Technical Report

No 58

Assessment of Non-Occupational Exposure to Chemicals

May 1994

ISSN-0773-8072-58

ECETOC

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European Centre for Ecotoxicology
and Toxicology of Chemicals

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CONTENTS

SUMMARY

The main objective of the work described in this report is to review the assumptions and equations used to assess non-occupational exposure to chemicals. The approach recommended in this report to assess consumer exposure and indirect human exposure has been evaluated for several representative chemicals with different properties and use patterns.

A step-wise approach is recommended to assess consumer exposure. The first step consists of an initial evaluation to establish whether a potential exposure exists. If the substance itself is a consumer product or if the substance is contained in a preparation/article which is a consumer product, direct exposure of the consumer is possible. It is then necessary to estimate the extent, frequency and duration of exposure. The assessment of extent, duration and frequency requires an understanding of the substance and/or product use category and use scenario. Information on the use and function of the substance/product should therefore be provided in the dataset to allow a meaningful exposure assessment. Typical product use scenarios are discussed for common consumer products such as cosmetics, household products, aerosol products, paints and plasticisers. Recommendations are made for typical quantities per application, and frequencies of application. The second step consists of an evaluation of all potential exposure routes (oral, dermal, inhalation) to allow the estimation of the total exposure of the consumer to a particular substance. Comprehensive consumer exposure assessments require measured data to assess the extent of dermal, oral and inhalation exposure to products and their components. Realistic exposure assessments can also be achieved using reasonable calculations and justifiable assumptions for key exposure parameters. In this report some practical approaches are described to predict uptake via oral, dermal and inhalation routes taking into account the bioavailability of the substance. Use of default values in the absence of data may often lead to an overestimation of the exposure dose. A check for realism in the exposure assessment is therefore recommended to ensure that the final assessment is realistic and not overly conservative.

Similarly to the consumer exposure assessment, a step-wise approach is recommended to assess indirect human exposure. The first step (screening phase) consists of an initial evaluation to establish whether air, water or soil compartments are likely to be exposed to the substance (i.e. environmental exposure assessment) and whether human exposure via air, water, soil and food intake is likely to occur (i.e. indirect exposure). It is recommended that if environmental exposure occurs at a regional level, indirect exposure of the public can be expected and should be assessed. Environmental exposure can be estimated if it is known how and in what quantity a substance enters the environment and how it is subsequently distributed and transformed in these receiving

compartments (i.e. air, water, soil). The proposed environmental exposure scheme to obtain release estimations and environmental concentrations for water, air and soil at the regional level has been discussed in detail in ECETOC Technical Report No. 51 "Environmental Hazard Assessment of Substances" (1993a) and is further developed in a forthcoming ECETOC Technical Report on "Environmental Exposure Assessment" (1994a).

If indirect exposure is likely to occur, then it is necessary to estimate the relation between the concentration in each contact medium (air, water, soil) and transfer to food products and drinking water. In addition, it is necessary to assess dietary characteristics and food sourcing for the average individual. Comprehensive indirect exposure assessments (investigative phase) require measured concentration data for air, water, soil and food products, and measured data on ingestion (food, water, soil) and inhalation rates. In the absence of measured data, some practical approaches (screening phase) are described to predict the concentrations in air, water and soil at a regional level, and to assess transfer of chemicals from these media to drinking water and food products. Quantitative structure activity relationships (QSARs) are discussed to relate partition between water, soil and plants, and between animal diet, lipid tissue, and food product. In addition, average food baskets for all EC member countries have been compiled to estimate the potential dose to which the average adult or child may be exposed.

The total non-occupational exposure (consumer and indirect) or resulting total estimated intake for the average individual can then be used in the human health risk assessment and compared with intake criteria, such as acceptable and tolerable daily intakes.

SECTION 1. INTRODUCTION

In recent years there has been growing concern about environmental contamination and exposure of the general population to chemicals. Many substances are released to receiving environmental compartments due to losses in production, processing, formulation and use, or due to losses from waste treatment and recycling processes.

The development of risk assessment procedures for chemicals has received considerable attention from regulators, academia and industry. Impending changes in EEC legislation have accelerated the need to define the principles and consider the practical details of exposure, effect and hazard assessment.

A scientifically-based risk assessment strategy for substances requires a comprehensive and integrated assessment of local and regional emissions, transport, distribution and transformation processes (ECETOC, 1993a). The environmental exposure can be estimated if it is known how and in what quantity a substance enters the environment and how it is subsequently distributed and transformed in the receiving compartments (e.g. air, water, soil). The effect of transport and transformation processes on the distribution and concentration of substances in the different environmental compartments may be predicted by using mathematical models (OECD, 1989; Braat *et al*, 1991; OECD, 1991; ECETOC, 1992a), assessed in experimental laboratory simulation models, or possibly measured in actual environments if specific analytical techniques have been developed for the substance of interest. The end product of an environmental exposure assessment is typically a predicted or measured concentration for ambient air, surface water, ground water, surface soil, and root-zone soil at the local (PEC_{local}) or regional ($PEC_{regional}$) scale.

When contaminants enter the environment, man may be exposed through multiple exposure pathways. The link between man, environment and chemical exposure is through inhalation, ingestion, and dermal contact as visualised in Figure 1.

The prediction of a potential dose to which human populations are exposed through air, water, soil and food throughout a lifetime is often referred to as indirect exposure assessment. The average daily dose is dependent on the concentration in each contact medium (air, water, soil, food) and the intake or uptake factor for each contact medium. This implies that the environmental exposure assessment of substances will be linked to an estimation of human exposure through food consumption. Transfer functions and food consumption patterns will need to be assessed to predict this exposure. It should be pointed out that although each individual step in the exposure

Figure 1 The Link Between Man, The Environment and Chemical Exposure

assessment relies on justifiable assumptions, the potential dose must be interpreted with care. Error and uncertainty may propagate through the assessment and the potential dose is therefore only an approximate value at screening level.

Direct exposure of the consumer to a substance can be expected if the substance itself is a consumer product or if the substance is contained in a preparation or article available on the market. Exposure to the substance of interest leads to a dose which is the quantity of the substance received via the relevant exposure routes i.e. via dermal contact, ingestion or inhalation. To establish this dose, it is necessary to understand the variety of uses (and foreseeable misuses) of the substance itself or the substance in a preparation/article, the quantity of substance typically used in such scenarios and the frequency and duration of substance use. Only when such data are available, an estimation of the total realistic exposure for the consumer to the substance of interest is feasible for all possible routes.

The total human exposure can be estimated for each target population (e.g. workers, consumers, public) for which exposure to the substance can be reasonably foreseen. When a new substance is initially introduced to the market place, it is more likely that the exposure is direct rather than indirect. The new substance is often a part of an article or product and exposure can result from migration, evaporation, and/or leaching and is influenced by the physico-chemical characteristics of the substance and specific consumer habits. For existing substances it may be appropriate to investigate direct and indirect exposure.

The difficulty in exposure assessment lies in the complex nature of the transfer pathways. ECETOC therefore formed a Task Force with the following terms of reference:

- define the principles and practical considerations for evaluating direct and indirect human exposure to substances,
    - to which consumers are exposed,
    - which are released into the environment from diffuse and localised sources;
- Review critically the approach used by regulators in assessing consumer exposure and indirect exposure to man for well-documented representative substances;
- Recommend possible practical procedures for assessing the probability and magnitude of direct and indirect human exposure.

The main objective of this report is to review the assumptions and equations used to assess consumer and indirect human exposure to substances. Occupational exposure i.e. exposure of workers is not considered in this report.

The recommended approach and equations have been compiled in the software package HAZCHEM (ECETOC, 1994b) in order to allow an initial evaluation of indirect exposure. This is illustrated with representative case studies. The concept as discussed in this report is applicable to all substances, whether 'new' or 'existing'.

SECTION 2. BACKGROUND

2.1 LEGISLATION

The 7th Amendment of Directive 67/548/EEC (EEC, 1992) came into force on 31st October 1993. Article 3.2. requires that risk assessment be carried out according to principles to be laid down in a Commission Directive on Risk Assessment of New Substances (93/67/EEC) which was adopted in April 1993. The specific guidance on how to conduct exposure and effect assessment and risk characterisation has been described in Technical Guidance Documents. The purpose of these Technical Guidance Documents is to assist the notifier and the assessor in the risk characterisation and, if necessary, in deciding on what further testing would be required and its timing. This guidance is to be used in conjunction with the Risk Assessment Directive (93/67/EEC). Technical Guidance Documents were adopted on 31st October 1993.

The EC Council Regulation on the evaluation and control of the environmental risks of existing substances (EEC, 1993) requires competent authorities to evaluate the risks to man and environment of existing substances. This regulation was adopted on 23rd March 1993, and came into force on 4th June 1993. Its implementation requires a Commission Regulation on priority setting and risk assessment of Existing Substances. This Directive will refer to a large extent to the Commission Directive on Risk Assessment of New Substances, and its respective Technical Guidance Documents.

2.2 SCIENTIFIC DEVELOPMENTS

The protection of man and the environment has generated numerous activities in the fields of toxicology, industrial hygiene, occupational safety, epidemiology, environmental impact assessment, environmental quality and engineering-reliability studies. In the past decade, risk characterization, risk analysis, risk assessment and risk management have grown to new and exciting 'risk' disciplines. Risk assessment methods are developed to address a wide range of health and environmental risk situations, including air pollution, occupational exposure to chemicals or radiation, consumer exposure, disposal or hazardous waste sites, hazardous substances in the food chain, and introduction of new substances or technologies.

Industry has widely used risk analyses to determine the environmental and health associated implications of both existing and new production technologies. Risk assessment methods are systematically applied to assist the decision making process, i.e. set management priorities by assessing the magnitude of the risks involved. The methods for the evaluation and control of existing and new substances within the framework of EC Council Regulation on Existing Substances and the 7th Amendment of Directive 67/548/EEC will be further developed to allow an integrated human and environmental risk characterisation of the substance.

In this context, the Dutch National Institute of Public Health and Environmental Protection (RIVM) has developed on behalf of the Netherlands Ministry of Housing, Spatial Planning and the Environment (VROM) and the Ministry of Welfare, Health and Cultural Affairs (WVC) a risk assessment software package USES (Uniform System for the Evaluation of Substances) which integrates DRANC (Dutch Risk Assessment New Chemicals), PRISEC (Priority Setting Existing Chemicals) and ESPE (Evaluation System Pesticides) (RIVM, VROM, WVC, 1994; see also Vermeire *et al*, 1992). DRANC was used in The Netherlands to evaluate risks to man and the environment for New Chemicals, but was replaced by USES in 1994. PRISEC is a regional multi-media model which assumes steady-state conditions but not equilibrium between compartments. It is a "level-3" model in the classification scheme of Mackay (1979) and was developed as software package to prioritise chemicals which should undergo risk assessment. Similarly, activities within Health and Welfare Canada and the Californian EPA have resulted in the development of software packages used for the evaluation of risk to both environment and man (Mackay *et al*, 1991; McKone, 1993).

SECTION 3. CONSUMER EXPOSURE

3.1 INTRODUCTION

External exposure for the consumer may be defined as the quantity of a substance to which an individual is potentially exposed via the oral, inhalation or dermal route. The internal exposure or uptake can be defined as the quantity of the substance which has been absorbed into the systemic circulation per unit bodyweight. Consumers can be exposed via preparations, for example, cosmetic products, aerosol products, household cleaning products etc. Consumers can also be exposed via articles, for example, through skin contact with textiles from which substances may be leached. Exposure of consumers to substances in a typical consumer product is not easy to quantify. Estimation of the exposure requires a knowledge of the approximate concentration of the substance in the product which may occasionally be obtained from the label or directly from the manufacturer. Exposure estimates also require an understanding of the product use scenarios and the route(s) of exposure. The estimated exposure level can then be used as part of a meaningful risk assessment process by comparing it with the No Observed Adverse Effect Level (NOAEL) of the substance. The margin of safety for the consumer exposed to the substance of interest can then be calculated. In the absence of measured data, maximum predicted exposure is generally used as a default. If the safety margins appear small, it is very important to strive towards developing a realistic estimate of each potential exposure whenever possible using real life data. This is to ensure that the exposure estimate is not grossly exaggerated as a result of using maximum default values.

A step-wise approach is advocated to assess the exposure to man. The first step in the process is an initial evaluation to establish whether a potential exposure exists. It is then necessary to estimate the intensity, frequency and duration of exposure to the hazardous agent.

3.2 DURATION OF EXPOSURE

An estimate of the duration of exposure is important when preparing a consumer exposure assessment. Consumers may be exposed for varying lengths of time when using preparations or articles. Depending on the normal use or reasonably foreseeable misuse of the actual preparation or article, the exposure may consist of a single dose of a substance over a short period of time or of repeated doses of the substance over a longer time period. Consumers may experience acute exposure to a substance through a single low-frequency event e.g. the use of a paint-stripping solvent in the home. Accidental misuse of a product can also lead to acute and often high

Table 1 Definitions of Symbols Used in Consumer Exposure Calculations

U	= estimated total uptake	(mg/kg)
U_{oral}	= estimated oral uptake	(mg/kg)
I_{oral}	= amount of substance ingested	(mg/kg)
B_{oral}	= bioavailability for oral exposure (default = 1)	
I_{inh}	= amount of substance inhaled	(mg/kg)
C_{air}	= average concentration of substance in air	(mg/m^3)
V_{inh}	= ventilation rate of an adult (default = $0.8 m^3/h$)	(m^3/h)
t	= duration of exposure	(h)
BW	= bodyweight of an adult	(kg)
U_{inh}	= estimated uptake of substance by lungs via inhalation	(mg/kg)
B_{inh}	= bioavailability for inhalation exposure (default =0.75; Linders, 1990)	
E_{derm}	= amount of substance in contact with the skin surface	(mg)
C_{derm}	= average concentration of substance in skin surface layer	(mg/cm^3)
T_{derm}	= thickness of surface layer (default = 0.01; Vermeire *et al*, 1993)	(cm)
S_{derm}	= surface area of exposed skin	(cm^2)
U_{derm}	= estimated uptake via the skin	(mg/kg)
J	= flux of substance through the skin (permeation rate)	($mg/cm^2/h$)
D_{derm}	= diffusion coefficient of substance in stratum corneum	(cm^2/h)
d_{derm}	= thickness of stratum corneum (default = 0.0025cm)	(cm)
K_m	= partition coefficient of substance (stratum corneum/water)	
K_p	= skin permeability coefficient of substance ($K_p = D_{derm} \cdot K_m / d_{derm}$)	(cm/h)
Mw	= molecular mass of substance	(g/Mol)
K_{ow}	= octanol/water partition coefficient	
Lt	= lag time	(h)
UPS	= uptake before saturation	(mg/cm^2)
A	= amount of substance deposited per unit area on dishes	(mg/cm^2)
FA_{oral}	= fraction of deposited substance ingested	
S_{dish}	= area of dishes in contact with substance	(cm^2)
dS/dt	= release of solvent per unit time	(g/h)
R	= evaporation rate	($g/m^2/h$)
a	= area painted per unit time	(m^2/h)
A_p	= surface area to painted	(m^2)
A_{ev}	= evaporating surface of wet paint	(m^2)
M	= mass of solvent applied per unit area	(g/m^2)
t_d	= drying time between one element being painted and being completely dry (= M/R)	(h)
t_a	= time required to paint total area (A_p/a)	(h)
S(t)	= release rate as function of time	
V1	= volume of room of consumer product application	(m^3)
V2	= remaining volume of house	(m^3)
V1 +V2	= volume of house	(m^3)
C1	= average concentration of substance in the room of consumer product application	(mg/m^3)
C2	= average concentration of substance in remaining house	(mg/m^3)
ACH	= room air changes per hour (default = 1)	
Q21 = Q12	= exchange rate between V1 and V2 (SCIES, 1991)	(m^3/h)
Q10	= exchange rate between V1 and the outside air	(m^3/h)
Q20	= exchange rate between V2 and the outside air	(m^3/h)

exposures e.g. accidental ingestion of a product from the container by a child. Longer-term exposure to preparations and articles also occurs through the repeated use of a product over a period of several days or longer e.g. an individual painting several rooms in a house or a consumer regularly using a personal care product such as a deodorant. A realistic estimate of the duration of exposure should be made based on a knowledge of the typical product uses and on the reasonably foreseeable misuses and accidental misuses of the product.

By analogy therefore, for each use category of the chemical, it can be established whether the exposure of the consumer is characterised as acute, i.e. single or multiple doses within a short period such as from the use of a paint stripping solvent; subchronic, i.e. repeated or continuous exposure extending over several days such as could occur during and after painting of a room or rooms; or chronic, i.e. repeated or continuous exposure extending over periods of years or even the whole life span such as could arise from daily use of the same spray deodorant.

3.3 ROUTE OF EXPOSURE (ORAL / DERMAL / INHALATION)

Information on the use and function of a substance should be provided in the data set. Subsequently it can be decided to which product group the substance belongs, and which exposure route(s) need to be considered for the exposure assessment.

3.3.1 Oral Exposure

Consumers may ingest substances in food products and drinking water. In addition, substances in preparations such as detergents may also be ingested inadvertently, e.g. detergent residues on eating utensils which have not been rinsed with clean water. Consumers may also ingest the non-respirable fraction of inhaled airborne aerosols or dusts (see Section 3.3.2).

Intake by the oral route is normally measured in mg/(kg·event) for acute exposures or mg/(kg·day) for longer exposures. In the absence of measured data, a screening assessment can be made using simple calculations and justifiable assumptions.

Bioavailability

The amount of a substance which is taken up by the body will depend on its bioavailability. The main factor when considering absorption through the gastrointestinal tract is the solubility of the substance. Other factors include chemical reactivity, particularly with either the stomach acid or enzymes. Many substances which are water-insoluble and chemically inert can be considered to be non-bioavailable. They can of course still have local effects on the gastrointestinal tract itself. In the absence of relevant data on a substance, one should assume 100% bioavailability.

A simple equation therefore for calculating uptake (i.e. absorption) of a substance is as follows (Vermeire *et al*, 1993):

$$U_{oral} = I_{oral} \cdot B_{oral} \qquad (1)$$

Where:-

U_{oral} = estimated oral uptake [mg/kg BW]
I_{oral} = amount of substance ingested [mg/kg BW]
B_{oral} = bioavailability for oral exposure

3.3.2 Inhalation Exposure

Consumers may be exposed to gases, mists (i.e. liquid aerosols) and dusts. Similarly to the oral exposure assessment, a screening inhalation assessment can be made using simple calculations and justifiable assumptions in the absence of measured data. In order to estimate the amount inhaled, a knowledge of the concentration of the substance in the inhaled air is necessary. The total amount inhaled can be calculated as follows (Vermeire *et al*, 1993):

$$I_{inh} = \frac{C_{air} \cdot V_{inh} \cdot t}{BW} \qquad (2)$$

Where:-

I_{inh} = amount of substance inhaled [mg/kg BW]
C_{air} = average concentration of substance in air [mg/m^3]
V_{inh} = ventilation rate of an adult (default = 0.8) [m^3/h]
t = duration of exposure [h]
BW = bodyweight of an adult [kg]

The approach described above represents a worst case assessment at the screening phase because it assumes complete absorption of the substance inhaled.

Bioavailability

The amount of substance which is taken up by the body via the inhalation route will depend on the bioavailability. A number of factors need to be considered including vapour pressure, solubility, particle size, particle shape, air velocity, ventilation rate and the fact whether nose or mouth breathing is used.

In addition, when considering particulates, it must be remembered that they only partially enter the respiratory system. Once inhaled, the particles may undergo deposition or they may be exhaled without deposition. This so-called aspiration efficiency drops slowly for particle sizes of Mass Median Air Diameters (MMAD) greater than 10 μm. Only particles small enough to reach the alveolar region of the lung are available for direct pulmonary absorption (respirable fraction). Depending on solubility, there may be absorption higher up in the respiratory tract. Deposited particles can be cleared to the pharynx and swallowed. Uptake therefore depends not only on pulmonary absorption but also on absorption through the mucous membranes of the nose, mouth and upper respiratory tract. In addition, uptake through the gastrointestinal tract may occur for that fraction of the substance which is swallowed. This fraction is also important when considering the local effects of insoluble and durable substances on the lungs themselves.

Given a knowledge of bioavailability, the uptake can be calculated as follows (Vermeire *et al*, 1993):

$$U_{inh} = \frac{C_{air} \cdot V_{inh} \cdot B_{inh} \cdot t}{BW} = I_{inh} \cdot B_{inh} \qquad (3)$$

Where:-

U_{inh} = estimated uptake of substance by lungs via inhalation [mg/kg BW]
C_{air} = average concentration of substance in air [mg/m^3]
V_{inh} = ventilation rate of an adult (default = 0.8) [m^3/h]
B_{inh} = bioavailability for inhalation exposure (default value = 0.75) (Linders, 1990)
t = duration of exposure [h]
BW = bodyweight [kg].

3.3.3 Dermal Exposure

The skin of consumers may be exposed directly to substances or to articles e.g. aqueous solutions, suspensions or emulsions, solids (in whole or powder form) or gases (vapours or aerosols). The potential for dermal absorption from such exposures is likely to be most significant in the cases of liquids or solids. Examples include contact with textiles, cleaning solutions and handling of articles. It is also possible that exposure to some vapours or aerosols could lead to significant dermal absorption. Dermal exposure depends on the concentration of a substance in immediate contact with the skin.

Two stages are necessary for estimating dermal uptake. The first step is to calculate the exposure to the skin surface i.e. external exposure. The second step is to calculate the uptake via the skin. The first step is the easiest and the following equation can be used:

$$E_{derm} = C_{derm} \cdot T_{derm} \cdot S_{derm} \qquad (4)$$

Where:-

E_{derm} = amount of substance in contact with the skin surface [mg]

C_{derm} = average concentration of substance in skin surface layer [mg/cm^3]

T_{derm} = thickness of surface layer (default = 0.01 cm) (Vermeire *et al*, 1993)

S_{derm} = surface area of exposed skin [cm^2] (see Table 2).

Bioavailability

Whatever the approach, it will be necessary to consider the question of systemic bioavailability, or in other words, the facility of the substance to penetrate the skin barrier. The rate of penetration through the skin is not simple to estimate. It is a function of the differential solubility of the substance in water and fat, its polarity and molecular size on the one hand, and, on the other hand, environmental factors (temperature, humidity, etc) and skin dependent variables (skin condition, health, anatomical region, etc).

