NATIONAL INSTITUTE OF PUBLIC HEALTH AND ENVIRONMENTAL PROTECTION
BILTHOVEN, THE NETHERLANDS

Reportnr. 670203001

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Soil-plant and plant-mammal transfer factors

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June 1990

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Verzendlijst

CONTENTS

SUMMARY

In order to assess the lifetime hazard of ingestion exposure of man to new substances, the RIVM Assessment System for New Substances links environmental concentrations in water and soil to human exposure applying transfer factors. This report discusses indirect human exposure to new substances via consumption of fruits, vegetables, grains, meat, and dairy products. A limited validation study of the RIVM Assessment System for New Substances had previously shown that this part of the model needed further study with regard to the estimation of transfer factors. On the basis of an evaluation of recent research in this area, the present report proposes what is considered to be an improvement of the RIVM Assessment System for New Substances. Being aware of a persisting high degree of uncertainty in the model estimates, it is recommended to use the biotransfer factor correlations with K_{ow} as determined by Travis & Arms (1988) to estimate the concentration of a substance in meat and dairy products. Concerning the uptake of chemicals in plants from soil, it is suggested to estimate the stem concentration factor from the K_{ow} using the extrapolation method based on the experimental work of Briggs et al. (1982, 1983).

SAMENVATTING

Het RIVM Beoordelingssysteem Nieuwe Stoffen schat het gevaar van levenslange orale blootstelling van de mens aan nieuwe stoffen in door middel van overdrachtsfactoren die verband leggen tussen de concentraties in water en bodem en de humane blootstelling. Dit rapport behandelt de indirecte blootstelling van de mens aan nieuwe stoffen via de consumptie van vruchten, graanproducten, vlees en melkproducten. Een eerdere beperkte validatiestudie van het RIVM Beoordelingssysteem heeft aangetoond dat deze module een betere schatting van overdrachtsfactoren vereist. Op basis van een evaluatie van recent onderzoek op dit gebied komt dit rapport tot een mogelijke verbetering van het Beoordelingssysteem. In het besef van een blijvende hoge mate van onzekerheid in de modelschattingen wordt aanbevolen om de bio-overdrachtsfactorcorrelaties met K_{ow} van Travis en Arms (1988) te gebruiken om de stofconcentraties in vlees en melkproducten te berekenen. Voorts wordt aanbevolen om eerst de stengel-concentratiefactor te schatten op basis van de K_{ow} met de extrapolatiemethode van Briggs et al. (1982, 1983) en deze factor vervolgens aan te wenden om stofconcentraties in planten te berekenen.

1. INTRODUCTION

The fate of a chemical substance is governed by its equilibrium distribution between environmental media such as soil, water, air, and biota and the concentration of the substance and its altered forms existing over time in media. A substance may be concentrated from soil by plants or animals, then passed up the food chain via herbivores, omnivores, and carnivores to finally man. An animal may concentrate the substance without noticeable effects. The next consumer in the food chain may further concentrate the material. This process is called: biomagnification.

In order to assess the lifetime hazard of ingestion exposure of man in the RIVM Assessment System for New Substances a steady-state model was constructed (Roghair, 1988; Fig. 1). This model links environmental concentrations of organic substances in water and soil to human exposure applying transfer factors. These transfer factors incorporate information on environmental transport and partitioning and human dietary intakes. Concentrations in surface water in mg/dm^3 and in soil in mg/kg dwt are thus converted to daily exposure of man via drinking water and food (fish, meat, dairy products, food crops) in mg/kg bw/day. At steady state, transfer factors give a simple expression of the final disposition of substances taken in at constant rate. It is recognized that it may not be justified to assume that there is a steady state, particularly if there are wide variations. Although these factors only apply to defined environmental conditions, they can be assumed to have wider applicability for reasonably comparable circumstances.

