bw.d
W	receptor's weight	kg
x	index indicating summer or winter	-
X_a	the thickness of the air sublayer	m
y	index indicating indoor or outdoor	-
Y	the distance the breathing zone is above the air-soil interface	m
Y_V	vegetative productivity	kg/m2
z	index indicating meat, fat or dairy products	-

APPENDIX 4

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APPENDIX 5

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