Depending on exposure and/or toxicity, the dermal penetration can be assumed to be negligible for highly lipophilic substances i.e. $\log K_{ow} > 5$. Dermal penetration is limited not by the stratum corneum but by other physiological constituents of the skin such as the aqueous layer or capillary clearance (Kasting and Robinson, 1993). The dermal penetration is considered to be very low for substances with a $\log K_{ow} < -1$ (i.e. very hydrophillic substances) and for substances with a relative molecular mass over 700 (Vermeire *et al*, 1993). Some substances have been tested for skin permeability in *in vitro* systems and these data are available in the literature. It may be possible to gain some estimate of permeability from the ratio of LD_{50} dermal/LD_{50} oral. A high ratio will be indicative of poor absorption (see ECETOC, 1993b).

Table 2 Mean surface area by body part for the adult male (EPA, 1989)[1]

Body part	Mean surface area [cm^2][2]
Head	1,180
Trunk	5,690
Upper extremities	3,190
arms	2,280
upper arms	1,430
forearms	1,140
hands	840
Lower extremities	6,360
legs	5,050
thighs	1,980
lower legs	2,070
feet	1,120
Total	19,400

[1] Values for children can be found in Appendix D.

[2] Total and subtotals do not reflect the sum of the individual body parts.

In other cases, it may be possible to calculate the dermal permeation rate using the $\log K_{ow}$. This approach is used by McKone and Howd (1992) and is described below. Whichever way it is done, either by experimental methods or by theoretical models, the actual uptake of a substance through the skin can be estimated by:

$$U_{derm} = \frac{J \cdot S_{derm} \cdot t}{BW} \tag{5}$$

Where:-

U_{derm} = estimated uptake via skin [mg/kg BW]

J = permeation rate [mg/(cm^2·h)]

S_{derm} = surface area of exposed skin [cm^2]

t = duration of exposure [h]

BW = bodyweight [kg].

The Approach of McKone and Howd

McKone and Howd (1992) have compiled experimental data on skin permeation. The permeation rate for human epidermis is usually measured *in vitro*. A glass cell, separated into two compartments by the isolated *stratum corneum*, is used. One compartment is filled with the aqueous solution of the substance. The other compartment may contain distilled water, which is continuously stirred. From the experimental data, the authors developed a generalised approach for estimation of the permeation coefficient and the lag time for permeation based on the octanol/water partition coefficient and the molecular mass of the substance.

The permeation rate or dermal flux J of a chemical through the *stratum corneum* of the skin may be described by:

$$J = \frac{D_{derm} \cdot C_{derm} \cdot K_m}{d_{derm}} \tag{6}$$

or with K_p

$$J = C_{derm} \cdot K_p \tag{7}$$

Where:-

D_{derm} = diffusion coefficient of substance in *stratum corneum* [cm^2/h]

C_{derm} = average concentration of substance in skin surface layer [mg/cm^3]

d_{derm} = thickness of *stratum corneum* (0.0025 cm)

K_m = partition coefficient *stratum corneum*/water of the substance

K_p = permeability coefficient, substance-specific [cm/h]
= $D_{derm} \cdot K_m / d_{derm}$

For most substances, if a figure is available, it will be K_p. This can be used directly in the dermal uptake equation (5) as follows:

$$U_{derm} = \frac{K_p \cdot C_{derm} \cdot S_{derm} \cdot t}{BW} \tag{8}$$

In older literature, the percentage of a substance absorbed is sometimes available. This figure can usually be converted to a K_p value before being used in other scenarios.

Theoretical Prediction of Permeability Coefficient

McKone and Howd (1992) studied the published data on skin permeation rates for many substances in water solution and derived the following estimate of K_p in relation to molecular weight and the octanol/water partition coefficient:

$$K_p = Mw^{-0.6}\left[0.33 + \frac{d_{derm}}{2.4\cdot10^{-6} + 3\cdot10^{-5}\cdot K_{ow}^{0.8}}\right]^{-1} \tag{9}$$

Where:-

Mw = molecular mass of substance [g/Mol]
d_{derm} = thickness of *stratum corneum* (0.0025 cm)
K_{ow} = octanol/water partition coefficient

Using Equation (9) for the data of 51 chemicals, 68% of the predicted K_p values were within a factor of 3 and 95% and of the predicted K_p values within a factor of 9 of the measured value.

The permeation rate predicted by the above equation is only valid once a steady state has been reached. There is a lag time before the steady state, which is the time it takes for the chemical to penetrate the *stratum corneum.* McKone and Howd (1992) present the following equation for the lag time:

$$Lt = \frac{d_{derm}^2}{6\cdot D_{derm}} \tag{10}$$

Where:-

Lt = lag time [h]
d_{derm} = thickness of *stratum corneum* (0.0025 cm)
D_{derm} = diffusion coefficient of substance in *stratum corneum* [cm^2/h]

$$D_{derm} = Mw^{-0.6}\,\frac{2.4\cdot10^{-6} + 3\cdot10^{-5}\cdot K_{ow}^{0.8}}{0.64 + 0.25\,K_{ow}^{0.8}} \tag{11}$$

Where:-

Mw = molecular mass of substance [g/Mol]
K_{ow} = octanol/water partition coefficient

During the lag time the *stratum corneum* of the skin becomes loaded with the chemical. If it is assumed, that a linear concentration gradient from a concentration $C_{derm} \cdot K_m$ at the *stratum corneum* surface to zero at the lower surface, the amount of chemical in mg/cm^2 (skin), that must be absorbed from the water layer to achieve chemical saturation is given by:

$$UPS = \frac{d_{derm} \cdot K_m \cdot C_{derm}}{2} \qquad (12)$$

Where:-

UPS = uptake before saturation [mg/cm^2]

d_{derm} = thickness of *stratum corneum* [cm]

K_m = partition coefficient *stratum corneum*/water of the substance

C_{derm} = average concentration of substance in skin surface layer [mg/cm^3]

McKone and Howd (1992) derived the following empirical relation for K_m.

$$K_m = 0.64 + 0.25 K_{ow}^{0.8} \qquad (13)$$

The above equations enable the estimation of the uptake of substances from aqueous solutions in direct contact with skin, taking into account:

- the physico-chemical properties of the substance;
- the concentration of the substance in direct contact with the skin;
- the duration of the skin exposure.

If the period of dermal exposure (t) is shorter than the lag time (Lt), then the dermal absorption U_{derm} is given by:

$$U_{derm} = \frac{t \cdot S_{derm}}{Lt \cdot BW} \qquad (14)$$

If the period of dermal exposure is longer than the lag time, then the dermal absorption is

$$U_{derm} = (UPS + (t - Lt) \cdot Kp \cdot C_{derm}) \cdot \frac{S_{derm}}{BW} \tag{15}$$

The maximum skin permeation rate is limited by the aqueous solubility. This should be kept in mind for the evaluation of direct skin contact with pure substances with different water solubility. If two substances have the same permeation coefficient [cm/h], the solubility in water controls the final skin permeability rate.

If a preparation contains a substance at a level exceeding the water solubility, the skin permeation rate should be estimated as if the solution was fully saturated.

3.4 PRODUCT USE SCENARIOS

Typical product use scenarios are discussed below for common consumer products e.g. cosmetic products, household cleaning products, aerosol products, paints and plasticisers. In Section 3.5 more scenarios are illustrated.

3.4.1 Cosmetics

Cosmetics are used widely by both sexes and by all ages. Cosmetic products or personal care products include skin creams, lipsticks, anti-perspirant deodorants, shampoos, toothpastes etc. Cosmetics may be broadly grouped by product type based on (i) contact with mucous membranes (toothpaste, lipstick etc.), (ii) leave-on products (skin creams, anti-perspirant deodorants etc.) and (iii) rinse-off products (shampoo, shower gel etc.).

The consumer exposure estimate to a component in a cosmetic product is dependent on several factors including the concentration of the component in the finished product, the quantity of product used per application, the frequency of product use, the bodyweight, the surface area of application and the overall intake via dermal contact, ingestion or inhalation of the product.

The estimation of exposure to a substance in a cosmetic product is complicated due to the combined use of a number of cosmetics in actual life situations and due also to the fact that the frequency of application depends on the individual and on the individual product. The result of consumer surveys for a range of cosmetic products is given in Table 3. For example, toothpaste is used on average 1-2 times/day while a hair conditioner is used on average 1-2 times/week (see Table 3). The average quantity of a cosmetic product used per application differs also between the product types: about 1.4 g of toothpaste are used on average per application whereas 14 g is the average quantity per application for a hair conditioner. In the absence of specific data for product use, the use levels presented in Table 3 may serve as guidelines for exposure estimates.

Table 3 Examples of Exposure Levels of Some Typical Cosmetic Products (female user) (COLIPA, 1993)

Product Type	Typical Quantity per Application (g)	Frequency (Applications per day)	Exposure Levels (g/day)	
			normal use	extensive use
Mucous Membrane Contact				
toothpaste[1]	1.4	1 - 2	0.24	0.48
mouthwash[2]	10	1 - 5	1	5
lipstick	0.01	2 - 6	0.02	0.06
eye make-up				
powder	0.01	1 - 3	0.01	0.03
mascara	0.025	1	0.025	0.025
eye liner	0.005	1	0.005	0.005
Leave-On Products				
face cream	0.8	1	0.8	0.8
general purpose cream	1 mg/cm^2 skin	1 - 2	1.0	2.0
body lotion	8	1 - 2	8	16
anti-perspirant roll-on	0.5	1	0.5	0.5
hair styling products[4]	5	1 - 2	0.5	1
Rinse-Off Products[3)]				
make-up remover	2.5	1 - 2	2.5	5
shower gel	5	1 - 2	5	10
shampoo[4]	12	2 - 7/week	0.34	1.2
hair conditioner[4]	14	1 - 2/week	0.2	0.4

1 0.24g is assumed to be ingested per application.
2 Only 10% is ingested.
3 Multiply final exposure levels by 0.1 since 10 % rinse-off coefficient is assumed.
4 A partition coefficient of 10% is applied on the assumption that only 10% of product remains on scalp.

Product Use Patterns and Calculations:

When estimating exposure to substances in cosmetic products, the scenario giving rise to the highest exposure levels should be used. The type and quantity of product used is dependent on the sex of the consumer (e.g. shaving creams), age group (e.g. hair dyes), time of year (e.g. sun products for the skin), local habits and practices and fashion trends (e.g. hair colouring). A reference bodyweight should be used in each estimation. The sex of the consumer is important for the location of skin exposure for certain products e.g. shaving creams are used primarily on the face by males while they may be 'misused' by females for shaving their legs. For dermal exposure estimates, it is necessary to consider the surface area of application and the location(s) of exposure since different skin absorption for a substance may be seen depending on the site of application (Lotte *et al*, 1987). The percutaneous absorption of individual formulations of finished products and any potential formulation matrix effects should also be taken into account on a case by case basis. Oral exposure is obviously very important when considering a substance in a toothpaste or mouthwash since certain amounts of these products may be ingested especially by young children. Exposure via inhalation can occur from volatilization of components deposited on skin and hair or on other surfaces. Exposure via inhalation can also occur through the use of aerosol products e.g. hairsprays, deodorant sprays etc. Due to the variety of products used, inhalation exposure estimates are usually made on a case by case basis since, for example, pump sprays are likely to produce significantly lower levels of airborne material than the classical aerosol products. Other factors affecting exposure include the partitioning of the substance between two contact surfaces e.g. hair products bind preferentially to the hair and also to the scalp. Finally, even rinse-off cosmetic products may leave residues on the skin so that "rinse-off coefficients" after product application may be important. A rinse-off coefficient of 10% is a conservative estimate of product remaining on the skin (COLIPA, 1993).

An estimate of human exposure, expressed in mg/(kg·d), to a substance in a cosmetic product may need to take into account any or all of these factors. A comprehensive generalised approach would be as follows:

$$U = \frac{a \cdot b \cdot (c_1 + c_2 + c_3) \cdot d \cdot e}{BW}$$

Where:-

U = estimated total exposure [mg/(kg BW)]

a = Concentration of substance in finished product [%]

b = Quantity of product used per day [mg/day]

c_1 = Proportion absorbed through the skin [%]

c_2 = Proportion ingested [%]

c_3 = Proportion inhaled [%]

d = Partition coefficient (if applicable) (assume 10% max.)

e = Rinse-off coefficient (if applicable) (assume 10% max.)

BW = Bodyweight [kg]

In summary, any exposure to a cosmetic product has to take into account numerous factors and these often will be considered on a case by case basis. Whenever possible, actual data on the product categories used by consumers and the product use scenarios should be obtained to allow a realistic estimate of consumer exposure.

3.4.2 Household Cleaning Products

Household cleaning products are used frequently each day for a variety of purposes - laundry, dishwashing and for general household cleaning tasks. There are several potential routes of exposure and all must be considered when estimating the total exposure for the consumer to a particular substance (Hakkinen *et al*, 1991). For example, consumer use of a laundry product means dermal exposure via direct skin contact with the product or a solution thereof and also from product residues deposited on clothes washed with the detergent. Oral exposure to the product's components is possible if it is used for dishwashing via residues remaining on cooking utensils, dinnerware, glasses etc. Finally, there can be inhalation exposure from product dust generated during use and from possible volatilisation of product components while in the package, from solutions of the product and from product residues left on clothing or other surfaces.

Comprehensive consumer exposure assessments require measured data to assess the extent of possible dermal, oral and inhalation exposure to products and their components (Hakkinen, 1993). Realistic exposure assessments can also be developed using appropriate data from analogous product uses and justifiable values for key exposure elements. Obviously, data are needed on how household cleaning products are used by the consumer i.e. concentrations of product used for a particular task, how long a task takes, how often a specific task is performed and if there are uses different to those recommended by the manufacturer. Other relevant data include the amount of product deposited on fabric or utensils, the skin permeability constants of substances in products, the particle size for granular products etc. Studies on local habits and practices and "in home" observation studies provide useful data on real life situations. For example, a US study on how a granular detergent product was used by consumers showed that some consumers poured the product into a measuring cup and then into the washing machine. Others dipped the cup into the detergent while others poured the product directly into the machine from the container. By simulating these actions in a laboratory, the amount of detergent dust generated by pouring can be calculated and the duration of real consumer contact with the product can be assessed thus allowing an estimate of the amount of detergent dust a consumer might inhale (Hakkinen, 1993).

Product Use Patterns and Calculations:

The quantity of product used for each task and the frequency of use (jobs/week) for typical laundry and dishcare products are given in Table 4 (AIS, 1993). In the absence of specific data for product use, these use levels may serve as guidelines for calculations of consumer exposure. However, as in the case of cosmetic products, it is important to estimate real exposures on a case by case basis using as much measured data as possible. Finally, it is necessary to consider whether the separate values used in an exposure calculation are correlated (proportionally versus inversely) with each other and whether the combinations of tasks and task values used in a "worst case" scenario truly represent what a maximally exposed consumer is likely to do with a specific product. For example, it would be inappropriate to use the highest recorded task duration value, the highest recorded daily task frequency and the highest recorded product concentration for a cleaning product if the task duration is known to decrease as the daily task frequency increases and/or the concentration of product used for the task increases. Not conducting such a check for correlative interactions can result in an unduly conservative and unrealistic consumer exposure assessment.

Table 4 Estimation of Consumer Use of Typical Laundry and Cleaning Products in Europe (AIS, 1993)

		Northern Europe[1]		**Southern Europe**[1]	
		Quantity/Wash [g]	Frequency[2] Jobs/week	Quantity/Wash [g]	Frequency[2] Jobs/week
Regular Heavy Duty Detergents	Powder	55 - 185	3.5 - 5.2	165 - 290	2.7 - 4.8
	Liquid	100 - 215	3.7 - 4.8	105 - 230	1.8 - 4.9
Concentrated Heavy Duty Detergents	Powder	45 - 120	3.7 - 5.2	110 - 200	3.6 - 4.8
	Liquid	60 - 115	3.5 - 4.8	120 - 135	3.6 - 3.8
Hand Dish Washing Liquids	Regular	6.7 - 8.8	10.0 - 14.6	13.0 - 28.0	11.1 - 15.0
Machine Dish Washing Detergents	Regular Powder	30 - 40	3.4 - 4.8	45 - 50	4.1 - 5.1
	Conc. Powder	20 - 30	3.0 - 5.2	30 - 35	4.2 - 5.1
	Liquid	40 - 50	3.6 - 5.2	60 - 75	4.1 - 5.1
Fabric Conditioners	Regular	50 - 110	3.3 - 5.2	90 - 120	4.1 - 4.8
	Concentrate	35 - 70	3.8 - 5.5	50 - 90	4.0 - 4.5

[1] Includes estimation of some countries within Europe. Countries considered are not always the same for each product category. (Data are not available for all countries and each product category).

[2] Usually, consumers only use some of these products.

Some additional data which are important when calculating exposure levels to typical household cleaning products include the dilution of product used for each task. For this calculation, it is generally assumed that washing machines have a water volume of 20 litres in Europe. However, more modern cost-saving machines often have wash volumes of 12 - 15 litres. For US hand-dishwashing, a 0.2% solution is typically used i.e. 15ml of product diluted in about 7.5 litres of water (Hakkinen, 1993). If the handwashing is performed without gloves, then the skin area exposed is 720 cm^2 (for an adult female) and if the hands and forearms are immersed in the wash solution, then the area of exposed skin is 1680 cm^2 (Hakkinen, 1993). For calculations of deposits on dishes, one must consider whether consumers rinse dishes after washing in clear water or not and thus reduce actual oral exposure levels. The volatility of a substance deposited on dishes is also important since the material may have already evaporated before the dish is re-used.

The following examples are typical of calculations used for performing exposure assessments for a typical laundry or dishwashing product use scenario:

(i) direct skin contact with product or solution of product:

$$U_{derm} = \frac{K_p \cdot C_{derm} \cdot S_{derm} \cdot t}{BW} \tag{16}$$

Where:-

U_{derm} = estimated uptake via skin [mg/kg]
C_{derm} = concentration of substance in solution
= $C_{solution}$
K_p = skin permeability coefficient of substance
S_{derm} = surface area of exposed skin [cm^2]
t = duration of exposure [h]
BW = bodyweight [kg]

(ii) exposure from residue on clothing fabric:

$$U_{derm} = \frac{K_p \cdot C_{derm} \cdot S_{derm} \cdot t}{BW} \tag{17}$$

Where:-

U_{derm} = estimated dermal uptake from residue on clothing [mg/kg]
S_{derm} = surface area of exposed skin [cm^2]
t = duration of exposure [h]
BW = bodyweight [kg]
K_p = skin permeability coefficient of substance

C_{derm} is calculated from the mass of the substance estimated to be transferred to the skin divided by the volume of the skin surface water layer.

(iii) oral exposure from deposits on dishes, cooking utensils and glassware:

$$I_{oral} = \frac{A \cdot FA_{oral} \cdot S_{dish}}{BW} \qquad (18)$$

Where:-

I_{oral} = amount of substance ingested [mg/kg]
A = amount of substance deposited per unit area on dishes [mg/cm^2]
FA_{oral} = fraction of deposited substance ingested
S_{dish} = area of dishes in contact with substance [cm^2]
BW = bodyweight [kg]

3.4.3 Exposure to Aerosol Products

Aerosol products are designed for easy local application of, for example:

- hair lacquers;
- deodorizing agents;
- household cleaners;
- oven cleaners;
- aerosol paints;
- antistatic sprays;
- starch and sizing sprays.

They contain a preparation of active ingredient(s) mixed with a propellant, e.g. propane/butane or dimethylether and possibly other ingredients such as solvents. By using aerosol products, consumers are exposed to the contents of the spray-can. Propellants are completely released into the air. Active ingredients will stick generally on the site of application. However, one should take into account the extent of overspray, that is the fraction released into the air in the room of application. Dependent on the particle size, this fraction will settle on the furniture and the floor or may be inhaled by the consumer.

The amount of aerosol product released is dependent on its application. The propellant of a spray-can of paint will have been completely released after application. The solvent in the paint is only partly released to air due to overspray and the remaining part will be released during the drying time. The amount released may be derived from the volume or from the weight of the spray-can.

The resulting exposure concentration is dependent on the release rate, the physico-chemical properties of the constituents and the ventilation pattern and ventilation rate of the house. The release rate to air is dependent on the type of consumer product application. After the release, the final concentration during the day is controlled by the ventilation of the private house. The ventilation affects mainly the average consumer exposure and therefore a special section (3.4.4) will describe the approach in more detail. Only the simultaneous mathematical simulation of release and ventilation will provide the required information for peak and average lifetime exposure.

Other types of spray-cans are only used for regular applications of small amounts of product during a period of a few seconds. The duration for application of hairspray is on average assumed to be 10 seconds while releasing 6 to 15 g of product (Hartop *et al*, 1991). For a spray spot remover, the amount is about 2 to 6 g a time for 100 cm^2 fabric spot and for a starch and sizing spray, 6 to 8 g for a 2,000 cm^2 area (FLUSH, 1992).

The assessment of exposure to the propellant is of special interest. The propellant is completely released to the air and therefore it is the component producing the highest consumer exposure via inhalation. The resulting concentration is dependent on the volume of the room. A good example is the use of hair spray for 10 seconds in a room of 21 m^3 (Hartop *et al,* 1991). The spray-can of hair lacquer contained 50 % dimethylether. The results of this application are presented in Table 5 below.

The resulting concentration in the breathing zone in a room of 21 m^3 is more or less comparable to the nominal concentration, calculated from the released amount divided by the volume of the room (converted into ppm volume/volume) and assuming even dispersion of the aerosol.

Table 5 Concentration of Dimethylether in the Breathing Zone after Application of a Hair Lacquer, expressed as 10 Minute Time Weighted Average [TWA] (Hartop *et al*, 1991)

	ppm Dimethylether		
	Mean value	Maximum value	Minimum value
User TWA 10	114	143	82
Child TWA 10	89	97	86
User peak	1310	1577	1043
Child peak	717	762	672
Nominal	86	94	79

The peak concentrations are about a factor of 15 higher than the nominal concentrations, if aerosol is released into a room of a volume of 21 m^3. The aerosol propellant gas is initially diluted with air with a factor of 320 in the breathing zone of the hair spray user.