This report discusses human exposure to new organic substances via consumption of fruits, vegetables, grains, meat and dairy products. Other routes of human exposure have been described in previous reports of the risk assessment system (Roghair et al., 1988; de Nijs et al., 1988). A limited validation study of the RIVM Assessment System for New Substances had previously shown that this part of the model needed further study with regard to the estimation of transfer factors (de Nijs et al., 1988). As a consequence a literature research was initiated to reveal the latest developments in this area (van Keulen, 1990). The present report is a reflection of this research and proposes what is considered to be an improvement of the RIVM Assessment System for New Substances.
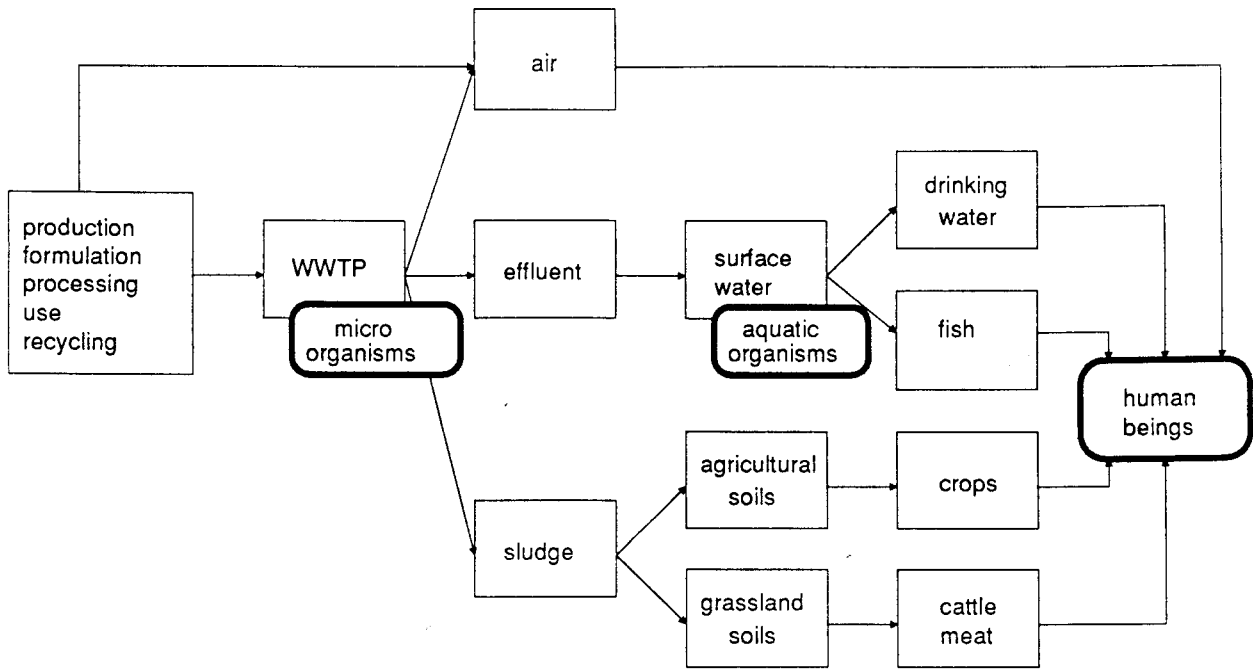
Fig. 1. Exposure estimate system

2. TRANSFER OF SUBSTANCES TO PLANTS

The transfer of substances to plants is of major importance to the exposure of man. Man is exposed by the intake of vegetables, fruits and grains contaminated by organic substances and by the intake of meat and dairy products from grazing animals.

In the transfer of substances from emission sources to plants different exposure pathways can be identified: via soil due to contamination of the soil (Fig. 2, pathway 1), via air due to the deposition of substances on the plant (Fig. 2, pathway 2). Man and cattle are exposed via transfer of substances to plants (Fig. 2, pathways 3, 4) because of adsorption of the compound to the plants exterior (leaves and roots) and uptake of the compound in the plant through the soil and air. The main exposure pathway for adsorption of substances to plant leaves is by deposition of contaminated particles from the air and dust from the soil. The roots are directly exposed to the soil and its solution. The direct transfer of substances to cattle, from soil by ingestion (pathway 5) and from contaminated air by inhalation (pathway 6), will be discussed in chapter 3.