Further exposure is dependent on the extent of ventilation of the room. The ventilation of a house will be discussed in Section 3.4.4.

3.4.4 Paints or Paint Removers

Application of paint or of paint remover results in release of solvents into the air.

The release rate depends on:

- the rate of application in m^2/h;
- the mass of paint or paint remover per surface area g/m^2;
- the rate of evaporation, related to the drying time of the paint or paint remover.

Bjerre (1989) described a six parameter mathematical exposure model for painters. The model is valid for solvents that evaporate from the wet paint layer at a constant rate. If a mixture of solvents is used in the paint, the release rate of the individual components is assumed to be equal.

$$\frac{dS}{dt} = R \cdot A_{ev} \qquad (19)$$

$$\frac{dA_{ev}}{dt} = a - \frac{A_{ev}}{t_d} \tag{20}$$

Where:-

dS/dt = Release of solvent [g/h]

R = evaporation rate [g/(m^2·h)]

a = area painted per unit time [m^2/h]

a = 0 if $t > t_a$.

t_a = time required to paint total area = A_p/a

A_p = surface area to be painted [m^2]

A_{ev} = evaporating surface of wet paint [m^2]

t = time unit [h]

M = mass of solvent applied per unit area [g/m^2]

t_d = drying time, i.e. time between one element being painted and being completely dry = M/R [h]

Examples of M, the mass of solvent per unit area, are:

- white spirit in paints: 47.6-91.6 g/m^2;
- methylene chloride in paint remover: 103-229 g/m^2.

Examples of R, the evaporation rate, are:

- white spirits in paints: 267-953 mg/(m^2·min);
- methylene chloride: 93-119 g/(m^2·min).

The final concentration is dependent on the release of solvent per time unit and on the extent of ventilation of the room and the remaining part of the house.

Releases of substances are not limited to the drying time but may continue at low levels for longer periods after application. This background release can be estimated as described above taking into account differences in evaporation rate R.

House ventilation

The ventilation rate of the house controls the average concentration of and consumer exposure to released airborne substances. Information on ventilation of houses is discussed by Andelman (1985) and McKone (1989). The basic starting points are the assumptions or real measurements on:

- ventilation rates between compartments within the house, especially the compartment of a specific consumer application;
- exchange rate of the air of the individual compartments of the house with the outside air.

The change of concentration with time in the room of consumer product application and the remaining part of the house may be described by:

$$\frac{dC_1}{dt} = \frac{[S(t) + Q_{21} \cdot C_2 - Q_{12} \cdot C_1 - Q_{10} \cdot C_1]}{V_1} \qquad (21)$$

$$\frac{dC_2}{dt} = \frac{[Q_{12} \cdot C_1 - Q_{21} \cdot C_2 - Q_{20} \cdot C_2]}{V_2} \qquad (22)$$

Where:-

S(t) = Release rate as function of time

V_1+V_2 = Volume of house [m^3]

V_1 = Volume of room of consumer product application [m^3]

V_2 = Remaining volume of house [m^3]

C_1 = Average concentration in the room of consumer product application [mg/m^3]

C_2 = Average concentration in the remaining volume of the house [mg/m^3]

Q_{21} = Q_{12} = Exchange rate between V_1 and V_2 [m^3/h] (SCIES, 1991)

Q_{10} = Exchange rate between V_1 and the outside air [m^3/h]. The concentration in the outside air is assumed to be zero
($Q_{10} = ACH \cdot V_1$)

Q_{20} = Exchange rate between V_2 and the outside air [m^3/h]. The concentration in the outside air is assumed to be zero
($Q_{20} = ACH \cdot V_2$)

ACH = Air Change per Hour [1/h]

In this example, only 2 compartments in a house are recognised. It is possible to design a ventilation scenario adapted to a specific situation. The presentation of simple differential equations is preferred, with which the concentration as function of time can be simulated by means of numerical integration. This provides a flexible approach to simulate complicated release rates in house compartments and ventilation patterns between house compartments.

3.4.5 Plasticisers

Plasticisers are used in a wide variety of products/articles available to consumers. For example, di-2-ethylhexyl phthalate (DEHP) is a commercially important chemical whose use is primarily as a plasticiser in polyvinylchloride (PVC). It may be present in concentrations up to 40%. As it is not chemically bound to the PVC it can diffuse out of the plastic and give rise to human exposure.

DEHP is found in a wide variety of products which include imitation leather, wall paper, floor covering, children's toys, footwear and rainwear as well in plastic bags and tubes for transfusion of blood and blood products. Although never widely used in food contact materials, its use has declined in this respect during recent years (UK-MAFF, 1987).

Products which could result in skin contact would be footwear, rainwear, PVC gloves etc. Products which could give rise to inhalation would be wallpaper, floor coverings etc. Plasticised PVC used in medical applications may give rise to intravenous and/or dermal exposure; these applications are not addressed in this report but an assessment is made by ECPI (1994).

Products which could result in skin contact would be footwear, rainwear, PVC gloves etc. Uptake through the skin can be estimated by using Equation 16. Products which could give rise to inhalation would be wallpaper, floor coverings etc. The amount of substance inhaled can be calculated by using Equation 2. Examples are given below.

3.5 CASE STUDIES ON CONSUMER EXPOSURE

3.5.1 Selection of Substances

The substances providing different properties have been chosen on the basis of:

- availability of a suitable database and
- illustrative for consumer exposure scenarios.

Two substances have been selected from ECETOC (1993a); dichloromethane and dimethylether have been added to the list. The substances are:

- linear alkylbenzene sulphonate (LAS);
- dimethylether;
- dichloromethane;
- diethylhexylphthalate (DEHP).

3.5.2 CONSUMER EXPOSURE TO LAS

The substance, LAS (linear alkylbenzene sulphonate), is an important synthetic surfactant used in many common household products e.g. detergents and other cleaning products. Direct exposure of the consumer to LAS occurs through the regular use of these products. Depending on the type of product and how it is used, exposure may occur via one or more routes i.e. dermal, inhalation and/or oral.

For estimation of consumer exposure to LAS, it is reasonable to consider first those scenarios which present substantial exposure during product use. Such scenarios for LAS exposure are represented here by usage of a regular granular laundry detergent (hand-laundering), usage of a hand-dishwashing liquid and additional exposure through the use of clothing or dishes washed with such products.

Basic Data for all Scenarios

- Adult average bodyweight is 66 kg (McKone and Daniels, 1991)
- Skin permeability coefficient (K_p) for LAS is 6×10^{-6} cm/h (Howes, 1975).

Dermal Absorption via Hand Laundering

The following additional data and assumptions are used:

- typical level of LAS in a granular laundry detergent is 10 %;
- product use concentration for handwash is 0.2 % (ca. 15 g product/7.5 l wash solution);
- concentration of LAS in wash solution (0.2 g product/100 ml · 10%) = 0.2 mg LAS/cm^3;
- duration of washing event is 15 minutes i.e. 0.25 h;
- exposed skin surface area (hands and forearms) is 1,980 cm^2 (Table 2).

The estimated dermal absorption or uptake (mg/kg) from direct skin contact with product or solution of product during hand laundering is calculated according to Eq. 8 as follows:

$$\begin{aligned} U_{derm} &= 6 \cdot 10^{-6}\ [\text{cm/h}] \cdot 0.2\ [\text{mg/cm}^3] \cdot 1980\ [\text{cm}^2] \cdot 0.25\ [\text{h}]\ /\ 66\ [\text{kg}] \\ &= 9 \cdot 10^{-6}\ [\text{mg/(kg}\cdot\text{event)}]. \end{aligned}$$

Assuming one event daily, then the absorption of LAS by a consumer via hand-laundering is approximately:

$$9 \cdot 10^{-6}\ [\text{mg/(kg}\cdot\text{d)}].$$

Dermal Absorption via Hand Dishwashing

The following additional data and assumptions are used:

- typical level of LAS in a hand dishwashing liquid is 20 %;
- product use concentration for dishwash is 0.3 % (15 ml product in 5 l water);
- concentration of LAS in wash solution (0.3 g product/100 ml · 20 %) = 0.6 mg LAS/cm^3;
- duration of dishwashing event is 15 minutes i.e. 0.25 h;
- exposed skin surface area (hands and lower arms) is 1980 cm^2 (Table 2).

The estimated dermal absorption or uptake [mg/kg] from direct skin contact with product or solution of product during hand dishwash is calculated according to Eq. 8 as follows:

$$\begin{aligned} U_{derm} &= 6 \cdot 10^{-6}\ [\text{cm/h}] \cdot 0.6\ [\text{mg/cm}^3] \cdot 1980\ [\text{cm}^2] \cdot 0.25\ [\text{h}]\ /\ 66\ [\text{kg}] \\ &= 27 \cdot 10^{-6}\ [\text{mg/(kg}\cdot\text{event)}]. \end{aligned}$$

Assuming 15 events per week (Table 4), then the absorption of LAS by a consumer via hand-dishwashing is approximately:

$$5.8 \cdot 10^{-5}\ [\text{mg/(kg}\cdot\text{d)}].$$

Dermal Absorption via Exposure from Residue on Clothing

The following additional data and assumptions are used:

- typical level of LAS in a granular laundry detergent is 10%;
- product use concentration for handwash is 0.2 % (ca. 15 g product/7.5 l wash solution);
- amount of LAS in wash solution = 1.5 g
- assume that the amount of LAS transferred to clothing is 10 % = 150 mg
- assume that the amount of LAS transferred to skin is 10 % of that on clothing = 15 mg
- exposed skin surface area (total body) is 19,400 cm^2 (Table 2);
- the thickness of the skin surface water layer containing the LAS is 0.006 cm;
- using the above data, the approximate total volume of skin surface water = 120 ml.

The estimated dermal uptake [mg/kg] from exposure to residue on clothing washed in a typical LAS-containing detergent is calculated according to Equation 16 as follows:

$$\begin{aligned} U_{derm} &= 6 \cdot 10^{-6} \, [cm/h] \cdot 15/120 \, [mg/cm^3] \cdot 19400 \, [cm^2] \cdot 24 \, [h] \, / \, 66 \, [kg] \\ &= 5.3 \times 10^{-3} \, [mg/(kg \cdot day)]. \end{aligned}$$

The above calculation is conservative since it assumes that (i) the total body is covered throughout the day with clothing; (ii) a skin surface water layer is universally present although only a small area of the body would continuously produce sweat over 24 hours; and (iii) a very large proportion (i.e. 10 %) of the LAS is transferred to clothing in the wash. More realistic estimates for dermal uptake of LAS would be an order of magnitude lower [10^{-4} mg/(kg·d)].

Oral Intake via Exposure to Deposits on Dishes

The following additional data and assumptions are used:

- typical level of LAS in a hand dishwashing liquid is 20 %;
- product use concentration for dishwash is 0.3 % (15 ml product in 5 l water);
- concentration of LAS in wash solution (0.3 g product/100 ml · 20 %) = 0.6 mg LAS/cm^3;
- assuming a volume of 0.25 ml wash solution remains on plate face and that the area of one side of a plate is 450 cm^2.

The estimated oral intake [mg/kg] from ingestion of detergent deposits is calculated according to Equation 18 as follows:

$$
\begin{aligned}
I_{oral} &= 0.33 \cdot 10^{-3}\ [\mathrm{mg/cm^2}] \cdot 1 \cdot 5400\ [\mathrm{cm^2}] / 66\ [\mathrm{kg}] \\
&= 2.7 \cdot 10^{-2}\ [\mathrm{mg} / (\mathrm{kg} \cdot \mathrm{d})].
\end{aligned}
$$

Since the value for S_{dish}, 5400 cm^2, represents the total area of dishes, glasses, other cooking utensils etc. to which a consumer would be exposed of per day (assumed equivalent to 12 plates), then the intake of LAS by a consumer via ingestion of deposits on dishes, plates etc. is approximately:

$$2.7 \cdot 10^{-2}\ [\mathrm{mg/(kg \cdot d)}].$$

Note that in this scenario, no account is taken of rinsing the dishes with clean water, of evaporation of substances from wet dishes or of wiping the dishes dry with a tea towel. The amount of volatilization of a substance from a washed dish will depend primarily on the physical/chemical properties of that substance. All of these typical events would significantly reduce the amount of residue which would be actually present on the dishes. Further, the calculation in this scenario assumes that all the residue remaining on the dish is reabsorbed during re-use of the dish and, most importantly, that it is also completely bioavailable once ingested by the consumer.

Total Exposure to LAS (combined dermal and oral)

Using the scenarios described here and conservative estimates for several data points (worst case scenarios), the total amount of LAS to which a consumer may be exposed is the sum of the following figures:

$9.0 \cdot 10^{-6}$ mg/kg (uptake due to hand laundering),
$2.7 \cdot 10^{-5}$ mg/kg (uptake due to hand dish washing),
$5.3 \cdot 10^{-3}$ mg/kg (uptake due to residue on clothing),
$2.7 \cdot 10^{-2}$ mg/kg (intake due to deposits on dishes),

giving a total figure of approximately $3 \cdot 10^{-2}$ mg LAS/kg bodyweight per day.

3.5.3 CONSUMER EXPOSURE TO DIMETHYLETHER AND DICHLOROMETHANE

The SCIES-model (1991) is based on simple equations for the estimation of the peak exposure and annual average exposure of consumers to household chemicals, i.e.:

- equations for the estimation of release rates, derived from a specific consumer scenario (amount of consumer product used per unit of time);
- the weight fraction, the vapour pressure and the molecular weight of the compound of interest, released to the indoor air;
- equations for the ventilation rate of the room of release with air from inside and outside the house, based on actual measurements in American homes with a tracer chemical;
- assumptions on activity pattern and residence inside and outside during the day. A distinction is made between the exposure of the active user and the one passively exposed.

The peak exposure in the SCIES-model is equal to the nominal concentration calculated by the amount released per unit of time, divided by the volume of the room and taking into consideration the ventilation rate. This peak exposure is not representative of the real peak exposure, when the compound is released within a short distance of the breathing zone of the consumer and the release time is relatively short. So the actual peak exposure may be higher than predicted by the SCIES-model.

In contrast, the release time of solvents in case of painting activities is exaggerated. For oil based paints it is estimated that the solvent will be released within 18 minutes, assuming a vapour pressure of 800 Pa. This is equivalent to a drying time of 18 minutes. The exaggerated release rate may compensate in some cases for the low estimations of the peak exposure.

Case Study Dimethylether

The SCIES-model was used to estimate consumer exposure to dimethylether by assuming the use of hair lacquer in a spray-can containing the substance as the aerosol propellant. The option chosen was "Aerosol Paints / Clear Coatings", because the option "Input your own scenario" used a time step of one hour instead of 5 minutes to estimate peak and average exposure. The output of the SCIES model is presented in Table 6.

The following assumptions are made by SCIES:

Table 6 Print file of SCIES: Aerosol hair lacquer with dimethyl ether as propellant.

```
Annual Frequency of Use  :     365     Events/Year
Mass of Product          :       7.000 grams
Duration of Use          :       0.003 Hours
Zone 1 Volume            :      21.000 cubic meters
Whole House Volume       :     292.000 cubic meters
House Air Exchange Rate  :       0.200 room air exchanges/h
User Inhalation Rate     :       1.300 cubic meter/h (during use)
Non-User Inhalation Rate :       1.100 cubic meter/h (& User after use)
Molecular Weight         :      46.000 g/mole
Vapour Pressure          :   3.258E+03 torr
Weight Fraction          :       0.500
Starting Time            :        9:00 AM

     OUTPUT SUMMARY
Evaporation Time                :   0.002 Hours
Release Time                    :   0.003 Hours (Duration of Exposure)
Duration Following Each Use     :  23.997 Hours
Interval Between Uses           :  24.000 Hours

User Potential Dose Rate From Inhalation      :    51859.189 mg/yr
Non-User Potential Dose Rate From Inhalation  :    17111.217 mg/yr

 --------------------------------------------------------------------
                                                Average          Peak
                                                [mg/m3]        [mg/m3]
                                                -------        -------
Concentration in zone of release
     During period of use                       157.292        157.292
     During period after use                      6.259        139.936

Concentration in Zone 2
     During period of use                         0.000          0.000
     During period after use                      2.149          7.580

Concentration to which User and
Non-User are exposed
     Person Using Product (user)                  5.378        157.292
     Person Not Using Product (non-user)          1.776          7.580
```

- immediate dilution in the room of use because of the high vapour pressure of dimethyl ether;
- the spray-can being used in a room with a volume V_1 of 21 m^3;
- the total volume VT of the house being 292 m^3;
- the volume of the house minus the volume of the room of use being $V_2 = VT - V_1$ [m^3];
- the air change per hour with outside air being the same for all rooms (ACH = 0.2/h);
- the ventilation rate from the room of use inside the house being $0.4326 \cdot (V_1 + V_2) \cdot ACH$ [m^3/h];
- the ventilation rate to outside air of the room of use being $V_1 \cdot ACH$;
- the ventilation rate to outside air of the remaining part of the house being $V_2 \cdot ACH$;
- the spray-can with hair lacquer being used every day;
- each time the spray-can is used, an amount of 3.5 g is released into the air;

- no attention is paid to maximum concentrations in the breathing zone which may be 10 times higher than the concentration originating from instantaneous mixing with the air of the room of use.

The SCIES model estimates:

- an average concentration of 6.3 mg/m^3 in the room of use averaged over 24 hours;
- an average concentration of 2.1 mg/m^3 in the remaining part of the house;
- a peak exposure of 157 mg/m^3 in the room of use;
- a peak exposure of 7.6 mg/m^3 in the remaining part of the house.

An actual peak concentration in the breathing zone of about 1,310 ppm (2,510 mg/m^3) was reported by Hartop *et al* (1991).

Case Study Dichloromethane

An example is presented for dichloromethane as a constituent of paint remover. In this case the scenario of oil based paint was used. The data are presented in Table 7 below.

3.5.4 Consumer Exposure to DEHP

Exposure assessments have been conducted into the use of DEHP in food contact materials (UK-MAFF, 1987) and its use in children's toys, pacifiers and teethers (Turnbull and Rodricks, 1989). In both cases estimated exposures were extremely low. In the case of food contact it was estimated that the maximum daily intake of DEHP would be no more than 0.02 mg. For a 66 kg person this would be $3 \cdot 10^{-4}$ [mg/(kg·day)]. In the case of children's toys etc. exposures were estimated to range from $2.4 \cdot 10^{-4}$ - $9.3 \cdot 10^{-4}$ [mg/(kg·day)].

In March 1989 the US Chemical Manufacturers Association Phthalate Esters Panel produced a publication which described a step by step approach of estimating consumer exposure to DEHP from PVC consumer products (CMA, 1989). The guide confines itself to assessing exposure from skin contact or inhalation. Using human *in vitro* absorption data and *in vivo* data from rats, a human skin absorption rate of DEHP was estimated to be $2.5 \cdot 10^{-5}$ [$mg/(cm^2 \cdot h)$]. A table in the guide gives rates for products with varying DEHP contents.

The following paragraphs describe scenarios where dermal absorption and exposure via inhalation to DEHP could occur.

Table 7 **Print file of SCIES: Paint remover, containing 30% (w/w) dichloromethane**

```
   Annual Frequency of Use :      6   Events/Year
   Mass of Product         :    500.0 grams
   Duration of Use         :      0.1 Hours
   Zone 1 Volume           :     40.0 cubic meters
   Whole House Volume      :    292.0 cubic meters
   House Air Exchange Rate :      0.2 room air exchanges/h
   User Inhalation Rate    :      1.3 cubic meter/h (during use)
   Non-User Inhalation Rate:      1.1 cubic meter/h (& User after use)
   Molecular Weight        :     84.0 g/mole
   Vapour Pressure         :   4.753E+02 torr
   Weight Fraction         :      0.3
   Starting Time           :       1:00 PM

 OUTPUT SUMMARY

   Evaporation Time               :  0.006   Hours
   Release Time                   :  0.1     Hours (Duration of Exposure)
   Duration Following Each Use    : 1460      Hours
   Interval Between Uses          : 1460      Hours

   User Potential Dose Rate From Inhalation      :    37600 mg/yr
   Non-User Potential Dose Rate From Inhalation  :    12400 mg/yr


                                                      Average          Peak
                                                      [mg/m3]         [mg/m3]
                                                      -------         -------
   Concentration in zone of release
      During period of use                               3220            3420
      During period after use                               3.77         3190

   Concentration in Zone 2
      During period of use                                 12.5            24.9
      During period after use                               1.38          264

   Concentration to which User and
   Non-User are exposed
      Person Using Product (user)                           3.87         3420
      Person Not Using Product (non-user)                   1.28          264
```

Example of Skin Absorption

The following assumptions are made: a person wears PVC gloves containing 30% DEHP for 2 hours per day.

Uptake through the skin can be estimated using Equation 17:

with $J = 2.5 \cdot 10^{-5}$ [mg/(cm²·h)]

$S_{derm} = 840$ cm² (Table 2)

This results in:

$$U_{derm} = (2.5 \cdot 10^{-5} \cdot 840 \cdot 2) / 66 = 6.4 \cdot 10^{-4} \text{ [mg/(kg BW·d)]}$$

Example of Inhalation Exposure

Consider a room with floor coverings and wallpaper used as an office for 8 h/d. The floor coverings and wallpaper contain DEHP. The air concentration will depend on the size of the room and the surface area of floor and wallpaper. This can be estimated from figures given in the CMA guide. The following assumptions are made:

- Average concentration of DEHP in the office atmosphere is $1.5 \cdot 10^{-3}$ mg/m^3;
- Ventilation rate of occupant: 1.5 m^3/h;
- Time spent in office: 8 hours per day.

Using Equation 2, the amount of DEHP inhaled is as follows:

$$I_{inh} = (1.5 \cdot 10^{-3} \cdot 1.5 \cdot 8) / 66 = 2.7 \cdot 10^{-4} \text{ [mg/(kg BW · d]}$$

Using the default value of 0.75 for bioavailability, the uptake by inhalation can be calculated from Equation 3 as follows:

$$U_{inh} = (18 \cdot 10^{-3} \cdot 0.75) / 66 = 2 \cdot 10^{-4} \text{ [mg/(kg BW·d)]}$$

SECTION 4. INDIRECT EXPOSURE

4.1 INTRODUCTION

Indirect exposure is defined as exposure of the public via the environment, i.e. air, water, soil and food. It should be pointed out that in this report the exposure assessment is targeted at the protection of the average individual of an EC member state - i.e. air, water and soil concentrations are assessed regionally and average diets are assessed for the region under consideration. This assumption is consistent with the observation that (1) people move around locally and in the region; and (2) food habits and sourcing may vary throughout the year. The average daily dose for each of these routes is the product of the average exposure concentrations in each contact medium (air, water, soil, food) with the average intake or uptake factor.

The total daily intake for human beings is calculated by summing the individual parts of the exposure:

$$DI = \frac{1}{BW} \cdot \sum_{i(\text{air,water,soil,food})} C_i \cdot I_i \qquad (23)$$

Where:-

DI = total daily intake of a substance [mg/(kg BW·day)]
I_i = daily intake of medium i [kg wet weight/day, l/day or m^3/day]
C_i = actual predicted concentration in medium i [mg/kg wet weight, mg/l or mg/m^3]
BW = bodyweight [kg]

The resulting estimated total intake by the average individual is then usually compared with intake criteria, such as ADI or TDI (acceptable and tolerable daily intake, respectively).

It should be noted that the direct intake of soil by man was not included in this report. However, soil does play a significant role in the intake of substances through meat, milk and vegetation as described below.

Before engaging in a discussion on how to predict or assess the concentration in a certain food type, it is necessary to evaluate the food basket of the average individual. The sections on food consumption by food groups and age groups will therefore determine for which food types or intake media an exposure assessment is needed. Once this could be established, relevant transfer functions need to be developed which relate chemical concentrations in air, water and soil to food.

4.2 ESTIMATION OF FOOD CONSUMPTION BY FOOD GROUPS

The uptake of a substance through the food chain depends on the type and quantity of food consumed, on the concentration of the chemical and its bioavailability in the food. The concentration of the chemical can be measured or calculated through modelling. The type and quantity of food consumed, i.e. the food basket, must be obtained through statistical surveys of the general population. This information by age groups for European countries is not yet available.

An estimate of the average consumption can be made from published statistical data (Euromonitor, 1992). It should be pointed out that more detailed diet studies have been performed within several EC member countries. In addition, the values used in this report represent food consumption of the average individual. Deviations from average food baskets (e.g. vegetarian diet) should be evaluated on a case-by-case basis.

The main food groups have been selected to obtain results comparable to data reported by McKone and Daniels (1991) for the USA.

The grouping takes the following into account:

- the source of food: vegetable or animal origin;
- for vegetables: the part consumed, e.g. root, leaves or fruit;
- for animal products: 1) originated from land or water;
  2) meat or dairy product.

The Dutch DRANC model for risk assessment of new chemicals (Vermeire *et al*, 1992) also uses food basket information but is more simplified and therefore differs from McKone and Daniels and from the approach described in this report. The food groups are as follows:

This report	McKone and Daniels (1991)	Vermeire *et al* (1992)
Drinking water	Drinking water	Drinking water
Fruit and vegetables	Fruit and vegetables	Crops
Potatoes		
Cereals	Grains	
Milk and yoghurt	Milk	Milk
Butter and cheese		
Meat (pork, beef, poultry)	Meat	Beef
Fish and shellfish	Fish	Fish

Consumption per capita on a yearly basis by food group is shown in Table 8, Part 1.

The food groups used by McKone and Daniels (1991) and by Vermeire *et al* (1992) can only be considered as a very approximate description of typical European foods and more detail is required to reflect actual food consumption patterns.

As an example, both authors list "crops", either as such or as a combination of fruits and vegetables. However, the uptake of a chemical by man depends whether the part in the soil (root) or the part above the soil (leaves, fruit) is consumed. The presence of a substance e.g. in the root will mainly come through uptake from soil and pore water and not through atmospheric deposition. On the other hand, above ground vegetation will be contaminated both through soil uptake and atmospheric deposition. A differentiation should be made in order to achieve a sufficiently accurate estimate, reflecting the typical food consumption pattern. For this reason, potatoes have been considered separately as they are a very important food source in Europe, but not recognised by the two authors.

Milk consumption has been considered in all cases. However, milk is also used to produce yoghurt, butter and cheese. The levels in yoghurt would be approximately the same as in milk, but in butter and cheese a higher concentration of fat soluble substances can be expected. This may, for certain substances, lead to underestimation of exposure, if these foods are not included.

The type of meat is not specified by McKone and Daniels although it is believed to be beef. The DRANC model only considers beef and veal.

In reality pork is the most important meat in all European countries. Both model equations (Travis and Arms, 1988) assume 25 % fat content which coincides with the average fat content of pork. Also poultry and mutton/lamb are important in certain countries. Although data for meat are grouped, split data are available (Euromonitor, 1992).

Feed sources may differ significantly according to species and region. In order to establish the food chain, it is therefore important to consider the origin of the feed. Many crops, including imported products, are used for animal feed production, rather than for food consumption.

Fish is a relatively minor food source, except for Denmark, Portugal and Spain. Most fish will be from sea catches, rather than from inland waters. This means that an exposure estimate should preferably be based on contaminant concentrations in seas and oceans, rather than in lakes and rivers. In this report, however, concentrations in freshwater fish are estimated.

The data show clearly that the typical food consumption is highly variable from country to country and differences can be two- to three-fold, especially among vegetable foods (fruit, vegetables, cereals, potatoes). Use of the EC average figure gives a reasonable overall value and the evaluation of indirect exposure through food in the case studies of this report is therefore based on average ingestion figures.

4.3 EXTENT AND DURATION OF THE EXPOSURE

4.3.1 Average Daily Food Consumption

The raw data, given as consumption per capita per year (Table 8, Part 1), have been recalculated to show consumption per kg bodyweight per day (Table 8, Part 2). This places the data in a format comparable with McKone and Daniels (1991). Lifetime averages of food intake were calculated from the annual consumption per capita, assuming an average life span of 70 years and an average bodyweight of 58 kg[1] over this lifetime as used by McKone and Daniels (1991) for US food intake. The results shown in Table 8 (Part 2) appear reasonable for Europe and are of the same order of magnitude as for the US.

For use in the exposure calculations, the data were converted to consumable, dry weight quantities by applying correction factors for the edible portion and for water content (Table 8, Part 3). The conversion factors were obtained from the Dutch Food Tables and Recommended Quantities (Voorlichtingsbureau voor de Voeding, 1983).

4.3.2 Estimation of average daily food consumption by age groups

No data for food consumption during childhood have been identified. As it would be useful to consider this more vulnerable group separately, an estimate was made. The factor relating the food consumption of adults to that of children was calculated from the data of McKone and Daniels (1991):

---

[1] Calculated from the following data: child bodyweight of 27 kg for 15 years and adult bodyweight of 66 kg for 55 years.

Table 8 Average food consumption in the EC and its member countries
Part 1 Total average food consumption in kg per capita per year (Euromonitor, 1992)

Intake of	EC	B	DK	F	D	GR	IRL	I	NL	P	SP	UK	Range	
													min.	max.
Meat[1]	94.0	105.0	108.9	109.9	104.9	76.4	87.3	87.5	88.8	68.4	95.0	77.3	68.4	109.9
Beef and veal	22.0	22.3	18.1	30.7	23.7	19.0	19.0	26.8	19.3	13.6	11.5	17.0		
Pork	40.7	49.1	69.1	37.6	63.2	22.2	34.7	30.8	47.6	25.9	47.4	24.8		
Other	21.7	19.3	13.3	25.2	12.6	29.5	26.7	20.9	18.5	21.9	27.4	25.0		
Fish	10.1	10.2	41.8	7.5	7.4	7.2	12.6	10.1	9.8	24.7	20.3	3.5	3.5	41.8
Milk+yoghurt	82.4	67.8	74.2	65.8	65.8	66.9	173.6	69.7	79.3	52.1	102.6	122.3	52.1	173.6
Butter	4.9	8.6	6.9	8.6	8.5	1.0	5.5	2.4	3.9	0.9	0.6	4.2	0.6	8.6
Cheese	14.5	12.6	12.8	22.4	17.4	22.1	5.4	17.6	15.0	5.2	5.5	8.0	5.2	22.4
Fruit+vegetables	205.6	173.8	149.8	194.0	196.4	248.3	148.3	277.5	242.5	165.4	252.6	131.6	131.6	277.5
Cereals	116.5	98.7	93.1	101.8	99.6	145.2	144.7	160.0	74.5	125.4	97.7	119.6	74.5	160.0
Potatoes	83.3	97.6	62.9	73.6	69.6	86.4	140.2	38.0	87.0	111.5	107.0	106.7	38.0	140.2

[1] Total does not reflect the sum of the individual subgroups.

Table 8 **Average food consumption in the EC and its member countries**
Part 2 **Average food consumption in g per kg bodyweight per day**

Intake of	EC	B	DK	F	D	GR	IRL	I	NL	P	SP	UK	Range		US Data McKone (1991)
													min.	max.	
Meat	4.4	5.0	5.1	5.2	5.0	3.6	4.1	4.1	4.2	3.2	4.5	3.7	3.2	5.2	3.1
Beef and veal	1.0	1.1	0.9	1.5	1.1	0.9	0.9	1.3	0.9	0.6	0.5	0.8	0.5	1.5	
Pork	1.9	2.3	3.3	1.8	3.0	1.0	1.6	1.5	2.2	1.2	2.2	1.2	1.0	3.3	
Other	1.0	0.9	0.6	1.2	0.6	1.4	1.3	1.0	0.9	1.0	1.3	1.2	0.6	1.4	
Fish	0.5	0.5	2.0	0.4	0.3	0.3	0.6	0.5	0.5	1.2	1.0	0.2	0.2	2.0	0.3
Milk+yoghurt	3.9	3.2	3.5	3.1	3.1	3.2	8.2	3.3	3.7	2.5	4.8	5.8	2.5	8.2	5.6
Butter	0.2	0.4	0.3	0.4	0.4	0.0	0.3	0.1	0.2	0.0	0.0	0.2	0.0	0.4	no data
Cheese	0.7	0.6	0.6	1.1	0.8	1.0	0.3	0.8	0.7	0.2	0.3	0.4	0.2	1.1	no data
Fruit+vegetables	9.7	8.2	7.1	9.2	9.3	11.7	7.0	13.1	11.5	7.8	11.9	6.2	6.2	13.1	5.3
Cereals	5.5	4.7	4.4	4.8	4.7	6.9	6.8	7.6	3.5	5.9	4.6	5.6	3.5	7.6	4.0
Potatoes	3.9	4.6	3.0	3.5	3.3	4.1	6.6	1.8	4.1	5.3	5.1	5.0	1.8	6.6	no data

Note: averages over lifetime (70 years) assuming average bodyweight of 58 kg

Table 8 **Average food consumption in the EC and its member countries**
Part 3 **Average food consumption in g per kg bodyweight per day on consumable dry weight basis**

Intake of	EC	B	DK	F	D	GR	IRL	I	NL	P	SP	UK	Range		EF[1]	DF[2]
													min.	max.		
Meat	1.60	1.79	1.85	1.87	1.78	1.30	1.48	1.49	1.51	1.16	1.62	1.31	1.16	1.87	1	0.36
Beef and veal	0.35	0.36	0.29	0.49	0.38	0.31	0.31	0.43	0.31	0.22	0.18	0.27	0.18	0.49	1	0.34
Pork	0.79	0.95	1.34	0.73	1.22	0.43	0.67	0.60	0.92	0.50	0.92	0.48	0.43	1.34	1	0.41
Other	0.32	0.28	0.19	0.37	0.18	0.43	0.39	0.31	0.27	0.32	0.40	0.37	0.18	0.43	1	0.31
Fish	0.11	0.12	0.47	0.09	0.08	0.08	0.14	0.11	0.11	0.28	0.23	0.04	0.04	0.47	1	0.24
Milk+yoghurt	0.47	0.38	0.42	0.37	0.37	0.38	0.98	0.40	0.45	0.30	0.58	0.69	0.30	0.98	1	0.12
Butter	0.20	0.35	0.28	0.35	0.34	0.04	0.22	0.10	0.16	0.04	0.02	0.17	0.02	0.35	1	0.85
Cheese	0.38	0.33	0.33	0.58	0.45	0.57	0.14	0.46	0.39	0.14	0.14	0.21	0.14	0.58	1	0.55
Fruit+vegetables	1.17	0.99	0.85	1.10	1.11	1.41	0.84	1.57	1.37	0.94	1.43	0.75	0.75	1.57	0.8	0.15
Cereals	4.68	3.96	3.74	4.09	4.00	5.83	5.81	6.42	2.99	5.03	3.92	4.80	2.99	6.42	1	0.85
Potatoes	0.72	0.85	0.55	0.64	0.60	0.75	1.22	0.33	0.76	0.97	0.93	0.93	0.33	1.22	0.8	0.23

[1] Edible Fraction

[2] Dry-weight Fraction

Calculations can be performed as follows:

$$R = \frac{D_C}{D_A} \tag{24}$$

Where:-

D_C = average quantity of food consumed over childhood in kg/(kg BW·day)

D_A = average quantity of food consumed over adulthood in kg/(kg BW·day)

It is assumed that the food quantities listed in Table 8 apply to adults. Multiplication of these data with R gives an estimate for the food consumption of children. The data are presented in Table 9.

Table 9 Daily food consumption of children and adults

EC average in g of fresh weight per kgbw per day[1]			
Intake of	**Adult** D_A	**R**	**Child** D_C
Meat	4.4	1.57	6.9
Fish	0.5	1.23	0.6
Milk + yoghurt	3.9	4.24	16.5
Butter	0.2	4.24	0.8
Cheese	0.7	4.24	3.0
Fruit + vegetables	9.7	1.78	17.3
Cereals	5.5	2.47	13.6
Potatoes	3.9	1.78	6.9
Age[1]	16 - 70		0 - 15
Bodyweight[1]	66		27

[1] ratios and data as McKone and Daniels (1991).

4.4 ENVIRONMENTAL PATHWAYS

4.4.1 Introduction

The multiple exposure pathways which link man and the environment are illustrated in Figure 1 and the different food types to be considered have been discussed above.

In the absence of adequately measured concentrations for each contact medium (air, water, soil, food) multi-media fate and multiple-pathway exposure models can be used to obtain a predicted daily dose.

The environmental concentrations in air, water and soil can be estimated if it is known how and in what quantity a substance enters the environment and how it is subsequently distributed, transformed and (bio)degraded in these receiving compartments (ECETOC, 1992a). In multi-media models several environmental phases or compartments, such as water, air, soil and biomass are represented by separate boxes and complete mixing is assumed in each box (ECETOC, 1993a). The models allow the prediction of average concentrations in each of these environmental compartments which may represent very large areas or volumes. Since complete mixing seldom occurs in reality, it may well be that in some areas concentrations are below background, while in other areas concentrations may well exceed background concentrations.

As discussed by ECETOC (1993a) it is considered that the Mackay level 3 Fugacity Model is the most appropriate for screening purposes since the model formulation accounts for

- partitioning between media;
- degradation and advection in compartments;
- non-equilibrium between compartments; and
- mass transfer between compartments.

In this report, HAZCHEM (ECETOC, 1994b) has been used as a tool to illustrate the scope and limitations of such an assessment. In this model the exposure assessment is limited to the ingestion and inhalation routes. McKone (1992) discriminates additional routes and pathways, such as inhalation of gases and particles in outdoor air versus inhalation of gases and particles transferred from outdoor to indoor air. Inhalation of contaminants transferred from tap water and inhalation of soil vapours and particles that have been transferred to indoor air are also considered in the model of McKone.

Ingestion of soil and drinking water are considered as main intake routes in the models described by Mackay *et al* (1991), McKone (1993) and RIVM, VROM, WVC (1994), whereas description of dermal contact has been very limited. Only McKone (1993) described contact with soil, drinking water, and bathing water as being relevant dermal routes in locally contaminated areas.

The transfer functions which relate the chemical concentrations in air, water or soil to the contact medium (e.g. drinking water and food products) used in HAZCHEM are given in Table 10, and compared to equations used in MNSEM (Japan) (OECD, 1991), DRANC (The Netherlands), and CHEMCAN (Canada).

In this document Quantitative Structure-Activity Relationships (QSARs) will be discussed which have been used in HAZCHEM to relate partition between water, soil and plants, but also between animal diet and lipid tissue.

It is important to note that the reliability and accuracy for using these QSARs within the risk assessment scheme is difficult to assess. The exact domain for which the model is valid, and chemical inclusion or exclusion rules needs to be determined if indirect exposure QSARs are to be used with confidence within the risk assessment framework. It should also be noted that most of these transfer factors can be measured and that preference should be given to the experimental data, provided that adequate protocols and analytical methodology were employed. At the screening level each individual transfer will be assessed using structure-activity relationships which are based on justifiable assumptions. The overall exposure value must, however, be interpreted with care since error may propagate through the assessment.

4.4.2 Food chain

Indirect exposure of man to contaminants in food will be highly dependent on the assumptions made about the food basket throughout a lifetime (see Section 4.2). The prediction of a potential dose to which human populations are exposed will be largely dependent on dietary habits and food sourcing in addition to compound characteristics. Influences of food processing on content and transformation of parent substance have not been taken into account in this report.

The following sections will describe the relevant transfer functions which relate chemical concentrations in air, water and soil to those in food.

Bioconcentration water-fish

The predicted concentration in fish can be estimated using a predicted or measured bioconcentration factor (BCF) i.e. the ratio of the steady state concentration in the organism to the concentration of the chemical in the surrounding medium. The BCF is a measure of chemical partitioning, uptake, distribution and elimination at steady state.

Table 10 Comparison of Equations Used in HAZCHEM (ECETOC), MNSEM (Japan), DRANC (Netherlands) and CHEMCAN (Canada).

Part 1 Definitions

C_{air}	Concentration in air
C_{fish}	Concentration in fish
$C_{f,v,c}$	Concentration in fruits, vegetables and crops
C_{rv}	Concentration in root vegetables
C_{lv}	Concentration in leaf vegetables and cereals
C_{meat}	Concentration in meat
C_{milk}	Concentration in milk
C_{pw}	Concentration in pore water of soil
C_{soil}	Concentration in soil
C_{water}	Concentration in water
C_{gw}	Concentration in groundwater
Crw	Crop weight per m^2
D_{drw}	Daily dose of drinking water
D_{fish}	of eating fish
$D_{f,v,c}$	of ingesting fruits, vegetables and crops
D_{inh}	of inhalation
D_{meat}	of ingesting meat
D_{milk}	of ingesting milk
BCF_{fish}	Bioconcentration factor for fish
$BCF_{f,v,c}$	for fish, vegetables and crops
BCF_{meat}	for meat
BCF_{milk}	for milk
BCF_{rv}	for root vegetables
BCF_{pot}	for potatoes
BCF_{lv}	for leafy vegetables
BCF_{animal}	for animal (assumes edible portion)
I_{grass}	daily intake of grass by cows
$I_{soil,c}$	of soil by cows
I_{air}	of air by cows
g_l	Daily intake of substance by lactating cow
g_{nl}	by non-lactating cow
F_l	Daily feed rate by lactating cow
F_{nl}	by non-lactating cow
O_v	Dry weight / total weight of plant (0.2)
K_{ow}	Octanol/water partition coefficient
K_{wa}	Water/air partition coefficient
K_{pa}	Plant/air partition coefficient
H	Henry's Law constant
R	Gas constant
T	Temperature (K)
ρ	Density of solids

Table 10 Comparison of Equations used in HAZCHEM versus MNSEM, DRANC and CHEMCAN.
Part 2 Equations

Pathway	ECETOC HAZCHEM	Japan MNSEM	Netherlands DRANC	Canada CHEMCAN
Fish	$C_{fish} = C_{water} \cdot BCF_{fish}$ $BCF_{fish} = 0.048K_{ow}$	$C_{fish} = C_{water} \cdot BCF_{fish}$	$C_{fish} = C_{water} \cdot BCF_{fish}$ $\log BCF_{fish} = 0.79\log K_{ow}-0.40$	$C_{fish} = C_{water} \cdot BCF_{fish}$ $BCF_{fish} = 0.048K_{ow}$
Leaf vegetables and/or root vegetables	$C_{f,v,c} = C_{iw} \cdot TSCF \cdot SCF$ $TSCF = 0.748 \cdot$ $\exp[-(\log K_{ow}-1.76)^2/2.44]$ $SCF = 0.82+$ $10\exp(0.95\log K_{ow}-2.05)$ $C_{root,veg} = BCF_{pot} \cdot C_{iw}$ $BCF_{pot} = 0.82+$ $10\exp(0.77 \cdot \log K_{ow}-2.52)$	$C_{f,v,c} = C_{soil} \cdot BCF_{f,v,c} \cdot O_v$ $\log BCF_{f,v,c} =$ $1.588-0.578\log K_{ow}$	$C_{f,v,c} = C_{iw} \cdot TSCF \cdot SCF$ $TSCF = 0.748 \cdot$ $\exp[-(\log K_{ow}-1.76)^2/2.44]$ $SCF = 0.82+$ $10\exp(0.95\log K_{ow}-2.05)$	$C_{root,veg} = BCF_{rv} \cdot C_{lw}$ $BCF_{rv} = (0.82+0.14K_{ow})P_{root}$ $C_{lv} = BCF_{lv} \cdot C_{air}$ $BCF_{lv} = (0.19+$ $0.7 \cdot K_{wa} \cdot 0.05K_{pa}) \cdot$ $K_2/(K_2+K_G)$ $K_G = 0.004$ $1/K_2 = 126+5 \cdot 10^{-6}K_{pa}$ $K_{wa} = RT/H$ $K_{pa} = K_{ow} \cdot RT/H$
Meat	$C_{meat} =$ $BCF_{meat}(I_{pot} \cdot C_{pot}+I_{grass} \cdot C_{f,v,c}+$ $I_{soil} \cdot C_{soil}+I_{air} \cdot C_{air})$ $\log BCF_{meat} = \log K_{ow}-7.6$	$C_{meat} = BCF_{meat} \cdot g_{nl}$ $g_{nl} = F_{nl} \cdot C_{soil} \cdot BCF_{f,v,c}$ $\log BCF_{meat} = -7.735 +$ $1.033 \cdot \log K_{ow}$	$C_{meat} =$ $BCF_{meat}(I_{grass} \cdot C_{f,v,c}+$ $I_{soil} \cdot C_{soil}+I_{air} \cdot C_{air})$ $\log BCF_{meat} = \log K_{ow}-7.6$	$C_{animal} = BCF_{animal} \cdot C_{water}$ $BCF_{animal} = 0.05P \cdot K_{ow}$ P = animal fat content (kg/l)
Milk and/or dairy products	$C_{milk} = 0.04 \cdot$ $BCF_{milkfat} \cdot (I_{pot} \cdot C_{pot} +$ $I_{grass} \cdot C_{f,v,c}+I_{soil,c} \cdot C_{soil}+I_{air} \cdot C_{air})$ $C_{butter} = 0.8 \cdot$ $BCF_{milkfat} \cdot (I_{pot} \cdot C_{pot} +$ $I_{grass} \cdot C_{f,v,c}+I_{soil,c} \cdot C_{soil}+I_{air} \cdot C_{air})$ $C_{cheese} = 0.25 \cdot$ $BCF_{milkfat} \cdot (I_{pot} \cdot C_{pot} +$ $I_{grass} \cdot C_{f,v,c}+I_{soil,c} \cdot C_{soil}+I_{air} \cdot C_{air})$ $\log BCF_{milkfat} = \log K_{ow}-6.7$	$C_{milk} = BCF_{milk} \cdot g_l$ $g_l = F_l \cdot C_{soil} \cdot BCF_{f,v,c}$ $\log BCF_{milk} = -8.056 +$ $0.992 \cdot \log K_{ow}$	$C_{milk} = BCF_{milk} \cdot (I_{grass} \cdot C_{f,v,c} +$ $I_{soil,c} \cdot C_{soil}+I_{air} \cdot C_{air})$ $\log BCF_{milk} = \log K_{ow}-8.1$	

$$C_{fish} = BCF_{fish} \cdot C_w \qquad (25)$$

Where:-

C_{fish} = concentration in fish (mg/kg wet fish)

C_w = concentration in surface water (dissolved) (mg/l)

The bioconcentration of substances in fish is described as an equilibrium between water and fat, dependent on the hydrophobicity of the substance. Bioconcentration is therefore the net result of the uptake and distribution rate minus the elimination rate of the substance.