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       Atmosphere (gas, particles)
           |          |
           |         6|
           |          |
         2|          \|/
           |       CATTLE-------------------MAN
           |       /|\ /|\                  /|\
           |        |   |                    |
           |       3|   |                   4|
          \|/       |   |                    |
///////////plants/////pasture crops//////////////////////////////
         /|\              |
         1|              5|
           |              |
              Soil
```
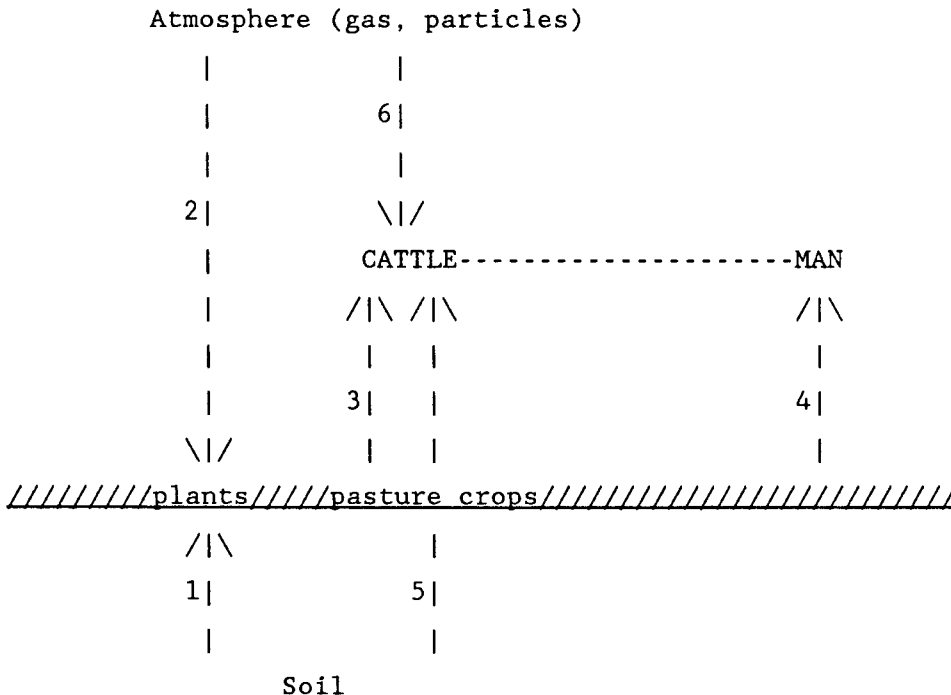
Fig. 2. The exposure pathways of man via plants and cattle

Chemical uptake by plants is a complex process that may involve a compound specific active and/or a passive process. In the latter process the chemical accompanies the transpiration water through the plant. Estimation of the uptake by the former process cannot be described with the scientific knowledge of today, but the research shows some relations to model the passive uptake of chemicals.

The passive uptake can be divided in penetration and uptake through the roots followed by transportation to the above ground parts and vegetative uptake directly from the surrounding air and penetration of adsorbed compound by the leaves. The uptake and transport in oil containing plants like carrots and cress should be considered as a special case of the former processes.

The final concentration of a substance in plants depends on many factors. Among the most important are the soil type, organic carbon and water content, plant type, physico-chemical properties of the compound, degradation and environmental conditions during growth of the plant. Recently, Ryan et al. (1988) developed a screening method for the potential plant uptake of neutral or weakly ionized organic chemicals. The concentration in plants depends on too many local or unknown parameters for a precise model estimation. The model of Ryan et al. (1988) gives an indication of the susceptibility of plant uptake for a certain chemical.

In the following paragraphs an outline is given of the estimation methods found in the literature. The different relations will be compared with each other.

2.1 Behaviour of chemicals in soil

Many processes impact organic chemicals in the soil environment. In a given situation, however, the processes are dependent on the physico-chemical properties of the compound and those of the soil. The environmental fate and impact on plants will be determined by the distribution of the chemical between vapour, solid and liquid phases in the soil, its transport and transformation rate in the system. Although Ryan et al. (1988) mention the degradation and volatilization of the organic compound in the soil, these processes have not been included in their model of the soil compartment. For a more extensive model formulation including leaching, degradation and

volatilization one is referred to Jury et al. (1983). At the moment only partitioning between solid and liquid phase in the soil is assumed.

The uptake of most chemicals in plants is dependent on the concentration in the soil-water phase which is determined by the partitioning with the solid phase in the soil. The partitioning of a compound between solids and solution is expressed as a linear sorption isotherm:

$$C_{abs} = K_d \cdot C_{liq} \qquad \text{Eq. 1}$$

where C_{abs} = the adsorbed concentration [mg/kg]
C_{liq} = the concentration in the soil solution [mg/dm^3]
K_d = adsorption coefficient