Since measured values of this bioconcentration factor are often lacking, QSAR methods are used to predict this BCF. Among the several relationships published, that of Mackay and Paterson (1982) is used in this report:

$$BCF_{fish} = 0.048 \cdot K_{ow} \qquad (26)$$

Where:-

BCF_{fish} = bioconcentration factor of fish (litre water/kg wet fish);

K_{ow} = octanol-water partition coefficient.

This equation is based on experimental data for several different classes of chemicals with a log K_{ow} ranging from approximately 1 to 6. The relationships cannot be used for extremely lipophilic chemicals; for chemicals with a log $K_{ow} \geq 6$, the BCF will not further increase with K_{ow}. Furthermore, the equation is not applicable for substances with a cross-section diameter greater than 9.5 Å (Opperhuizen, 1986) and/or for substances which are metabolised or which are sparingly soluble in water.

Bioconcentration soil-plant

It is increasingly recognized that vegetation serves as a vehicle for exposure to chemicals present in soil and atmosphere. Calculation methods are emerging, but considerable uncertainty still exists about the general validity of proposed algorithms (Briggs *et al*, 1982, 1983; Paterson and Mackay, 1989; Bacci *et al*, 1990; Riederer, 1990; Mackay *et al*, 1991; McKone, 1993).

It is assumed in this report that absorption from soil is controlled by the pore water concentration. The concentration in the pore water is described by:

$$C_{pw} = F_w \cdot C_{soil} \qquad (27)$$

Where:-

C_{pw} = concentration in pore water

C_{soil} = total soil concentration

F_w = ratio between pore water concentration and total soil concentration

$$F_w = \frac{1}{V_a \cdot \frac{H}{RT} + V_w + V_s \cdot f_{oc} \cdot K_{oc}} \qquad (28)$$

Where:-

V_a = air volume in soil (0.2 m^3/m^3)

V_w = water volume in soil (0.3 m^3/m^3)

V_s = solid volume in soil (0.5 m^3/m^3)

H = Henry constant (saturated vapour pressure [Pa]/solubility in water [Mol/m^3])

R = gas constant (8.314 J/(Mol·°K))

T = temperature [degree Kelvin]

f_{oc} = fraction organic carbon in soil

K_{oc} = partition coefficient soil organic carbon/water [kg/litre]

= $0.41 \cdot K_{ow} \cdot \rho_s / 1000$

K_{ow} = octanol/water partition coefficient

ρ_s = density soil solids (2400 kg/m^3)

Briggs *et al* (1982,1983) described methods for the estimation of concentration factors for plants:

- from pore water into root tissue (RCF=Root Concentration Factor)
- from pore water into the xylem fluid (TSCF=Transportation Stream Concentration Factor).
- from the xylem fluid in stems and leaves (SCF=Stem Concentration Factor).

The estimations were based on barley shoots and for a limited number of substances only.

The BCF root/vegetable (BCF_{rv}) is described by Equation 29:

$$BCF_{rv} = 10^{0.77 \cdot \log K_{ow} - 1.52} + 0.82 \qquad (29)$$

The BCF was based on roots with a relatively high peel content containing lipids. In order to get a more realistic BCF for potatoes, a crop with relatively high pulp and low peel content, this BCF_{rv} was lowered with a factor 10:

$$BCF_{potato} = 10^{0.77 \cdot \log K_{ow} - 2.52} + 0.82 \tag{30}$$

The concentration in potatoes in HAZCHEM is estimated as follows:

$$C_{potato} = BCF_{potato} \cdot F_w \cdot C_{soil} \tag{31}$$

The TSCF is described as:

$$TSCF = 0.784 \cdot \exp\left(-\frac{(\log K_{ow} - 1.78)^2}{2.44}\right) \tag{32}$$

and the SCF as:

$$SCF = 10^{(0.95 \cdot \log K_{ow} - 2.05)} + 0.82 \tag{33}$$

The concentration in stem and leaves is estimated by means of the TSCF and the SCF from the total concentration in soil as follows:

$$C_{lv.soil} = BCF_{lv} \cdot F_w \cdot C_{soil} \tag{34}$$

Where:-

$C_{lv.soil}$ = concentration in stem, leaves by absorption from pore water

$BCF_{lv.soil}$ = $TSCF \cdot SCF$

F_w = ratio between pore water concentration and total soil concentration

C_{soil} = total soil concentration

The $C_{lv.soil}$ and the C_{potato} are used in HAZCHEM for estimation of the contribution to the level in leaf vegetables and potatoes, respectively, by transfer of environmentally dispersed substances from soil to the human food chain.

Estimation of plant uptake from air

The plant may be contaminated by deposition from the air. The level of contamination is dependent on:

- the partitioning of the chemical over particulates and the gas phase in air;
- the deposition rate of the substance;
- the interception factor of the crop (Icf = 0.4);
- the crop weight per m^2 (Crw = 1.4 kg fresh weight);
- the elimination rate of the deposited chemical from the plant (Elr = 0.0014 per hour) (ECETOC, 1992b).

The deposition rate Dpr in $\mu g/m^2 \cdot h$ was estimated by:

$$Dpr = C_{air} \cdot (F_{part} \cdot V_{part} + (1 - F_{part}) \cdot V_{gas}) \cdot 3600 \qquad (35)$$

Where:-

C_{air} = air concentration [$\mu g/m^3$]
F_{part} = fraction of substance in air as particulate
= 0.00017 / (P + 0.00017)
V_{part} = deposition velocity particles = 0.01 m/s
P = saturated vapour pressure (Pa)

For the deposition velocity of gases the following assumptions are made:

V_{gas} = deposition velocity gases
= 0.0005 m/s if $H \leq 0.01$
= 0.0004 m/s if $0.1 < H < 100$
= 0.0003 m/s if $H > 100$
H = Henry constant (saturated vapour pressure [Pa]/solubility in water [Mol/m^3])

The concentration in vegetables due to deposition from air was estimated by assuming equilibrium between deposition and elimination processes:

$$C_{lv.air} = \frac{Dpr \cdot Icf}{Elr \cdot Crw} \qquad (36)$$

Where:-

$C_{lv.air}$ = Concentration in stem and leaves due to deposition [$\mu g/kg$]
Dpr = Deposition rate ($\mu g/m^2/h$)
Icf = Interception factor for crops

Elr = Elimination rate of deposited chemical [1/h]

Crw = Crop fresh weight per m^2

Finally a check is made whether $C_{lv.air}$ exceeds the concentration in the plant in equilibrium with air, based on fugacity considerations (equal fugacity in plant tissue and air):

$$Z_{plant} = \frac{F_{water} + F_{lipid} \cdot K_{ow}}{H} \tag{37}$$

Where:-

Z_{plant} = fugacity capacity constant in plant

F_{water} = water fraction (0.8 m^3/m^3)

F_{lipid} = lipid content (0.01 m^3/m^3) (Mackay, 1991)

$$Z_{air} = \frac{F_{air} + F_{prt} \cdot 6 \cdot 10^6}{RT} \tag{38}$$

Where:-

Z_{air} = fugacity capacity constant in air

F_{air} = volume fraction gas phase (1 m^3/m^3)

F_{prt} = volume fraction aerosol (10^{-11} m^3/m^3)

The concentration in plant in equilibrium with air based on fugacity considerations is given by:

$$C_{pl.fug} = \frac{Z_{plant} \cdot C_{air}}{Z_{air} \cdot 1000} \tag{39}$$

If these calculations result in $C_{lv.air} > C_{plfug}$, then it is assumed that $C_{lv.air} = C_{plfug}$.

The $C_{lv.air}$ is used in HAZCHEM for estimation of the contribution to the level in leaf vegetables and potatoes by transfer of environmentally dispersed chemicals from air to the human food chain.

Estimation of the concentration in plants after uptake from air and soil

The contributions $C_{lv.air}$ and $C_{lv.soil}$ are added in order to obtain the final concentration in stems and leaves C_{lv}.

$$C_{lv} = C_{lv.soil} + C_{lv.air} \tag{40}$$

Estimation of the level in meat and dairy products

For the estimation of the level in meat and milkfat the regression equations derived by Travis and Arms (1988) were used. The bioconcentration factor was defined as:

BCF = concentration in mg/kg milk or meat / uptake of substance (mg/day).

These authors have related the observed bioconcentration factors of chemicals in meat and milk to the octanol/water partition coefficient:

$$BCF_{meat} = 10^{\log K_{ow} - 7.6} \tag{41}$$

$$BCF_{milk} = 10^{\log K_{ow} - 8.1} \tag{42}$$

The dairy products, derived from cow milk, may have a variable content of milkfat, e.g. butter and cheese. Therefore the equation for the bioconcentration factor for dairy products was transformed to the bioconcentration factor for milkfat (on the basis of 4% milkfat in milk). In connection with the data of consumption and milkfat content of butter (0.8), cheese (0.25), milk and yogurt (0.04) the uptake of chemicals via milkfat can be more accurately estimated:

$$BCF_{milkfat} = 10^{\log K_{ow} - 6.7} \tag{43}$$

In order to estimate the expected level in meat and milkfat the daily intake of cattle in mg/d is needed.

This daily intake is estimated in HAZCHEM from the following exposure routes:

- 86 kg fresh feed, consisting of 90% of grass with the level C_{sl} (stem and leaf) and for 10% of fodder beets with the level of C_{potato};
- 0.576 kg of wet soil;
- 55 litre drinking water;
- 122 m^3 air.

The Daily Intake of Cattle (=DIC µg/kg) is estimated from:

$$DIC = 122 \cdot C_{air} + 55 \cdot C_{water} + 0.576 \cdot C_{soil} + 86 \cdot (0.9 \cdot C_{sl} + 0.1 \cdot C_{potato}) \quad (44)$$

Where:-

C_{air} = concentration in air [µg/m^3]
C_{water} = concentration in water [µg/kg]
C_{soil} = concentration in soil [µg/kg]
C_{sl} = concentration in stem and leaf [µg/kg]
C_{potato} = concentration in potato [µg/kg]

The concentration in meat and dairy products is estimated according to Equations (45)-(49) below:

$$C_{meat} = BCF_{meat} \cdot DIC \quad (45)$$

$$C_{milkfat} = BCF_{milkfat} \cdot DIC \quad (46)$$

$$C_{milk} = 0.04 \cdot BCF_{milkfat} \cdot DIC \quad (47)$$

$$C_{butter} = 0.80 \cdot BCF_{milkfat} \cdot DIC \quad (48)$$

$$C_{cheese} = 0.25 \cdot BCF_{milkfat} \cdot DIC \quad (49)$$

McKone (1993) has calculated error terms of ± 0.95 and ± 0.84 for the meat and milk regressions of Travis and Arms. These estimation errors correspond to coefficients of variation of 11 and 6, respectively.

Estimation of the concentration in drinking water

Groundwater and surface water may be used as a source for drinking water.

The concentration in groundwater is assumed to be equal to the pore water concentration at steady-state. This means that equilibrium has been achieved between the daily additions of the substance averaged over many years, and the daily elimination by degradation, leaching and volatilisation. The level in groundwater used as drinking water is estimated by averaging the pore water level in natural and arable soil. The groundwater is assumed not to be subjected to any purification prior to supply for drinking.

The concentration in the surface water is also taken to be equal to the predicted steady-state, in which equilibrium exists between the daily supply of the substance and its elimination by degradation, sedimentation and volatilisation. Surface water may be purified by means of two purification systems (Hrubec and Toet, 1992). The extent of removal is assumed to be dependent on the physico-chemical properties and biodegradation behaviour as outlined in Table 11.

Table 11 Purification Factors of Surface Waters as assumed by Hrubec and Toet (1992)

Physico-chemical properties and degradation behaviour	Purification	
	System 1 purification factors	System 2 purification factors
Henry coefficient	PF1 =	PF1 =
$H \leq 100$	1	1
> 100	0.5	0.5
log(octanol/water)	PF2 =	PF2 =
< 4	1	1
≥ 4 and ≤ 5	0.25	0.5
> 5	0.0625	0.25
Halflife days (bio)degradation	PF3 =	PF3 =
≥ 240	1	1
< 240	1	0.25
Total purification	$PFT1 = PF1 \cdot PF2 \cdot PF3$	$PFT2 = PF1 \cdot PF2 \cdot PF3$

The level in the drinking water is estimated by multiplying the surface water level with the greater factor of PFT1 or PFT2. If the drinking water level of purified surface water is lower than the level in ground water, then ground water is assumed to be used as drinking water (Vermeire *et al,* 1992).

4.4.3 Estimation of the Intake through Air

When direct release to the air compartment occurs, rapid dilution and effective photochemical transformation or degradation is usually observed. Removal and environmental partitioning will result in concentrations in air which are far below any effect concentration. However, due to this partitioning (e.g. plants, water) and differences in photochemical degradation rates the air compartment plays an important role in the indirect exposure assessment. Direct effects due to inhalation of air (PEC_{local} and $PEC_{regional}$) are taken into account in the model calculations by assuming an inhalation rate of 20 m^3/day.

In addition, it should be pointed out that indoor exposure may occur through release of substances from pre-treated construction materials (e.g. wood) and other building materials (e.g. carpets, walls). This slow release and background exposure is not discussed in this document.

4.5 CASE STUDIES ON INDIRECT EXPOSURE

4.5.1 Selection of Substances

The substances providing different properties have been chosen on the basis of:

- availability of a suitable database and
- illustrative for indirect exposure scenarios.

Three substances have been added to those used in the case studies of consumer exposure (see 3.5.1) resulting in a list of seven substances:

- linear alkylbenzene sulphonate (LAS);
- dimethylether;
- dichloromethane;
- benzene;
- diethylhexylphthalate (DEHP);
- 2,6 di-tert-butyl-4-methyl phenol (BHT);
- cypermethrine.

The HAZCHEM model has been used as multimedia Mackay level 3 model to predict the concentrations in air, water, soil and food products. The default settings for the EC region, EC waste water treatment plant and average EC diet are given in Appendix B. The details on the environmentally relevant input data on compound, release pattern and Mackay level 3 calculations can be found in Appendix C.

To evaluate the predicted concentrations, a comparison has been made between predicted and measured concentrations for the different substances in air, water, soil and food. Measured data have been compiled from the existing literature and ECETOC reports. Wherever possible background data have been selected for a realistic comparison between the predicted HAZCHEM value and measured value. However, it should be taken into consideration that measurements are often made locally near the pollution source and/or on a contaminated site.

The tables presented below summarise this comparison.

Table 12 Comparison of Measured Environmental Levels with Calculated Levels for Different Compartments

Part 1 Dichloromethane

MEDIUM	MEASURED	REFERENCE	CALCULATED (HAZCHEM)
Air (mg/m^3)	7-29 · 10^{-5} (mean background)	IPCS (1993a)	61·10^{-5}
Water (mg/l)	up to 10·10^{-3} (surface water) up to 2.6·10^{-3} (coastal water) 5-50·10^{-5} (surface water) up to 230 near sources (ground water)	IPCS (1993a) IPCS (1993a) OECD (1993) OECD (1993)	2.6·10^{-3} (surface water) 1.7·10^{-4} (ground water)
Sediment (mg/kg)	13·10^{-3} (median, 1 on 20% of all samples; EPA sediment sampling)	IPCS (1993a)	1.67·10^{-3}
Soil (mg/kg)			1.8·10^{-4} (arable) 3.4·10^{-6} (natural)
Food* (mg/kg)	up to 1·10^{-3} (drinking water, mean) up to 0.28 (butter) up to 0.3 (cereal) up to 0.1 (cheese) up to 0.3 (processed foods)	IPCS (1993a) OECD (1993) OECD (1993) OECD (1993) OECD (1993)	1.3·10^{-3} (drinking water) 3.4·10^{-4} (vegetables) 2.5·10^{-3} (fish) 9.4·10^{-7} (milk fat) 1.2·10^{-7} (meat)
Daily intake (mg/kg)	3·10^{-3} (inhalation)	OECD (1993)	2.3·10^{-4} (adult) 4.6·10^{-4} (child)

* Residues in food resulting from food processing with dichloromethane are not included.

Predicted air, water and sediment concentrations are in good agreement with reported measured values.

The comparison of predicted vs. measured concentration in food products is hampered by analytical detection limits, and most monitoring data relate to residues resulting from food processing.

The major indirect exposure pathway (> 80 %) is due to inhalation, and predicted levels are within one order of magnitude to the levels reported.

Table 12 **Comparison of Measured Environmental Levels with Calculated Levels for Different Compartments**

Part 2 **Cypermethrin**

MEDIUM	MEASURED	REFERENCE	CALCULATED (HAZCHEM)
Air (mg/m^3)			$0.14 \cdot 10^{-9}$
Water (mg/l)	$<1^*$-$2.9 \cdot 10^{-5}$ (rivers) $<1 \cdot 10^{-5}$ (surface water) $<1 \cdot 10^{-5}$, $7.5 \cdot 10^{-5}$ (groundwater)	House *et al* (1991)	$1.7 \cdot 10^{-7}$ (surface water) $1.8 \cdot 10^{-9}$ (ground water)
Sediment (mg/kg)	$<1^*$-$2.7 \cdot 10^{-3}$	House *et al* (1991)	$1 \cdot 10^{-3}$
Soil (mg/kg)	0.5-3.10^{-5}	Legrand *et al* (1991)	$9.3 \cdot 10^{-5}$ (arable) $2.5 \cdot 10^{-5}$ (natural)
Food (mg/kg)	Residues resulting from direct treatment of food crops or animals are not considered.	IPCS (1989; 1992a).	$0.1 \cdot 10^{-3}$ (vegetables) $0.4 \cdot 10^{-3}$ (meat) $3.2 \cdot 10^{-3}$ (milk fat) $16.8 \cdot 10^{-3}$ (fish) $4.2 \cdot 10^{-8}$ (drinking water)
Daily intake (mg/kg)			$1.33 \cdot 10^{-5}$ (adult) $2.26 \cdot 10^{-5}$ (child)

* Detection limit

Predicted concentrations in water and sediment are in good agreement with reported values in the literature.

The comparison of predicted vs. measured concentrations in food products is hampered by the absence of data.

The major indirect exposure pathway (> 60 %) is predicted due to fish consumption. Predicted concentrations in freshwater fish are of the order of 1 μg/kg.

Table 12 Comparison of Measured Environmental Levels with Calculated Levels for Different Compartments

Part 3: LAS

MEDIUM	MEASURED	REFERENCE	CALCULATED (HAZCHEM)
Air (mg/m^3)	-		10^{-16}
Water (mg/l)	$2 \cdot 10^{-3}$*	ECETOC (1993a)	$3 \cdot 10^{-5}$ (surface water) $5.4 \cdot 10^{-6}$ (ground water)
sediment (mg/kg)	1-10	ECETOC (1993a)	$4.8 \cdot 10^{-5}$
Soil (mg/kg)	0.9	ECETOC (1993a)	8.6 10^{-3} (arable)
Food (mg/kg)	<0.1-0.3 (fish)	Tokai *et al* (1990)	$2 \cdot 10^{-5}$ (vegetables) $6.6 \cdot 10^{-8}$ (meat) $5.2 \cdot 10^{-7}$ (milk fat) $9 \cdot 10^{-4}$ (fish) $3 \cdot 10^{-5}$ (drinking water)
Daily intake (mg/kg)			1.7 10^{-6} (adult) 3.1 10^{-6} (child)

* Detection Limit

Reported concentrations are related to local discharges from wastewater treatment plants. Regional background levels in water, sediment and soil are hampered due to relatively high detection limits in the analytical methodology.

Concentrations in fish measured in the Tokyo Bay are related to local discharges. Surface water concentrations averaged around 10 µg/l (BCF = 30).

The major indirect exposure pathway is predicted due to consumption of fish, vegetables and water.

Table 12 **Comparison of Measured Environmental Levels with Calculated Levels for Different Compartments**

Part 4 **BHT**

MEDIUM	MEASURED	REFERENCE	CALCULATED (HAZCHEM)
Air (mg/m^3)			$9.6 \cdot 10^{-8}$
Water (mg/l)	$0.1\text{-}14 \cdot 10^{-3}$ (Rhine)	BUA (1991) BUA (1991)	$8 \cdot 10^{-6}$ (surface water) $3.8 \cdot 10^{-9}$ (ground water)
Sediment (mg/kg)	$66\text{-}1690 \cdot 10^{-3}$		$1.4 \cdot 10^{-6}$
Soil (mg/kg)		BUA (1991)	$5 \cdot 10^{-6}$ (arable) $6 \cdot 10^{-9}$ (natural)
Food (mg/kg)	6-530 (various) $6\text{-}69 \cdot 10^{-3}$ (fish) $0.13\text{-}13 \cdot 10^{-3}$ (drinking water, USA)	IARC (1986) BUA (1991) BUA (1991)	$9.8 \cdot 10^{-7}$ (vegetables) $9.2 \cdot 10^{-8}$ (meat) $7.3 \cdot 10^{-7}$ (milk fat) $1.6 \cdot 10^{-4}$ (fish) $4 \cdot 10^{-8}$ (drinking water)
Daily intake (mg/kg)	1-2	IARC (1986)	$1.3 \cdot 10^{-7}$ (adult) $1.9 \cdot 10^{-7}$ (child)

Predicted concentrations in water and sediment are orders of magnitude lower than levels reported in literature.

The comparison of predicted vs. measured concentration in food products is hampered by use of BHT as a food additive.

The major indirect exposure pathway (> 60 %) is predicted due to fish consumption. Predicted fish concentrations are about 1 to 2 orders of magnitude lower than reported figures. From the data it can be concluded that indirect exposure is negligible as compared to direct consumer exposure from the use as of BHT as a food additive.

Table 12 Comparison of Measured Environmental Levels with Calculated Levels for Different Compartments

Part 5 DEHP

MEDIUM	MEASURED	REFERENCE	CALCULATED (HAZCHEM)
Air (mg/m^3)	0.4-2.9$\cdot10^{-6}$ ≤ 5$\cdot10^{-6}$ (remote areas)	IARC (1982) IPCS (1992b), UK-MAFF(1987)	0.6$\cdot10^{-6}$
Water (mg/l)	0.05-30$\cdot10^{-3}$ < 0.1-4.0$\cdot10^{-3}$ (rivers, lakes) up to 0.3 (rivers, lakes) 0.05-1.4$\cdot10^{-3}$ (ground water at waste water infiltration sites)	IARC (1982) IPCS (1992b) UK-MAFF (1987) UK-MAFF (1987)	1.2$\cdot10^{-3}$ (surface water) 0.13$\cdot10^{-6}$ (ground water)
Sediment (mg/kg)	1-70 (river sediment) (up to 1500 sediment near discharge points) 1.8-18.3 (Rhine) 0.1-8.9 (Weser)	IPCS (1992b) IPCS (1992b) Furtmann (1993) Furtmann (1993)	0.7
Soil (mg/kg)			0.1$\cdot10^{-3}$ (arable) 0.22$\cdot10^{-3}$ (natural)
Food (mg/kg)	0.01-10 (fish) < 1 (US food survey, 1974)	IPCS (1992b) UK-MAFF (1987)	0.8$\cdot10^{-3}$ (vegetables) 0.2$\cdot10^{-3}$ (meat) 1.4$\cdot10^{-3}$ (milk fat) 4.4 (fish) 3.5$\cdot10^{-5}$ (drinking water)
Daily intake (mg/kg)	4.5-30$\cdot10^{-3}$	IPCS (1992b)	2.3$\cdot10^{-3}$ (adult) 2.8$\cdot10^{-3}$ (child)

Predicted air, water and sediment concentrations are in good agreement with reported values in the literature.

The comparison of predicted vs. measured concentrations in food products is hampered by a different food contact today, and reported literature figures may therefore not reflect current use patterns. In addition, most monitoring data relate to leaching from packaging materials in food products.

The major indirect exposure pathway (> 96 %) is predicted due to fish consumption. Predicted freshwater fish concentrations are in good agreement with reported figures.

Table 12 Comparison of Measured Environmental Levels with Calculated Levels for Different Compartments

Part 6 Benzene

MEDIUM	MEASURED	REFERENCE	CALCULATED (HAZCHEM)
Air (mg/m^3)	$0.08-170.10^{-3}$ $0.5 - 6\ 10^{-3}$ (mean, rural and suburban areas) $6-40\ 10^{-3}$ (mean, urban areas)	ECETOC (1993a) IPCS (1993b) IPCS (1993b)	$0.56\ 10^{-3}$
Water (mg/l)	$0.1\ 10^{-4}$ $<0.1-10.10^{-4}$	ECETOC (1993a) IPCS (1993b)	$1.1\ 10^{-4}$
Sediment (mg/kg)	$<50.10^{-4}$ (sediment, USA, in 9% of samples taken)	IPCS (1993b)	$1.5\ 10^{-4}$ (sediment)
Soil (mg/kg)	$4\ 10^{-2}$ $0.5-3.10^{-5}$	ECETOC (1993a) IPCS (1993b)	$3.6\ 10^{-5}$ (arable) $6.2\ 10^{-6}$ (natural)
Food (mg/kg)	$3-88.10^{-3}$ (fish, Japan, 37 of 114 samples)	IPCS (1993b)	$2.5\ 10^{-5}$ (vegetables) $2.6 \cdot 10^{-7}$ (meat) $2.1 \cdot 10^{-6}$ (milk fat) $7.3 \cdot 10^{-4}$ (fish) $5.4 \cdot 10^{-5}$ (drinking water)
Daily intake (mg/kg)	Non-smokers: $3.3\ 10^{-3}$ (Canada) $6-22\ 10^{-3}$ (USA)	IPCS (1993b) IPCS (1993b)	$2.7\ 10^{-3}$ (adult) $5.4\ 10^{-3}$ (child)

Predicted air, water and sediment concentrations are in good agreement with reported values in the literature.

The comparison of predicted vs. measured concentrations in food products is hampered by the paucity of data. Predicted fish concentrations are significantly lower than the highest reported fish monitoring data in Japan but a mean value cannot be calculated.

The major indirect exposure pathway (> 80 %) is due to inhalation, and predicted levels are within one order of magnitude to the levels reported for non-smokers.

SECTION 5. CONCLUSIONS AND RECOMMENDATIONS

Before engaging in a non-occupational exposure assessment, the assessor should establish whether exposure to the substance/article is likely to occur. If so, the exposure assessment should be a step-wise process:

Consumer Exposure

1. The assessor should first consider those scenarios where greatest exposure to the product/article may be expected. Initially, "reasonable worst case" assumptions are made for these scenarios and an estimation of the exposure is developed using reasonable calculations and justifiable assumptions for key exposure elements. If the margin of safety is not considered adequate, the assumptions and data used in this first step need to be refined to provide a more accurate value for the exposure level.

2. Better estimates of the key parameters in exposure models should be developed. This will involve improved values for parameters such as room sizes, bodyweights, etc. which are relevant for individual geographies. In addition, improved data on product use scenarios for different product categories and different regions will give more realistic and region-specific estimates.

3. Suitable models for providing better estimates of internal exposure to substances of concern should be developed. Reasonable models are available for estimating the amount of a substance to which a consumer may be exposed externally. However, if the external exposure is of concern, then it is important to understand the uptake or absorption of the substance into the systemic circulation. Such "absorption models" should address all exposure routes (oral, dermal and via inhalation) and the different barrier membranes which these routes present. The models should also consider several factors including the physical/chemical parameters of the substance of interest; vehicle effects; physiology of the barrier membrane at the site of uptake (e.g. oral mucosa, skin in armpit region, etc.); metabolism of the substance during/after uptake and absorption into the barrier membrane versus into the systemic circulation (e.g. local effects after absorption into the skin versus transfer into the blood capillaries).

Indirect Exposure

1. The assessor should first consider whether environmental release and exposure may lead to human exposure. Initially, an estimation of the exposure can be made on the basis of simple transfer functions which relate partitioning between air, water, soil and plants, animal diet, lipid tissue and food products. It is recommended to assess air, water and soil concentrations on a regional basis and to use the diets for the average individual for that region.

2. Insights in the limitations and uncertainties of the transfer or quantitative structure activity relationships (QSARs) used in the indirect exposure assessment should be developed. These relations have been deduced for a limited range of classical hydrophobic substances and extrapolation beyond its domain is not recommended. Validation and/or reformulation of these QSARs for a wider range physico-chemical characteristics is needed if these "indirect QSARs" are to be used with confidence in the risk assessment process.

3. Better estimates of the variability in food habits and sourcing within and between regions should be compiled. In addition, the assessment could be further improved by incorporating measured concentration data for air, water, soil and food products where available.

APPENDIX A GLOSSARY OF TERMS

INDIRECT EXPOSURE:

Exposure of the public via the environment, i.e. air, water, soil and food. The transfer of contaminants from environmental compartment to living biota can be estimated by transfer factors which are estimated from physico-chemical properties and/or biological processes.

BIOACCUMULATION:

The net result of the uptake and distribution rate minus the elimination rate of the chemical. It is the resultant of biological and physico-chemical processes such as water/food ingestion and ad/absorption of chemicals.

BIOACCUMULATION FACTOR OR BIOCONCENTRATION FACTOR (BCF):

The ratio of the steady state concentration in an organism or a compartment within the organism vs. the concentration of the chemical in its surrounding medium (water, air, soil) or other biological compartment. The BCF is a measure of chemical partitioning, uptake, distribution and elimination at steady state exposure.

BIOAVAILABILITY

The ability of a substance to interact with the biosystem of an organism. Systemic bioavailability will depend on the chemical or physical reactivity of the substance and its ability to be absorbed through the gastrointestinal tract, respiratory tract or skin. It may be locally bioavailable at all these sites.

BIOMAGNIFICATION:

The accumulation and transfer of chemicals via the food chain (e.g. water - algae - invertebrate - fish - mammal) via ingestion with food, resulting in an increase of the internal concentration in organisms at the upper levels of this food chain.

ELIMINATION, DEPURATION OR CLEARANCE:

The removal of the substance and its metabolites from a medium (water, soil, air) or biotic compartment. The rate of elimination is expressed by its half-life or the time needed to eliminate 50% of the substance in a pollutant-free medium. This term is often referred to as the clearance or depuration time (CT_{50} or DT_{50}).

APPENDIX B. CASE STUDIES ON ENVIRONMENTAL AND INDIRECT EXPOSURE

B.1 DEFAULT SETTINGS FOR THE EEC

Input data on environment

total surface area (km^2)	2367020
water surface fraction	.013
arable land fraction	.612
height of air compartment (m)	1000
depth of water compartment (m)	3
depth of arable soil compartment (m)	.2
depth of natural soil compartment (m)	.05
depth of sediment compartment (m)	.03
conc. of susp. sed. in water (mg/l)	15
fraction org. carbon soil	.05
fraction org. carbon sediment	.05
fraction org. carbon susp. sed.	.1
wind velocity height 10 meter (m/sec)	5
backgr. level in air ($\mu g/m^3$)	0
advective inflow river water (m^3/sec)	0
backgr. level in water (mg/l)	0
burial rate of sediment (mm/year)	.1
rain precipitation excess (mm/year)	300

Advective residence time air (h)	85.4729
Advective residence time water (h)	1099.249

Input data on waste water treatment plant

number of inhabitant equivalents	3.5E+08
waste water/inhabitant/day (l/day)	200
concentration of primary sludge (g/l)	.22
O.C.-content of primary sludge (w/w)	.3
hydraulic retention time (hours)	7
sludge retention time (hours)	216
sludge conc. aeration tank (g/l)	2.5
O.C.-content of secondary sludge (w/w)	.37
sludge conc. effluent (mg/l)	40
discharge of compound in kg/hour	0
biodegradation rate (1/h)	3
μmax Monod-kinetics (1/h)	1.5
Michaelis-Menten constant (mg/l)	.5
biodegr. in adsorbed state (y/n)	n

Input of data on human food constituents in g/kg/day in the EC

adult intake of meat	4.4
adult intake of fish	.5
adult intake of milk/yoghurt	3.9
adult intake of butter	.2
adult intake of cheese	.7
adult intake of vegetables	9.7
adult intake of cereals	5.5
adult intake of potatoes	3.9
child intake of meat	6.9
child intake of fish	.6
child intake of milk/yoghurt	16.5
child intake of butter	.8
child intake of cheese	3

```
child intake of vegetables              17.3
child intake of cereals                 13.6
child intake of potatoes                6.9
```

B.2 OPTIONS FOR PRODUCTION AND USE OF SUBSTANCES

```
Data on production volume and use pattern of substance

Production/Use in kg/hour               0
                                                    type of main
                                     fraction        use   prod *
Agricultural chemicals                  0              0     0
Basic chemicals in chemical ind.        0              0     0
Chemicals for electric equipment   *    0              0     0
Chemicals personal & household use      0              0     0
Chemicals public areas -general-        0              0     0
Chemicals public areas -pesticides-     0              0     0
Chemicals public areas -detergents-     0              0     0
Chemicals leather processing       *    0              0     0
Chemicals for metal extr. & proc.  *    0              0     0
Fuel and fuel additives                 0              0     0
Chemicals photographic industry         0              0     0
Chemicals used in polymers              0              0     0
Chemicals pulp, paper, board       *    0              0     0
Chemicals as intermediates         *    0              0     0
Chemicals for textile processing        0              0     0
Chemicals paint, lacquer, varnish  *    0              0     0
Others                             *    0              0     0

* = Choice of main prod. and use type affects release!
    Inappropriate choice may yield worst case!

Information on main production and use type

0 = Not applied
1 = Closed systems non-isolated
2 = Isolated on site or continuous production
3 = Isolated off site or batch prod. dedicated equipment
4 = Batch production multipurpose equipment

Information on main use type

5 = Inclusion into matrix
6 = Non-dispersive use
7 = Wide dispersive use
```

APPENDIX C HAZCHEM CALCULATIONS

C.1 CASE STUDY DIMETHYL ETHER

Environmentally relevant input data on compound

```
name of substance                     dimethyl ether
CAS number                            115-10-6
vapour pressure             (Pascal)   101400
boiling point                     °C  -24.8
water solubility              (mg/l)   35300
log(octanol/water) part. coeff.        .1
molecular mass                       46.07
melting point                     °C  -138.5
environmental temperature         °C   15
degradation half life air    (hours)   130
degradation half life water  (hours)   100000
degradation half life soil   (hours)   100000
degradation half life sedim. (hours)   100000
part. coeff. prim. sludge WWTP (l/kg)  .155
part. coeff. sec. sludge WWTP  (l/kg)  .191
part. coeff. susp. part./w     (l/kg)  5.16E-02
part. coeff. sediment/water    (l/kg)  2.58E-02
part. coeff. soil/water        (l/kg)  2.58E-02
part. coeff. fish/water        (l/kg)  6.29E-02
part. coeff. earthworm/water   (l/kg)  1.28E-02
```

Data on prod. volume and use pattern of dimethyl ether

```
Production/Use in kg/hour              7370
                                                    type of main
                                     fraction        use   prod
Chemicals personal & household use     1              7      2
```

Environmental release pattern of dimethyl ether

```
Production volume kg/h                 7370
Release to air                         7370
Release to waste water                 0
Release to surface water               0
Release to soil                        0
Release to waste                       0
Total release                          7370
```

Emission rates to regional environmental compartments

```
Advective residence time air (h)       85.5
Advective residence time water (h)     1100
Direct emission to air (kg/h)          7370
```

Mackay level 3 calculation on dimethyl ether

```
Steady state mass in area   (kg)       434000
Mass % in air                          99.8
Mass % in water dissolved              7.25E-02
Mass % in water suspended              5.62E-08
Mass % in arable soil                  7.89E-02
Mass % in natural soil                 1.21E-02
Mass % in sediment                     5.88E-04
Mass % in fish                         4.57E-09
```

```
Overall residence time    h              58.8
Degradation residence time  h            188
Advection residence time h               85.6

Air conc µg/m3                           .183
Dissolved water conc mg/litre            3.41E-06
Suspended water conc mg/litre            2.64E-12
Arable soil conc ppm                     7.87E-07
Natural soil conc ppm                    7.88E-07
Sediment conc ppm                        2.16E-06
Susp.solids conc ppm                     1.76E-07
Fish conc ppm                            2.15E-07
```

Concentration in regional environmental compartments and in biota

```
concentration in air      µg/m3          .183
diss.conc. surface water  µg/l           3.41E-03
conc. in arable soil      µg/kg          7.87E-04
conc. in natural soil     µg/kg          7.88E-04
diss.conc. groundwater    µg/l           3.45E-03
diss.conc. drinking water µg/l           3.45E-03
conc. in vegetables       µg/kg          3.40E-03
conc. in root crop        µg/kg          2.84E-03
concentration in meat     µg/kg          7.21E-07
conc. in milk fat         µg/kg          5.73E-06
concentration in fish     µg/kg          2.15E-04
```

Human exposure assessment for adults

```
intake by inhalation          5.49E-05  mg/kg/day
intake by drinking water      1.04E-07  mg/kg/day
intake by vegetables          3.30E-08  mg/kg/day
intake by cereals             1.87E-08  mg/kg/day
intake by potatoes            1.11E-08  mg/kg/day
intake by fish                1.07E-10  mg/kg/day
intake by meat                3.17E-12  mg/kg/day
intake by cheese              1.00E-12  mg/kg/day
intake by butter              9.16E-13  mg/kg/day
intake by milk/yoghurt        8.93E-13  mg/kg/day

Predicted intake              5.51E-05  mg/kg/day
```

Human exposure assessment for children

```
intake by inhalation          1.10E-04  mg/kg/day
intake by drinking water      2.07E-07  mg/kg/day
intake by vegetables          5.88E-08  mg/kg/day
intake by cereals             4.62E-08  mg/kg/day
intake by potatoes            1.96E-08  mg/kg/day
intake by fish                1.29E-10  mg/kg/day
intake by meat                4.97E-12  mg/kg/day
intake by cheese              4.29E-12  mg/kg/day
intake by milk/yoghurt        3.78E-12  mg/kg/day
intake by butter              3.66E-12  mg/kg/day

Predicted intake              1.10E-04  mg/kg/day
```

C.2 CASE STUDY DICHLOROMETHANE

Environmentally relevant input data on compound

name of substance		dichloromethane
CAS number		75-09-2
vapour pressure	(Pascal)	46000
boiling point	°C	40.7
water solubility	(mg/l)	16500
log(octanol/water) part. coeff.		1.3
molecular mass		85
melting point	°C	-95
environmental temperature	°C	20
degradation half life air	(hours)	4000
degradation half life water	(hours)	1000
degradation half life soil	(hours)	1000
degradation half life sedim.	(hours)	1000
part. coeff. prim. sludge WWTP	(l/kg)	2.45
part. coeff. sec. sludge WWTP	(l/kg)	3.02
part. coeff. susp. part./w	(l/kg)	.818
part. coeff. sediment/water	(l/kg)	.409
part. coeff. soil/water	(l/kg)	.409
part. coeff. fish/water	(l/kg)	.998
part. coeff. earthworm/water	(l/kg)	.246

Data on prod. volume and use pattern of dichloromethane

Production/Use in kg/hour 25000

	fraction	type of main use	type of main prod
Basic chemicals in chemical ind.	.2	6	2
Chemicals personal & household use	.2	7	2
Chemicals for metal extr. & proc.	.2	7	2
Chemicals photographic industry	.2	7	2
Chemicals paint, lacquer, varnish	.2	7	2

Environmental release pattern of dichloromethane

Production volume kg/h	25000
Release by production	250
Release by compounding	406
Release by commercial use	119000
Release by private use	128000
Release by recovery	0
Release to air	10800
Release to waste water	13500
Release to surface water	0
Release to soil	995
Release to waste	0
Total release	25300

input data on waste water treatment plant

discharged compound is dichloromethane

number of inhabitant equivalents	3.5E+08
waste water/inhabitant/day (l/day)	200
concentration of primary sludge (g/l)	.22
O.C.-content of primary sludge (w/w)	.3

```
hydraulic retention time (hours)          7
sludge retention time (hours)             216
sludge conc. aeration tank (g/l)          2.5
O.C.-content of secondary sludge (w/w)    .37
sludge conc. effluent (mg/l)              40
discharge of compound in kg/hour          13500
biodegradation rate (1/h)                 .3
µmax Monod-kinetics (1/h)                 0
Michaelis-Menten constant (mg/l)          0
biodegr. in adsorbed state (y/n)         n
```

Fate of compound dichloromethane in WWTP
(Namkung & Rittmann 1987)

```
total influent concentration (mg/l)         4.62

effluent concentration (dissolved mg/l)     1.34
effluent concentration (suspended mg/l)     1.63E-04

amount biodegraded per hour (kg)            7610
amount volatilized per hour (kg)            1940
removed via primary sludge per hour (kg)    4.84
removed via second. sludge per hour (kg)    .960
removed via effl./hour (dissolved kg)       3920
removed via effl./hour (suspended kg)       .474

primary sludge production per hour (kg)     428000
second. sludge production per hour (kg)     236000

comp. conc. in primary sludge (mg/kg)       11.3
comp. conc. in second. sludge (mg/kg)       4.06

percentage removal by primary sludge        3.60E-02
percentage removal by biodegradation        56.5
percentage total removal                    70.9
```

Emission rates to regional environmental compartments
of dichloromethane

```
Direct emission to air (kg/h)             10800
Direct emiss. to arable soil (kg/h)       995

WWTP emission to air (kg/h)               1940
WWTP emission to water (kg/h)             3920
WWTP emission to arable soil (kg/h)       5.80
```