Organic compounds are primarily sorbed by the organic carbon in the soil. The soil adsorption coefficient can be expressed as the product of the fraction organic carbon and the organic carbon distribution coefficient (K_{oc}) :

$$K_d = K_{oc} \cdot f_{oc} \qquad \text{Eq. 2}$$

There have been many investigations showing the relationship between K_{oc} and the octanol-water partitioning coefficient (K_{ow}) (see Ryan et al., 1988).

The concentration in the soil solution will decrease with increasing K_d but the final plant concentration will also be determined by leaching, degradation and volatilization of the compound and other processes resulting in a decrease of the exposure time and therefore of the concentration in the plant.

To be able to compare the different estimation methods relative to the total soil concentration C_s and the effect of soil sorption, a simple mass balance equation for the soil system has been used:

$$\rho \cdot C_s = \rho \cdot C_{abs} + \theta \cdot C_{liq} \qquad \text{Eq. 3}$$

where C_s = the total concentration of the organic chemical in the soil [mg/kg wwt]
ρ = the soil bulk density [g/cm^3]
θ = the soil-water content by volume [cm^3/cm^3].

Using the linear adsorption to the organic carbon content in the soil (eq. 1 and 2), equation 3 can be rewritten to express the concentration in the soil solution relative to the total concentration:

$$C_{liq} = \frac{\rho}{\rho \cdot K_{oc} \cdot f_{oc} + \theta} \cdot C_s \qquad \text{Eq. 4}$$

To estimate the K_{oc} the following relation of Karickhoff (1981) has been chosen:

$$\log(K_{oc}) = 0.989\log(K_{ow}) - 0.346 \qquad \text{Eq. 5}$$

A standard soil with a soil bulk density ρ of 1.4 g/cm^3, a soil water content θ of 0.4 cm^3/cm^3 and 0.05 g/g organic matter has been used in the comparisons with a standard total soil concentration of 1 μg/g.

2.2 Plant uptake of substances

2.2.1 Uptake from soil

Shone and Wood (1974) studied the uptake of simazine by 6-day old barley plants. They defined a transportation stream concentration factor (TSCF) for the relationship between simazine transport and water uptake:

$$TSCF = \frac{\text{mg simazine in shoots per cm}^3 \text{ water transpired}}{\text{mg simazine per cm}^3 \text{ of external solution}}$$

Water was taken up preferentially to simazine in the experiments and the TSCF was always less than unity. Shone and Wood (1974) further showed that the translocation of herbicides to the plant stems could not be inferred from the concentration in the plants roots. They defined a root concentration factor (RCF) for the uptake and sorption of a chemical by a plant root:

$$RCF = \frac{\text{concentration in root [mg/kg fresh weight]}}{\text{concentration in external solution [mg/dm}^3]}$$

Briggs et al. (1982, 1983) evaluated 18 chemicals and found a relationship between the RCF and the K_{ow} for both living and macerated roots. The difference between living and macerated roots was interpreted as the result of two processes:

- a partitioning between the organic material of the root and the external solution, effective in both living and macerated roots and

- a fraction of root that is aqueous and equal in concentration to the external solution only present in living roots and constant for all compounds, 0.82.

The RCF for living roots is given by equation 6:

$$\log(RCF_{Briggs} - 0.82) = 0.77\log(K_{ow}) - 1.52 \quad (n = 7, \ r = 0.981) \qquad \text{Eq. 6}$$

Other investigations, by Topp et al. (1986) showed a similar relationship between the RCF and the octanol-water partitioning coefficient:

$$\log(RCF_{Topp}) = 0.63\log(K_{ow}) - 0.959 \quad (n = 9, \ r = 0.896) \qquad \text{Eq. 7}$$