Mackay level 3 calculation on dichloromethane

```
Steady state mass in area   (kg)          1770000
Mass % in air                             82.1
Mass % in water dissolved                 13.4
Mass % in water suspended                 1.64E-04
Mass % in arable soil                     4.43
Mass % in natural soil                    1.30E-02
Mass % in sediment                        .112
Mass % in fish                            1.33E-05

Overall residence time   h                100
Degradation residence time  h             3750
Advection residence time h                103

Air conc µg/m3                            .613
Dissolved water conc mg/litre             2.56E-03
Suspended water conc mg/litre             3.14E-08
Arable soil conc ppm                      1.80E-04
```

```
Natural soil conc ppm                       3.44E-06
Sediment conc ppm                           1.67E-03
Susp.solids conc ppm                        2.09E-03
Fish conc ppm                               2.55E-03

Concentration in regional environmental compartments
and in biota of dichloromethane

concentration in air       µg/m3            .613
diss.conc. surface water   µg/l             2.56
conc. in arable soil       µg/kg            .180
conc. in natural soil      µg/kg            3.44E-03
diss.conc. groundwater     µg/l             .170
diss.conc. drinking water  µg/l             1.28
conc. in vegetables        µg/kg            .238
conc. in root crop         µg/kg            .284
concentration in meat      µg/kg            1.18E-04
conc. in milk fat          µg/kg            9.40E-04
concentration in fish      µg/kg            2.55

Human exposure assessment for adults

intake by inhalation           1.84E-04  mg/kg/day
intake by drinking water       3.84E-05  mg/kg/day
intake by vegetables           2.31E-06  mg/kg/day
intake by cereals              1.31E-06  mg/kg/day
intake by fish                 1.28E-06  mg/kg/day
intake by potatoes             1.11E-06  mg/kg/day
intake by meat                 5.21E-10  mg/kg/day
intake by cheese               1.64E-10  mg/kg/day
intake by butter               1.50E-10  mg/kg/day
intake by milk/yoghurt         1.47E-10  mg/kg/day

Predicted intake               2.28E-04  mg/kg/day


Human exposure assessment for children

intake by inhalation           3.68E-04  mg/kg/day
intake by drinking water       7.74E-05  mg/kg/day
intake by vegetables           4.12E-06  mg/kg/day
intake by cereals              3.24E-06  mg/kg/day
intake by potatoes             1.96E-06  mg/kg/day
intake by fish                 1.53E-06  mg/kg/day
intake by meat                 8.16E-10  mg/kg/day
intake by cheese               7.05E-10  mg/kg/day
intake by milk/yoghurt         6.20E-10  mg/kg/day
intake by butter               6.02E-10  mg/kg/day

Predicted intake               4.55E-04  mg/kg/day
```

C.3 CASE STUDY CYPERMETHRIN

Environmentally relevant input data on compound

```
name of substance                            cypermethrin
CAS number                                   52315-07-8
vapour pressure                   (Pascal)     1.9E-07
boiling point                           °C     0
water solubility                    (mg/l)     .009
log(octanol/water) part. coeff.                6.3
molecular mass                               416.3
melting point                           °C     80
environmental temperature               °C     15
degradation half life air          (hours)     1000
degradation half life water        (hours)     120
degradation half life soil         (hours)     3000
degradation half life sedim.       (hours)     1000
part. coeff. prim. sludge WWTP     (l/kg)      245000
part. coeff. sec. sludge WWTP      (l/kg)      303000
part. coeff. susp. part./w         (l/kg)      81800
part. coeff. sediment/water        (l/kg)      40900
part. coeff. soil/water            (l/kg)      40900
part. coeff. fish/water            (l/kg)      99800
part. coeff. earthworm/water       (l/kg)      55100
```

Data on prod. volume and use pattern of cypermethrin

```
Production/Use in kg/hour                      11
                                                          type of main
                                             fraction      use    prod
Agricultural chemicals                         .95           7      4
Chemicals personal & household use            .05           7      4
```

Environmental release pattern of cypermethrin

```
Production volume kg/h                         11

Release by production                          .0771
Release by compounding                         .044
Release by commercial use                      10.4
Release by private use                         .277
Release by recovery                            0

Release to air                                 1.05
Release to waste water                         .0687
Release to surface water                       1.04
Release to soil                                8.64
Release to waste                               0

Total release                                  10.8
```

input data on waste water treatment plant

```
discharged compound is cypermethrin

number of inhabitant equivalents               3.5E+08
waste water/inhabitant/day (l/day)             200
concentration of primary sludge (g/l)          .22
O.C.-content of primary sludge (w/w)           .3
hydraulic retention time (hours)               7
sludge retention time (hours)                  216
sludge conc. aeration tank (g/l)               2.5
O.C.-content of secondary sludge (w/w)         .37
sludge conc. effluent (mg/l)                   40
```

```
discharge of compound in kg/hour        .0687
biodegradation rate (1/h)               .01
µmax Monod-kinetics (1/h)               1.5
Michaelis-Menten constant (mg/l)        .5
biodegr. in adsorbed state (y/n)       y
```

Fate of compound cypermethrin in WWTP (Namkung & Rittmann 1987)

```
total influent concentration (mg/l)         2.36E-05

effluent concentration (dissolved mg/l)     9.39E-08
effluent concentration (suspended mg/l)     1.14E-06

amount biodegraded per hour (kg)            1.34E-02
amount volatilized per hour (kg)            5.03E-09
removed via primary sludge per hour (kg)    4.50E-02
removed via second. sludge per hour (kg)    6.72E-03
removed via effl./hour (dissolved kg)       2.74E-04
removed via effl./hour (suspended kg)       3.32E-03

primary sludge production per hour (kg)     428000
second. sludge production per hour (kg)     236000

comp. conc. in primary sludge (mg/kg)       .105
comp. conc. in second. sludge (mg/kg)       2.84E-02

percentage removal by primary sludge        65.5
percentage removal by biodegradation        19.6
percentage total removal                    94.8
```

Emission rates to regional environmental compartments of cypermethrin

```
Advective residence time air (h)        85.5
Advective residence time water (h)      1100

Direct emission to air (kg/h)           1.05
Direct emission to water (kg/h)         1.04
Direct emiss. to arable soil (kg/h)     8.64

WWTP emission to air (kg/h)             5.03E-09
WWTP emission to water (kg/h)           3.59E-03
WWTP emission to arable soil (kg/h)     5.17E-02
```

Mackay level 3 calculation on cypermethrin

```
Steady state mass in area   (kg)        43200
Mass % in air                           7.82E-02
Mass % in water dissolved               3.59E-02
Mass % in water suspended               4.41E-02
Mass % in arable soil                   93.3
Mass % in natural soil                  3.80
Mass % in sediment                      2.73
Mass % in fish                          3.58E-03

Overall residence time   h              3870
Degradation residence time  h           4020
Advection residence time h              100000

Air conc µg/m3                          1.43E-05
Dissolved water conc mg/litre           1.68E-07
Suspended water conc mg/litre           2.06E-07
Arable soil conc ppm                    9.27E-05
Natural soil conc ppm                   2.47E-05
```

```
Sediment conc ppm                               10.0E-04
Susp.solids conc ppm                            1.37E-02
Fish conc ppm                                   1.68E-02
```

Concentration in regional environmental compartments and in biota of cypermethrin

```
concentration in air      µg/m3             1.43E-05
diss.conc. surface water  µg/l              1.68E-04
conc. in arable soil      µg/kg             9.27E-02
conc. in natural soil     µg/kg             2.47E-02
diss.conc. groundwater    µg/l              1.79E-06
diss.conc. drinking water µg/l              4.20E-05
conc. in vegetables       µg/kg             .105
conc. in root crop        µg/kg             6.10E-04
concentration in meat     µg/kg             .403
conc. in milk fat         µg/kg             3.20
concentration in fish     µg/kg             16.8
```

Human exposure assessment for adults

```
intake by fish                  8.38E-06  mg/kg/day
intake by meat                  1.77E-06  mg/kg/day
intake by vegetables            1.02E-06  mg/kg/day
intake by cereals               5.76E-07  mg/kg/day
intake by cheese                5.60E-07  mg/kg/day
intake by butter                5.12E-07  mg/kg/day
intake by milk/yoghurt          4.99E-07  mg/kg/day
intake by inhalation            4.28E-09  mg/kg/day
intake by potatoes              2.38E-09  mg/kg/day
intake by drinking water        1.26E-09  mg/kg/day

Predicted intake                1.33E-05  mg/kg/day
```

Human exposure assessment for children

```
intake by fish                  1.01E-05  mg/kg/day
intake by meat                  2.78E-06  mg/kg/day
intake by cheese                2.40E-06  mg/kg/day
intake by milk/yoghurt          2.11E-06  mg/kg/day
intake by butter                2.05E-06  mg/kg/day
intake by vegetables            1.81E-06  mg/kg/day
intake by cereals               1.43E-06  mg/kg/day
intake by inhalation            8.57E-09  mg/kg/day
intake by potatoes              4.21E-09  mg/kg/day
intake by drinking water        2.52E-09  mg/kg/day

Predicted intake                2.26E-05  mg/kg/day
```

C.4 CASE STUDY LAS

Environmentally relevant input data on compound

```
name of substance                      LAS
CAS number
vapour pressure              (Pascal)   1E-10
boiling point                     °C    400
water solubility               (mg/l)   350
log(octanol/water) part. coeff.         2.5
molecular mass                         347
melting point                     °C    10
environmental temperature         °C    20
degradation half life air     (hours)   20
degradation half life water   (hours)   35
degradation half life soil    (hours)   350
degradation half life sedim.  (hours)   17
part. coeff. prim. sludge WWTP (l/kg)   2800
part. coeff. sec. sludge WWTP  (l/kg)   2800
part. coeff. susp. part./w     (l/kg)   1000
part. coeff. sediment/water    (l/kg)   1000
part. coeff. soil/water        (l/kg)   1000
part. coeff. fish/water        (l/kg)   30
part. coeff. earthworm/water   (l/kg)   10
```

Data on prod. volume and use pattern of LAS

```
Production/Use in kg/hour               29300

                                                   type of main
                                      fraction      use   prod

Chemicals public areas -detergents-     1             7     4
```

Environmental release pattern of LAS

```
Production volume kg/h                  29300

Release to air                          0
Release to waste water                  29300
Release to surface water                0
Release to soil                         0
Release to waste                        0

Total release                           29300
```

input data on waste water treatment plant

```
discharged compound is LAS

number of inhabitant equivalents        3.5E+08
waste water/inhabitant/day (l/day)      200
concentration of primary sludge (g/l)   .22
O.C.-content of primary sludge (w/w)    .3
hydraulic retention time (hours)        7
sludge retention time (hours)           216
sludge conc. aeration tank (g/l)        2.5
O.C.-content of secondary sludge (w/w)  .37
sludge conc. effluent (mg/l)            40
discharge of compound in kg/hour        29300
biodegradation rate (l/h)               .041
µmax Monod-kinetics (l/h)               1.5
Michaelis-Menten constant (mg/l)        .5
biodegr. in adsorbed state (y/n)       y
```

Fate of compound LAS in WWTP (Cowan *et al*, 1992)

total influent concentration (mg/l)	10.0
effluent concentration (dissolved mg/l)	1.85E-02
effluent concentration (suspended mg/l)	2.07E-03
amount biodegraded per hour (kg)	21700
amount volatilized per hour (kg)	1.12E-11
removed via primary sludge per hour (kg)	7430
removed via second. sludge per hour (kg)	12.2
removed via effl./hour (dissolved kg)	53.9
removed via effl./hour (suspended kg)	6.04
primary sludge production per hour (kg)	428000
second. sludge production per hour (kg)	236000
comp. conc. in primary sludge (mg/kg)	17400
comp. conc. in second. sludge (mg/kg)	51.8
percentage removal by primary sludge	25.4
percentage removal by biodegradation	74.3
percentage total removal	99.8

Emission rates to regional environmental compartments of LAS

Advective residence time air (h)	85.5
Advective residence time water (h)	1100
WWTP emission to air (kg/h)	1.12E-11
WWTP emission to water (kg/h)	60.0
WWTP emission to arable soil (kg/h)	7450

Mackay level 3 calculation on LAS

Steady state mass in area (kg)	3760000
Mass % in air	6.69E-14
Mass % in water dissolved	7.43E-02
Mass % in water suspended	1.12E-03
Mass % in arable soil	99.9
Mass % in natural soil	0
Mass % in sediment	1.51E-03
Mass % in fish	2.23E-06
Overall residence time h	501
Degradation residence time h	501
Advection residence time h	1460000
Air conc µg/m3	1.06E-15
Dissolved water conc mg/litre	3.03E-05
Suspended water conc mg/litre	4.55E-07
Arable soil conc ppm	8.65E-03
Natural soil conc ppm	0
Sediment conc ppm	4.82E-05
Susp.solids conc ppm	3.03E-02
Fish conc ppm	9.09E-04

Concentration in regional environmental compartments and in biota of LAS

concentration in air	µg/m3	1.06E-15
diss.conc. surface water	µg/l	3.03E-02
conc. in arable soil	µg/kg	8.66
conc. in natural soil	µg/kg	0
diss.conc. groundwater	µg/l	5.41E-03

```
diss.conc. drinking water µg/l          3.03E-02
conc. in vegetables       µg/kg         2.01E-02
conc. in root crop        µg/kg         1.16E-02
concentration in meat     µg/kg         6.57E-05
conc. in milk fat         µg/kg         5.22E-04
concentration in fish     µg/kg         .910
```

Human exposure assessment for adults

```
intake by drinking water      9.11E-07  mg/kg/day
intake by fish                4.55E-07  mg/kg/day
intake by vegetables          1.95E-07  mg/kg/day
intake by cereals             1.11E-07  mg/kg/day
intake by potatoes            4.54E-08  mg/kg/day
intake by meat                2.89E-10  mg/kg/day
intake by cheese              9.12E-11  mg/kg/day
intake by butter              8.34E-11  mg/kg/day
intake by milk/yoghurt        8.13E-11  mg/kg/day
intake by inhalation          3.19E-19  mg/kg/day

Predicted intake              1.72E-06  mg/kg/day
```

Human exposure assessment for children

```
intake by drinking water      1.82E-06  mg/kg/day
intake by fish                5.46E-07  mg/kg/day
intake by vegetables          3.48E-07  mg/kg/day
intake by cereals             2.73E-07  mg/kg/day
intake by potatoes            8.01E-08  mg/kg/day
intake by meat                4.53E-10  mg/kg/day
intake by cheese              3.91E-10  mg/kg/day
intake by milk/yoghurt        3.44E-10  mg/kg/day
intake by butter              3.34E-10  mg/kg/day
intake by inhalation          6.38E-19  mg/kg/day

Predicted intake              3.07E-06  mg/kg/day
```

C.5 CASE STUDY BHT

Environmentally relevant input data on compound

```
name of substance                           BHT
CAS number                                  128-37-0
vapour pressure                 (Pascal)     .3
boiling point                         °C     265
water solubility                  (mg/l)     .66
log(octanol/water) part. coeff.              4.6
molecular mass                              220
melting point                         °C     70
environmental temperature             °C     20
degradation half life air      (hours)       17
degradation half life water    (hours)       240
degradation half life soil     (hours)       133
degradation half life sedim.   (hours)       120
part. coeff. prim. sludge WWTP (l/kg)        4900
part. coeff. sec. sludge WWTP  (l/kg)        6040
part. coeff. susp. part./w     (l/kg)        1630
part. coeff. sediment/water    (l/kg)        816
part. coeff. soil/water        (l/kg)        816
part. coeff. fish/water        (l/kg)        1990
part. coeff. earthworm/water   (l/kg)        835
```

Data on prod. volume and use pattern of BHT

```
Production/Use in kg/hour                    2000

                                                         type of main
                                             fraction     use   prod
Fuel and fuel additives                        .1          7      2
Chemicals used in polymers                     .5          5      2
Others                                         .4          5      2
```

Environmental release pattern of BHT

```
Production volume kg/h                       2000

Release by production                        1.02
Release by compounding                       4
Release by commercial use                    19.8
Release by private use                       .160
Release by recovery                          0

Release to air                               11.8
Release to waste water                       3.00
Release to surface water                     .020
Release to soil                              10.1
Release to waste                             0

Total release                                24.9
```

input data on waste water treatment plant

```
discharged compound is BHT

number of inhabitant equivalents             3.5E+08
waste water/inhabitant/day (l/day)           200
concentration of primary sludge (g/l)        .22
O.C.-content of primary sludge (w/w)         .3
hydraulic retention time (hours)             7
sludge retention time (hours)                216
sludge conc. aeration tank (g/l)             2.5
```

```
O.C.-content of secondary sludge (w/w)  .37
sludge conc. effluent (mg/l)            40
discharge of compound in kg/hour        3.00
biodegradation rate (1/h)               3
µmax Monod-kinetics (1/h)               1.5
Michaelis-Menten constant (mg/l)        .5
biodegr. in adsorbed state (y/n)      n
```

Fate of compound BHT in WWTP (Namkung & Rittmann, 1987)

```
total influent concentration (mg/l)          1.028E-03

effluent concentration (dissolved mg/l)      3.15E-05
effluent concentration (suspended mg/l)      7.60E-06

amount biodegraded per hour (kg)             1.78
amount volatilized per hour (kg)             1.92E-02
removed via primary sludge per hour (kg)     1.04
removed via second. sludge per hour (kg)     4.49E-02
removed via effl./hour (dissolved kg)        9.18E-02
removed via effl./hour (suspended kg)        2.22E-02

primary sludge production per hour (kg)      428000
second. sludge production per hour (kg)      236000

comp. conc. in primary sludge (mg/kg)        2.42
comp. conc. in second. sludge (mg/kg)        .190

percentage removal by primary sludge         34.6
percentage removal by biodegradation         59.5
percentage total removal                     96.2
```

Emission rates to regional environmental compartments of BHT

```
Advective residence time air (h)        85.5
Advective residence time water (h)      1100

Direct emission to air (kg/h)           11.8
Direct emission to water (kg/h)         .020
Direct emiss. to arable soil (kg/h)     10.1

WWTP emission to air (kg/h)             1.92E-02
WWTP emission to water (kg/h)           .114
WWTP emission to arable soil (kg/h)     1.08
```

Mackay level 3 calculation on BHT

```
Steady state mass in area   (kg)        2390
Mass % in air                           9.52
Mass % in water dissolved               .310
Mass % in water suspended               7.59E-03
Mass % in arable soil                   90.1
Mass % in natural soil                  .018
Mass % in sediment                      6.98E-02
Mass % in fish                          6.17E-04

Overall residence time   h              103
Degradation residence time  h           116
Advection residence time h              895

Air conc µg/m3                          9.60E-05
Dissolved water conc mg/litre           8.02E-08
Suspended water conc mg/litre           1.96E-09
Arable soil conc ppm                    4.94E-06
Natural soil conc ppm                   6.45E-09
```

```
Sediment conc ppm                       1.41E-06
Susp.solids conc ppm                    1.31E-04
Fish conc ppm                           1.60E-04
```

Concentration in regional environmental compartments and in biota of BHT

```
concentration in air      µg/m3         9.60E-05
diss.conc. surface water  µg/l          8.02E-05
conc. in arable soil      µg/kg         4.94E-03
conc. in natural soil     µg/kg         6.45E-06
diss.conc. groundwater    µg/l          3.79E-06
diss.conc. drinking water µg/l          4.01E-05
conc. in vegetables       µg/kg         9.81E-04
conc. in root crop        µg/kg         8.59E-05
concentration in meat     µg/kg         9.21E-05
conc. in milk fat         µg/kg         7.31E-04
concentration in fish     µg/kg         .1595582
```

Human exposure assessment for adults

```
intake by fish                7.98E-08  mg/kg/day
intake by inhalation          2.88E-08  mg/kg/day
intake by vegetables          9.51E-09  mg/kg/day
intake by cereals             5.39E-09  mg/kg/day
intake by drinking water      1.20E-09  mg/kg/day
intake by meat                4.05E-10  mg/kg/day
intake by potatoes            3.35E-10  mg/kg/day
intake by cheese              1.28E-10  mg/kg/day
intake by butter              1.17E-10  mg/kg/day
intake by milk/yoghurt        1.14E-10  mg/kg/day

Predicted intake              1.26E-07  mg/kg/day
```

Human exposure assessment for children

```
intake by fish                9.57E-08  mg/kg/day
intake by inhalation          5.76E-08  mg/kg/day
intake by vegetables          1.70E-08  mg/kg/day
intake by cereals             1.33E-08  mg/kg/day
intake by drinking water      2.40E-09  mg/kg/day
intake by meat                6.35E-10  mg/kg/day
intake by potatoes            5.93E-10  mg/kg/day
intake by cheese              5.49E-10  mg/kg/day
intake by milk/yoghurt        4.83E-10  mg/kg/day
intake by butter              4.68E-10  mg/kg/day

Predicted intake              1.89E-07  mg/kg/day
```

C.6 CASE STUDY DEHP

Environmentally relevant input data on compound

name of substance		DEHP
CAS number		117-82-7
vapour pressure	(Pascal)	.000022
boiling point	°C	370
water solubility	(mg/l)	.041
log(octanol/water) part. coeff.		4.88
molecular mass		390
melting point	°C	-46
environmental temperature	°C	20
degradation half life air	(hours)	24
degradation half life water	(hours)	720
degradation half life soil	(hours)	1025
degradation half life sedim.	(hours)	4500
part. coeff. prim. sludge WWTP	(l/kg)	9330
part. coeff. sec. sludge WWTP	(l/kg)	11500
part. coeff. susp. part./w	(l/kg)	3110
part. coeff. sediment/water	(l/kg)	1560
part. coeff. soil/water	(l/kg)	1560
part. coeff. fish/water	(l/kg)	3790
part. coeff. earthworm/water	(l/kg)	1670

Environmental release pattern of DEHP

Production volume kg/h	50000

		type of main	
	fraction	use	prod
Chemicals used in polymers	1	5	2

Release to air	62.1
Release to waste water	28.5
Release to surface water	348
Release to soil	2.28
Total release	440.88

input data on waste water treatment plant

discharged compound is DEHP

number of inhabitant equivalents	3.5E+08
waste water/inhabitant/day (l/day)	200
concentration of primary sludge (g/l)	.22
O.C.-content of primary sludge (w/w)	.3
hydraulic retention time (hours)	7
sludge retention time (hours)	216
sludge conc. aeration tank (g/l)	2.5
O.C.-content of secondary sludge (w/w)	.37
sludge conc. effluent (mg/l)	40
discharge of compound in kg/hour	28.5
biodegradation rate (l/h)	3
μmax Monod-kinetics (l/h)	1.5
Michaelis-Menten constant (mg/l)	.5
biodegr. in adsorbed state (y/n)	n

Fate of compound DEHP in WWTP (Namkung & Rittmann, 1987)

total influent concentration (mg/l)	9.77E-03
effluent concentration (dissolved mg/l)	2.47E-04

```
effluent concentration (suspended mg/l)      1.14E-04

amount biodegraded per hour (kg)             14.0
amount volatilized per hour (kg)             3.15E-04
removed via primary sludge per hour (kg)     12.8
removed via second. sludge per hour (kg)     .672
removed via effl./hour (dissolved kg)        .721
removed via effl./hour (suspended kg)        .332

primary sludge production per hour (kg)      428000
second. sludge production per hour (kg)      236000

comp. conc. in primary sludge (mg/kg)        29.9
comp. conc. in second. sludge (mg/kg)        2.84

percentage removal by primary sludge         44.8
percentage removal by biodegradation         49.1
percentage total removal                     96.3
```

Emission rates to regional environmental compartments of DEHP

```
Advective residence time air (h)         85.5
Advective residence time water (h)       1100

Direct emission to air (kg/h)            62.1
Direct emission to water (kg/h)          348
Direct emiss. to arable soil (kg/h)      2.28

WWTP emission to air (kg/h)              3.15E-04
WWTP emission to water (kg/h)            1.05
WWTP emission to arable soil (kg/h)      13.4
```

Mackay level 3 calculation on DEHP

```
Steady state mass in area   (kg)         1004000
Mass % in air                            .136
Mass % in water dissolved                10.5
Mass % in water suspended                .490
Mass % in arable soil                    5.45
Mass % in natural soil                   1.92
Mass % in sediment                       81.5
Mass % in fish                           3.98E-02

Overall residence time   h               2280
Degradation residence time   h           3120
Advection residence time h               8490

Air conc µg/m3                           5.76E-04
Dissolved water conc mg/litre            1.14E-03
Suspended water conc mg/litre            5.33E-05
Arable soil conc ppm                     1.26E-04
Natural soil conc ppm                    2.90E-04
Sediment conc ppm                        .692
Susp.solids conc ppm                     3.55
Fish conc ppm                            4.33
```

Concentration in regional environmental compartments and in biota of DEHP

```
concentration in air       µg/m3         5.76E-04
diss.conc. surface water   µg/l          1.14
conc. in arable soil       µg/kg         .126
conc. in natural soil      µg/kg         .290
diss.conc. groundwater     µg/l          1.67E-04
```

```
diss.conc. drinking water µg/l          .571
conc. in vegetables       µg/kg         .789
conc. in root crop        µg/kg         1.83E-03
concentration in meat     µg/kg         .175
conc. in milk fat         µg/kg         1.39
concentration in fish     µg/kg         4330
```

Human exposure assessment for adults

```
intake by fish                2.17E-03  mg/kg/day
intake by drinking water      1.71E-05  mg/kg/day
intake by vegetables          7.66E-06  mg/kg/day
intake by cereals             4.34E-06  mg/kg/day
intake by meat                7.68E-07  mg/kg/day
intake by cheese              2.43E-07  mg/kg/day
intake by butter              2.22E-07  mg/kg/day
intake by milk/yoghurt        2.16E-07  mg/kg/day
intake by inhalation          1.73E-07  mg/kg/day
intake by potatoes            7.15E-09  mg/kg/day

Predicted intake              2.20E-03  mg/kg/day
```

Human exposure assessment for children

```
intake by fish                2.60E-03  mg/kg/day
intake by drinking water      3.43E-05  mg/kg/day
intake by vegetables          1.37E-05  mg/kg/day
intake by cereals             1.07E-05  mg/kg/day
intake by meat                1.20E-06  mg/kg/day
intake by cheese              1.04E-06  mg/kg/day
intake by milk/yoghurt        9.15E-07  mg/kg/day
intake by butter              8.87E-07  mg/kg/day
intake by inhalation          3.45E-07  mg/kg/day
intake by potatoes            1.26E-08  mg/kg/day

Predicted intake              2.66E-03  mg/kg/day
```

C.7 CASE STUDY BENZENE

Environmentally relevant input data on compound

```
name of substance                         benzene
CAS number                                71-43-2
vapour pressure                (Pascal)    11000
boiling point                        °C    75
water solubility                 (mg/l)    1800
log(octanol/water) part. coeff.            2.13
molecular mass                           78
melting point                        °C    5.5
environmental temperature            °C    20
degradation half life air       (hours)    134
degradation half life water     (hours)    570
degradation half life soil      (hours)    215
degradation half life sedim.    (hours)    1700
part. coeff. prim. sludge WWTP  (l/kg)     16.6
part. coeff. sec. sludge WWTP   (l/kg)     20.5
part. coeff. susp. part./w      (l/kg)     5.53
part. coeff. sediment/water     (l/kg)     2.77
part. coeff. soil/water         (l/kg)     2.77
part. coeff. fish/water         (l/kg)     6.74
part. coeff. earthworm/water    (l/kg)     1.90
```

Data on prod. volume and use pattern of benzene

```
Production/Use in kg/hour                  1800000

                                                       type of main
                                         fraction       use   prod
Fuel and fuel additives                    .5            7     2
Chemicals as intermediates                 .5            2     2
```

Environmental release pattern of benzene

```
Production volume kg/h                     1800000

Release to air                             22000
Release to waste water                     688
Release to surface water                   0
Release to soil                            115
Release to waste                           0

Total release                              22800
```

input data on waste water treatment plant

```
discharged compound is benzene

number of inhabitant equivalents           3.5E+08
waste water/inhabitant/day (l/day)         200
concentration of primary sludge (g/l)      .22
O.C.-content of primary sludge (w/w)       .3
hydraulic retention time (hours)           7
sludge retention time (hours)              216
sludge conc. aeration tank (g/l)           2.5
O.C.-content of secondary sludge (w/w)     .37
sludge conc. effluent (mg/l)               40
discharge of compound in kg/hour           688
biodegradation rate (1/h)                  .3
µmax Monod-kinetics (1/h)                  1.5
```

```
Michaelis-Menten constant (mg/l)        .5
biodegr. in adsorbed state (y/n)       n
```

Fate of compound benzene in WWTP
(Namkung & Rittmann 1987)

```
total influent concentration (mg/l)          .236

effluent concentration (dissolved mg/l)      5.97E-02
effluent concentration (suspended mg/l)      4.89E-05

amount biodegraded per hour (kg)             338
amount volatilized per hour (kg)             173
removed via primary sludge per hour (kg)     1.67
removed via second. sludge per hour (kg)     .289
removed via effl./hour (dissolved kg)        174
removed via effl./hour (suspended kg)        .143

primary sludge production per hour (kg)      428000
second. sludge production per hour (kg)      236000

comp. conc. in primary sludge (mg/kg)        3.90
comp. conc. in second. sludge (mg/kg)        1.22

percentage removal by primary sludge         .242
percentage removal by biodegradation         49.2
percentage total removal                     74.7
```

Emission rates to regional environmental compartments
of Benzene

```
Advective residence time air (h)         85.5
Advective residence time water (h)       1100
Direct emission to air (kg/h)            22000
Direct emiss. to arable soil (kg/h)      115
WWTP emission to air (kg/h)              173
WWTP emission to water (kg/h)            174
WWTP emission to arable soil (kg/h)      1.96
```

Mackay level 3 calculation on benzene

```
Steady state mass in area   (kg)         1350000
Mass % in air                            98.1
Mass % in water dissolved                .738
Mass % in water suspended                6.12E-05
Mass % in arable soil                    1.14
Mass % in natural soil                   3.03E-02
Mass % in sediment                       1.34E-02
Mass % in fish                           4.98E-06

Overall residence time   h               60.2
Degradation residence time  h            195
Advection residence time h               87.1

Air conc µg/m3                           .561
Dissolved water conc mg/litre            1.08E-04
Suspended water conc mg/litre            8.98E-09
Arable soil conc ppm                     3.56E-05
Natural soil conc ppm                    6.16E-06
Sediment conc ppm                        1.54E-04
Susp.solids conc ppm                     5.98E-04
Fish conc ppm                            7.30E-04
```

Concentration in regional environmental compartments and in biota of benzene

```
concentration in air       µg/m3          .561
diss.conc. surface water   µg/l           .108
conc. in arable soil       µg/kg          3.56E-02
conc. in natural soil      µg/kg          6.16E-03
diss.conc. groundwater     µg/l           8.57E-03
diss.conc. drinking water  µg/l           .054
conc. in vegetables        µg/kg          2.53E-02
conc. in root crop         µg/kg          1.39E-02
concentration in meat      µg/kg          2.49E-04
conc. in milk fat          µg/kg          1.98E-03
concentration in fish      µg/kg          .730
```

Human exposure assessment for adults

```
intake by inhalation           1.68E-04  mg/kg/day
intake by drinking water       1.62E-06  mg/kg/day
intake by fish                 3.65E-07  mg/kg/day
intake by vegetables           2.46E-07  mg/kg/day
intake by cereals              1.39E-07  mg/kg/day
intake by potatoes             5.42E-08  mg/kg/day
intake by meat                 1.10E-09  mg/kg/day
intake by cheese               3.46E-10  mg/kg/day
intake by butter               3.16E-10  mg/kg/day
intake by milk/yoghurt         3.09E-10  mg/kg/day

Predicted intake               1.71E-04  mg/kg/day
```

Human exposure assessment for children

```
intake by inhalation           3.37E-04  mg/kg/day
intake by drinking water       3.25E-06  mg/kg/day
intake by vegetables           4.38E-07  mg/kg/day
intake by fish                 4.38E-07  mg/kg/day
intake by cereals              3.45E-07  mg/kg/day
intake by potatoes             9.59E-08  mg/kg/day
intake by meat                 1.72E-09  mg/kg/day
intake by cheese               1.48E-09  mg/kg/day
intake by milk/yoghurt         1.31E-09  mg/kg/day
intake by butter               1.27E-09  mg/kg/day

Predicted intake               3.41E-04  mg/kg/day
```

APPENDIX D BODY SURFACE AREAS FOR CHILDREN (EPA, 1989)

Table D.1 Median Total Body Surface Area (m^2)

Age (year)	Male	Female
3 < 6	0.728	0.711
6 < 9	0.931	0.919
9 < 12	1.16	1.16
12 < 15	1.49	1.48
15 < 18	1.75	1.60

Table D.2 Percentage of Total Body Surface Area by Part of Body

Age (year)	Head	Trunk	Arms	Hands	Legs	Feet
< 1	18.2	35.7	13.7	5.3	20.6	6.54
3 < 4	13.6	31.9	14.4	6.07	26.8	7.21
6 < 7	13.1	35.1	13.1	4.71	27.1	6.90
9 < 10	12.0	34.2	12.3	5.30	28.7	7.58
12 < 13	8.74	34.7	13.7	5.39	30.5	7.03
17 < 18	7.58	31.7	17.5	5.13	30.8	7.28

BIBLIOGRAPHY

AIS (1993). Unpublished data. Association Internationale de la Savonnerie et de la Detergence, Brussels.

Andelman, J.B. (1985). Inhalation exposure in the home to volatile organic contaminants of drinking water. The Science of the Total Environment 47, 443-460.

Bacci, E., Calamari, D., Gaggi, C. and Viyhi, M. (1990). Bioconcentration of organic chemical vapors in plant leaves: experimental measurements and correlation. Environ. Sci. Technol. 24, 885-889.

Bjerre, A. (1989). Assessing exposure to solvent vapour during the application of paints etc. Model calculations versus common sense. Annals of Occupational Hygiene 33 (4), 507-517.

Braat, L., Bakema, A.H., de Boer, K.F., Kok, R.M., Meijers, R. and van Minnen, J.G. (1991). EXPECT: outline of an integrated model for environmental scenario analysis and impact assessment, National Institute of Public Health and Environmental Protection (RIVM), Report No. 259102001, Bilthoven.

Briggs, G.G., Bromilow, R.H. and Evans, A.A. (1982). Relationships between lipophilicity and root uptake and translocation of non-ionised chemicals by barley. Pestic. Sci. 13, 495-504.

Briggs, G.G., Bromilow, R.H. Evans, A.A. and Williams, M. (1983). Relationships between lipophilicity and the distribution of non-ionised chemicals in barley shoots following uptake by roots. Pestic. Sci. 14, 492-500.

BUA (1991). Beratergremium für umweltrelevante Altstoffe. Butylhydroxytoluol. Stoffbericht 58, Weinheim.

CMA (1989). How to comply with proposition 65: DEHP exposure. Chemical Manufacturers Association, Washington, DC.

COLIPA (1993). Document 93/067, unpublished. Brussels.

De Nijs, A.C.M., C. Toet, T.G. Vermeire, P. van der Poel and J. Tuinstra (1992). Dutch Risk Assessment of New Chemicals "DRANC". Sci. Total Environ., submitted.

De Nijs, A.C.M. and T.G. Vermeire (1990). Soil-plant and plant-mammal transfer factors. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 670203001.

ECETOC (1992a). Estimating environmental concentrations of chemicals using fate and exposure models. Technical Report No. 50.

ECETOC (1992b). Hazard assessment of chemical contaminants in soil. Technical Report No. 40 and Revised 'Appendix 3'.

ECETOC (1993a). Environmental Hazard Assessment of Substances. Technical Report No. 51.

ECETOC (1993b). Percutaneous absorption. Monograph No. 20.

ECETOC (1994a). Environmental exposure assessment. Technical Report No. XX.

ECETOC (1994b). HAZCHEM, a mathematical model for use in risk assessment of substances. Special Report, in preparation.

ECPI (1994). Medical applications of plasticised PVC. European Council for Plasticisers & Intermediates, Brussels, in preparation.

EEC (1992). Council Directive 92/32/EEC of 30 April 1992 amending for the 7th time Council Directive 67/548/EEC on the approximation of laws, regulations and administrative provisions relating to the classification, packaging and labelling of substances ("7th Amendment"). Off. J. of the European Communities L 154/1.

EEC (1993). Council Regulation 793/93 of 23 March 1993 on the evaluation and control of the risks of existing substances. Off. J. of the European Communities L 84/1.

EPA (1989). Exposure factors handbook. Office of Health and Environmental Assessment, Exposure Assessment Group, US Environmental Protection Agency, EPA/600/8-89/043, PB90-106774. Washington, DC.

Euromonitor, European Marketing Data and Statistics 1992, ISBN: 0 86338 403 X, © Euromonitor Plc 1992.

FLUSH (1992). User's Manual. Final Draft Report prepared for the U.S. Environmental Protection Agency, Exposure Evaluation Division, Office of Pollution Prevention and Toxics by: Versar Inc., 6580 Versar Center, Springfield, Virginia 22151, January 14, 1992.

Furtmann, K. (1993). Phthalate in der aquatischen Umwelt. LWA-Materialien Nr. 6/93, Landesamt für Wasser und Abfall Nordrhein-Westfalen, Düsseldorf.

Hakkinen, P.J., Kelling, C.K. and Callender, J.C. (1991). Exposure assessment of consumer products: human body weights and total body surface areas to use, and sources of data for specific products. Vet. Hum. Toxicol. 33 (1), 61-65.

Hakkinen, P.J. (1993). Cleaning and laundry products, human exposure assessments. In: Handbook of Hazardous Materials, Academic Press Inc., pp. 145-151.

Hartop, P.J., Cook, T.L. and Adams, M.G. (1991). Simulated consumer exposure to dimethylether and propane/butane in hairsprays. International Journal of Cosmetic Science 13, 161-167.

House, W.A., Farr, I.S. and Orr, D.R. (1991). Pesticides in soils and water. BCPC Monograph, pp. 183-192.

Howes, D. (1975). The percutaneous absorption of some anionic surfactants. J. Soc. Cosmet. Chemists, 26, 47-63.

Hrubec, J. and Toet, C. (1992). Predictability of the removal of organic compounds by drinking water treatment. RIVM report No. 714301007.

IARC (1982). International Agency for Research on Cancer, Some industrial chemicals and dyestuffs. Monograph Vol. 29, Lyon.

IARC (1986). International Agency for Research on Cancer, Some naturally occurring and synthetic food components, furocoumarins and ultraviolet radiation. Monograph Vol. 40, Lyon.

IPCS (1989). International Programme on Chemical Safety. Environmental Health Criteria 82, Cypermethrin. Geneva.

IPCS (1992a). International Programme on Chemical Safety. Environmental Health Criteria 142, Alpha-cypermethrin. Geneva.

IPCS (1992b). International Programme on Chemical Safety. Environmental Health Criteria 131, Diethylhexyl phthalate. Geneva.

IPCS (1993a). International Programme on Chemical Safety. Environmental Health Criteria for methylene chloride. Draft Report WHO/IPS/93.12, Geneva.

IPCS (1993b). International Programme on Chemical Safety. Environmental Health Criteria 150, Benzene. Geneva.

Kasting, G.B. and Robinson, P.J. (1993). Can we assign an upper limit to skin permeability? Pharmaceutical Research, 10 (6), 930-931.

Legrand, M.F., Costentin, E. and Bruchet, A. (1991). Occurence of 38 pesticides in various French surface and ground waters. Environ. Technol. 12 (11), 985-996.

Linders, J.B.H.J. (1990). Risicobeordeling voor de mens bij blootstelling aan stoffen. Uitgangspunten en veronderstellingen (Risk assessment for man exposed to chemical substances. Principles and premises.) RIVM Report No. 725201003, Bilthoven.

Lotte, C., Rougier, A., Wilson, D.R. and Maibach, H.I. (1987). *In vivo* relationship between transepidermal water loss and percutaneous penetration of some organic compounds in man: effect of anatomic site. Arch. Dermatol. Res., 279, 351-356.

Mackay, D. (1979). Finding fugacity feasible. Environ. Sci. Technol., 13, 1218-1223.

Mackay, D. (1991). Multimedia Environmental Models: The fugacity approach. Lewis Publishers Inc., Chelsea, Mi. (ISBN 0-87371-242-0).

Mackay, D. and Paterson, S. (1982). Fugacity revisited. Environ. Sci. Technol. 16, 654-660.

Mackay, D., Paterson, S. and Tam, D.D. (1991). Assessments of chemical fate in Canada: continued development of a fugacity model. A report prepared for Health and Welfare Canada, Toronto, September 1991.

McKone Th.E. (1989). Household exposure models. Toxicology Letters 49, 321-339.

McKone, T.E. and Daniels, J.I. (1991). Estimating human exposure through multiple pathways from air, water, and soil. Reg. Toxicol. and Pharmacol., 13, 36-61.

McKone, Th.E. (1993). CalTOX, a multimedia total exposure model for hazardous-wastes sites. Report UCRL- CR-111456PtII, final draft. California Environmental Protection Agency, Sacramento, Ca., December 1993.

McKone, Th.E. and Howd, R.A. (1992). Estimating dermal uptake of nonionic organic chemicals from water and soil: I. Unified fugacity-based models for risk assessments. Risk Analysis 12 (4), 543-557.

McKone, Th.E. (1993). The precision of QSAR methods for estimating intermedia transfer factors in exposure assessments.

MNSEM. Multi-phase non-steady state equilibrium model, Version 1.4.5. Model information K. Yoshida, Mitsubishi-kasai Institute of Toxicological and Environmental Sciences, Japan.

NTP (1982). National Toxicology Program, NTP Technical Report on the carcinogenesis bioassay of di-(2-ethylhexyl) phthalate (CAS No. 117-81-7) in F 344 rats and B6C3F mice (feed study), NIH Publ. No. 82-1773, Washington, DC.

OECD (1989). Compendium of environmental exposure assessment methods for chemicals. OECD Environment Monographs, No 27, Paris.

OECD (1991). The OECD workshop on the application of simple models for environmental exposure assessment. 11 - 13 December 1991, Berlin.

OEDC (1993). Methylene chloride. Draft status report. Paris.

Opperhuizen, A. (1986). Bioconcentration of hydrophobic chemicals in fish. Aquatic Toxicology and Environmental Fate, 9th Vol., ASTM STP 921. Poston, T.M. and Purdy, R. (eds.), Philadelphia, pp. 304-315.

Paterson, S. and Mackay, D. (1989). Modeling the uptake and distribution of organic chemicals in plants. In: Intermedia Pollutant Transport: Modeling and Field Measurements, Allen, D.T., Cohen, Y. and Kaplan, I.R. (eds), Plenum Press, New York, NY, 283-292.

Riederer, M. (1990). Estimating partitioning and transport of organic chemicals in the foliage/atmosphere system: discussion of a fugacity-based model. Environ. Sci. Technol. 24, 829-837.

RIVM, VROM and WVC (1994). Uniform system for the evaluation of substances (USES), version 1.0. National Institute of Public Health and Environmental Protection (RIVM), Ministry of Spatial Planning and the Environment (VROM), Ministry of Welfare, Health and Cultural Affairs (WVC). The Hague. Distribution No. 11144/150.

SCIES (1991). Screening-Level Consumer Inhalation Exposure Software (SCIES): Description and User's Manual Version 3.0. Prepared for U.S. Environmental Protection Agency, Office of Toxic Substances, Exposure Evaluation Division, Exposure Assessment Branch by Versar Inc., 6580 Versar Center, Springfield, Virginia 22151, November 22, 1991.

Tokai, A., Kikuchi, M., Wakabayashi, M. and Yoshida, T. (1990). Environmental behavior of selected chemicals in Tokyo bay with relation to their physicochemical and biochemical properties. J. Chem. Soc. Japan, Chemistry and Industrial Chemistry (Nippon Kagaku Kaishi), 9, 982-991.

Travis, C.C. and Arms, A.D. (1988). Bioconcentration of Organics in Beef, Milk and Vegetation. Envir. Sci. and Technol. 22(3), 271-274.

Turnbull, D. and Rodricks, J.V. (1989). A comprehensive risk assessment of DEHP as a component of baby pacifiers, teethers, and toys. In: Paustenbach, D.J. (ed.), The risk assessment of environmental and human health hazards: A textbook of case studies. John Wiley & Sons, New York.

UK-MAFF (1987). Ministry of Agriculture, Fisheries and Food. Survey of plasticiser levels in food contact materials and in foods. Food Surveillance Paper No. 21, London.

Vermeire, T.G., van Iersel, A.A.J., de Leeuw, F.A.A.M., Peijnenburg, W.J.G.M., van der Poel, P., Taalman, R.D.F.M. and Toet, C. (1992). Initial assessment of the hazards and risks of new chemicals to man and the environment, National Institute of Public Health and Environmental Protection, Bilthoven, The Netherlands, Report No. 679102006 (January 1992).

Vermeire, T.G., van der Poel, P., van de Laar, R.T.H. and Roelfzema, H. (1993). Estimation of consumer exposure to chemicals: application of simple models. The Sci. of the Total Environ., 136, 155-176.

Voorlichtingsbureau voor de Voeding (1983). Nederlandse voedingsmiddelentabel - Aanbevolen hoeveelheden energie en voedingsstoffen, 's Gravenhage, The Netherlands, 34th Edition, September 1983.

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