Briggs et al. (1982, 1983) also proposed a bell shaped relationship between TSCF and the octanol-water partition coefficient (K_{ow}):

$$TSCF_{Briggs} = 0.748 \ e^{-[(\log(K_{ow}) - 1.78)^2/2.44]} \quad (n = 17, \ r \text{ not reported}) \quad \text{Eq. 8}$$

At low Kow values the translocation of the chemical is limited by the lipid membrane in the root. At high K_{ow} values the rate of transport decreases because of the high lipophilicity of the compounds resulting in a strong retention by the roots. All TSCF values were below unity, indicating passive transport of the chemical with the concentration gradient.

Analogous to the RCF, Briggs et al (1983) proposed a stem concentration factor for the transportation stream solution (SCF_{tss}) defined as:

$$SCF_{tss} = \frac{\text{concentration in stem [mg/kg fresh weight]}}{\text{concentration in transportation stream solution [mg/dm}^3]}$$

The macerated stem sorption of organic substances was related to the K_{ow}. For living plants a similar contribution of aqueous phase is assumed in the stem as has beeen found for the roots:

$$\log(SCF_{tss} - 0.82) = 0.95\log(K_{ow}) - 2.05 \quad (n = 8, \; r = 0.98) \qquad \text{Eq. 9}$$

To calculate the concentration in the stem relative to the concentration in the soil solution (SCF_{liq}) one must multiply SCF_{tss} with the TSCF, the partitioning of the transportation stream concentration and the external soil solution:

$$SCF_{liq} = SCF_{tss} \quad . \quad TSCF_{Briggs} =$$

$$(0.82 + 10^{[0.95\log(K_{ow}) - 2.05]}) \; . \; (0.748e^{-[(\log(K_{ow}) - 1.78)^2/2.44]} \qquad \text{Eq. 10}$$

Travis and Arms (1988) give an statistical/empirical relationship between experimentally determined plant concentration factors and the octanol-water partitioning coefficient based on 28 data pairs from literature. The SCF_{Travis} is expressed in (μg/kg dry wt)/(μg/kg dry soil), the concentration in the above ground parts relative to the soil concentration.

$$\log(SCF_{Travis}) = 1.588 - 0.578\log(K_{ow}) \quad (n = 29, \; r = 0.73) \qquad \text{Eq. 11}$$

2.2.2 Uptake from air

The exposure of plants to organic chemicals in the air can be divided in two different pathways:

- volatilization from the soil and subsequent deposition from the air onto the plant, a local process and

- emission of chemicals to the air and subsequent wet and dry deposition of gas and particles onto the plant, a regional process.

In most (laboratory) experiments of plant uptake due to soil-borne organics no attempts have been made to discriminate between root uptake and subsequent translocation and vegetative uptake of vapour from volatilization of the compound from the soil. Several studies (Beall and Nash, 1971; Fries and Marrow, 1981) show the relative importance of uptake from the air.

Topp et al. (1986) examined the relative importance of foliar uptake to root uptake and translocation based on laboratory experiments with [14]C labelled

chemicals and barley seedlings. Their study showed a relationship between the foliar uptake and the volatized compound:

% Foliar Uptake = 46.11 + 28.95log(% volatized)   Eq. 12

where % Foliar Uptake = the % foliar uptake of total ^{14}C uptake

     % volatized   = the amount of volatized ^{14}C labelled compound as the % of the total ^{14}C applied.

McKone and Ryan (1989) give an estimation method for the plant absorption/uptake due to wet and dry deposition of contaminated particles from the air. In their study of human exposure to chemicals in food chains they give an estimation of the amount of chemical deposited on plants from the air. All parameters, maximum and minimum values with their distribution have been estimated to model the human exposure and the uncertainty using Monte Carlo simulation techniques. The steady state concentration in vegetation is approximated based on a mass balance:

$$V_{dp} \cdot C_{pf} = M_f \cdot R_v \cdot C_v$$ Eq. 13

so C_v is:

$$C_v = \frac{V_{dp} \cdot C_{pf}}{M_f \cdot R_v}$$ Eq. 14

where V_{dp} = the deposition factor of atmospheric particles on food crops [m/day], which is the ratio of deposition rate on vegetation in mg/m^2.day to the air concentration in mg/m^3

    C_{pf} = the concentration in air, particle fraction $[mg/m^3]$

    C_v = the concentration in fresh vegetation [mg/kg fresh weight]

    M_f = the annual average inventory of food crops per unit area [kg fresh weight/m^2], ranging from 1.0 up to 9.0 kg/m^2 (median, 3.0, log-uniform distribution)

    R_v = the removal rate constant of chemicals from vegetation surfaces, ranging from 0.01 to 1.0 (median 0.03, log-uniform distribution).

The total deposition rate on vegetation, V_{dp}, is approximated:

$$V_{dp} = 0.8 \cdot V_t(dry) + V(wet) \qquad\qquad Eq. 15$$

where the first term reflects the dry deposition and the second the wet deposition on vegetation. The dry deposition on vegetation is estimated as a fraction, 0.8, of the total dry deposition rate, V_t. McKone and Ryan (1989) show that in general the dry deposition exceeds by far the wet deposition. The total dry deposition rate varies over a large range from 1 up to 100,000 m/day. In their simulations McKone and Ryan (1989) use a log-normal distribution with a geometric mean of 300 m/day and a standard deviation of 30 for the deposition on vegetation.

2.3 Comparison of the estimation methods

In this paragraph the different methods to calculate the root and stem concentration will be compared. For a discussion about differences in the experiments and analytical routines one is referred to the original literature and Ryan et al. (1988).

The root concentration can be estimated using the method of Briggs et al. (1982, 1983) and Topp et al. (1986). In figure 3 the root concentration factor calculated with both methods is plotted against the octanol-water partition coefficient on a log-log scale. The root concentration factor is calculated as both the ratio relative to the soil liquid phase, C_{liq}, (RCF) and the total soil concentration, C_s, (RCFS). The RCFS decreases while RCF increases at higher log K_{ow} values for both methods (Briggs et al., 1982, 1983; Topp et al., 1986) because the effect of soil sorption is larger. For both ratio's the concentration factor differs only slightly for log K_{ow} smaller than 2. The difference results from the constant factor for living roots of Briggs, 0.82. He presumes that a fraction of the roots aqueous phase is always in equilibrium with the external solution.

The stem concentration factor is also plotted against the octanol-water partition coefficient on a log-log scale (Fig. 4). The concentration factors have been calculated using the methods of Briggs et al. (1982, 1983) and Travis and Arms (1988). The method of Travis and Arms has been adjusted for the differences in the units of the concentration ratio.

Root Concentration Factor
relative to the total soil concentration and the soil liquid phase
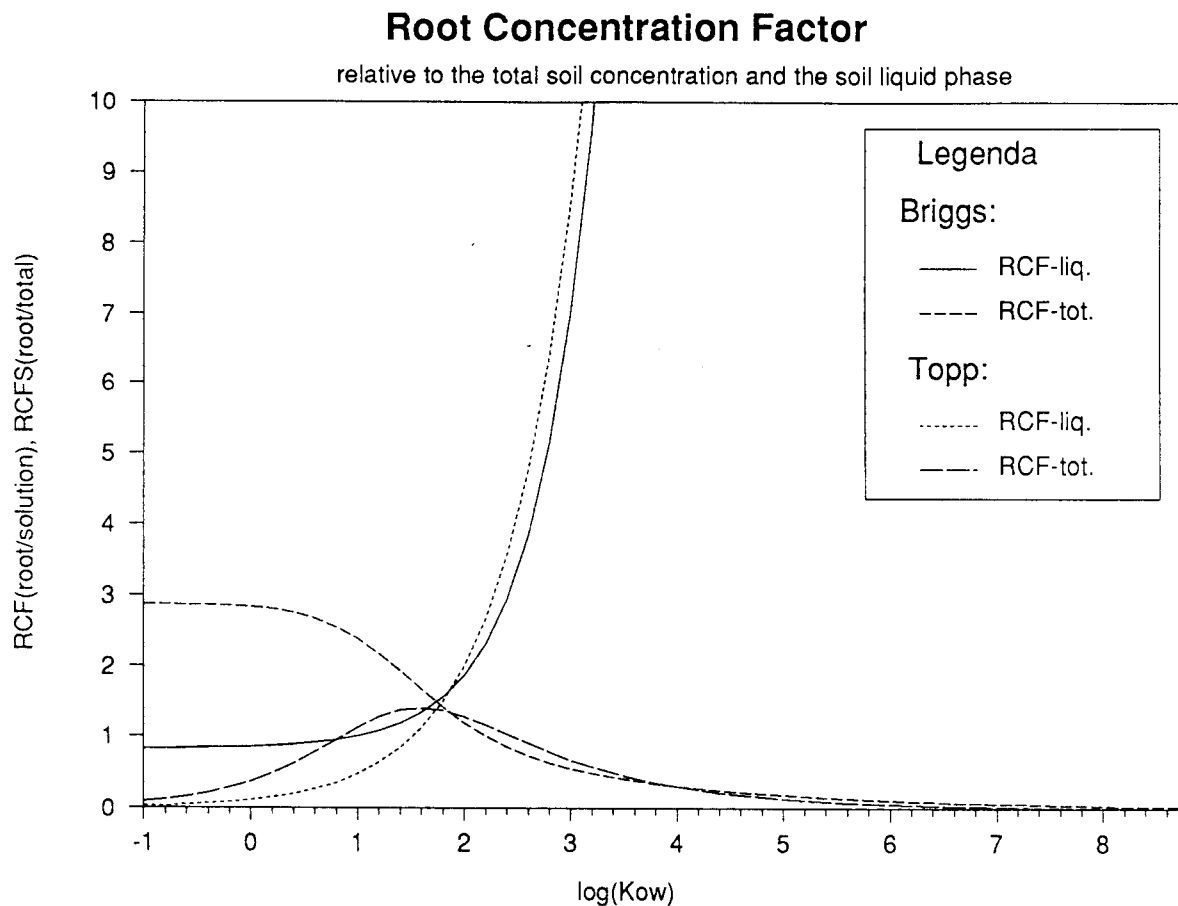
Fig. 3. The comparison of different estimation methods for the root concentration factor

The stem concentration, expressed in mg/kg dry weight, has been converted to mg/kg fresh weight by multiplying with a constant factor of 0.25 taken from McKone and Ryan (1989). The soil concentration is also expressed in mg/kg dry weight and has been adjusted for the weight of the soil solution:

$$C_s = C_{dry} \cdot \frac{1}{1 + \theta \cdot \rho}$$ Eq. 16

where θ = the water volume content by volume assumed to be 0.4 cm^3/cm^3

ρ = the density of water, 1 g/cm^3.

Stem Concentration Factor

relative to the total soil concentration and the soil liquid phase
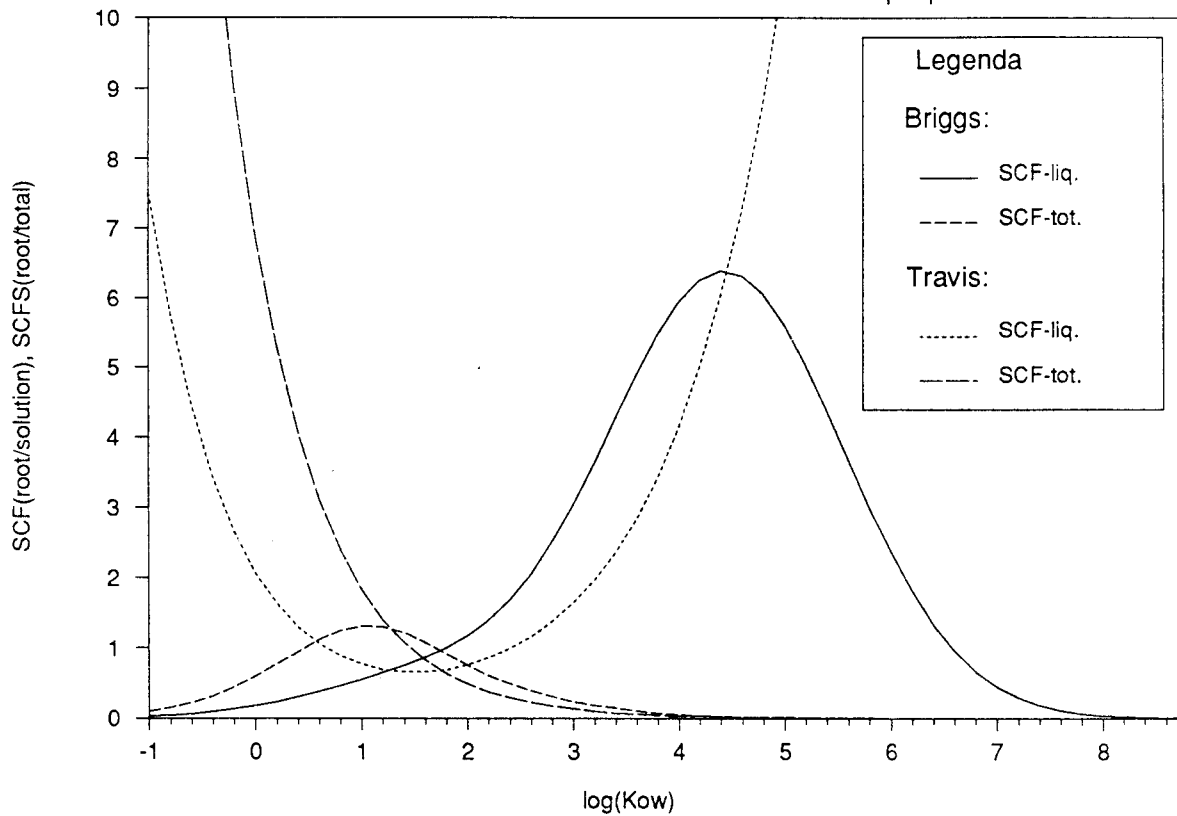
Fig. 4. The comparison of different estimation methods for the stem concentration factor

As for the root concentration factor, the effect of soil sorption causes the SCFS to decrease while SCF increases at higher log K_{ow}. The methods differ because Travis and Arms (1988) assume a linear relationship between log SCF and log K_{ow} while Briggs et al. (1982, 1983) found a bell shaped relationship between the log of the transpiration stream concentration factor (TSCF) and the log K_{ow}. Briggs et al. (1982, 1983) suggest that at low log K_{ow} values the lipid membrane limits the translocation of the chemical in the root and at high log K_{ow} values the transporation rate decreases because of the increasing lipophilicity of the compounds. It is surprising to see that for the more generally occurring log K_{ow} values, between 1 and 6, the difference between both methods is very small. Although the difference at high and low log Kow between the extrapolation methods is high, it will result in a negligible effect on the final plant concentration and the exposure of man.

3. TRANSFER OF SUBSTANCES TO MAMMALS

In the following, the exposure of man via intake of meat and dairy products contaminated by the transfer of substances from pasture-crops and from the atmosphere to grazing mammals will be discussed. The model pathway includes the indirect transfer of substances to cattle by ingestion of substances taken up by or deposited onto pasture crops (Fig. 2, pathway 3). The transfer of substances from soil or air (Fig.2, pathways 1 and 2, respectively) to pasture crops was discussed in chapter 2. Other potentially important pathways are the direct transfer of substances from contaminated soil by ingestion (Fig.2, pathway 5) and from contaminated air by inhalation of gas and particles (Fig.2, pathway 6) (McKone & Ryan, 1989). Ingestion of substances by cattle via drinking water will not be considered as data are insufficient at present to estimate the exposure via this route.

3.1 Fate of substances in mammals

The fate of a substance ingested via food or inhaled by a specific mammal depends on too many factors for an accurate and precise estimation of tissue concentrations by modelling or structure-activity relationships. These factors include rate of uptake, metabolic fate and rate, strain, age and physical condition of the animal, food consumption and food conversion, and climatic conditions.

In order that a substance may be absorbed into the bloodstream it must cross one or more semi-permeable lipoprotein membranes. Most membranes have an electric potential that may effectively preclude the ready penetration of charged chemical species. Absorption is faster under conditions in which ionization is suppressed, i.e. low pH for acids and high pH for bases. The absorption of a chemical therefore depends on its physico-chemical properties, molecular size, shape, degree of ionization, and lipid solubility. Absorption of an ingested solid in the gastrointestinal tract will be impaired if dissolution in the gastro-intestinal tract does not take place. Food or soil in the gastrointestinal tract can enhance or delay absorption e.g. by producing a non-absorbable complex or by affecting gastric emptying, gut motility, pH, and microflora. The lung represents a poor barrier to a substance entering the blood. Volatile compounds will be absorbed only

partially, and the unabsorbed fraction will be eliminated and not retained for subsequent absorption, as in the gut (WHO, 1978; Hayes, 1982).

Once absorbed, the distribution of a substance is determined by the relative plasma concentration, the rate of blood flow through various organs and tissues, the rate by which the chemical penetrates the cell membranes, and the binding sites that are immediately available in the plasma and tissues. When the plasma concentration is high and the cell membranes do not provide significant barriers to diffusion, distribution is mainly to organs with high blood flow such as brain, liver, and kidney. Lipid-soluble substances tend to be distributed and localized in adipose tissue in accordance with their lipid to water partitioning coefficient. A major factor that can affect distribution of a substance is its affinity to bind to proteins and other macromolecules of the body, localizing it temporarily and modifying its initial pattern of distribution and rates of absorption, metabolism, and excretion (WHO, 1978; Hayes, 1982).

The concentration of a substance in blood plasma and tissues further is a function of its elimination from the body by excretion via urine and exhalation and its metabolic transformation (WHO, 1978). Fat-soluble substances may remain for a long time in adipose tissues and thus be shielded from metabolic turnover (Moriarty & Walker, 1987).

Although the above summary shows that many variables determine the plasma and tissue concentration of a substance in the body, an approximation - which may be adequate for an initial assessment using a steady-state model - can be found from the physico-chemical properties of the substance. A first approximation of the distribution can be based on that which would be found between homogeneous compartments at thermodynamic equilibrium using partitioning coefficients. However, it should always be kept in mind that compartments are not homogeneous, thermodynamic equilibrium is usually not attained and the real partitioning coefficients are not known.

3.2 Partitioning coefficients

When cattle ingest chemical substances together with food or soil or inhale these from air, the substances can be thought of being distributed between the medium of intake and the lipophilic structures of the body such as membranes, lipoprotein micelles (e.g. in milk) and fat depots. Water-soluble

substances, apart from some metallic compounds, are unlikely to persist within organisms (Moriarty & Walker, 1987). They are, in general, also unlikely to reach tissues of cattle given their low levels in pasture crops (see chapter 2), their reduced passage of lipoprotein membranes, and limited adsorption to soil particles.

The distribution between animal fat and medium of intake can be expressed by the animal fat/diet distribution factor K_{ad}:

$$K_{ad} = \frac{\text{steady-state concentration of pollutant in animal fat}}{\text{constant concentration in medium of intake}}$$

The K_{ad} [(mg/kg)/(mg/kg dwt) or (mg/kg)/(mg/m^3)] can be related to the partitioning coefficient between n-octanol and water, the K_{ow}: the larger the value of K_{ow}, or the lower the solubility in water, the greater the tendency for molecules to move into lipophilic structures. Several equations are available which correlate K_{ad} with the n-octanol/water-partitioning coefficient K_{ow}.

Kenaga (1980) derived a correlation for 23 compounds:

$$\log K_{ad} = 0.5\log (K_{ow}) - 3.457 \quad (r = 0.79) \qquad \text{Eq. 17}$$

As the compounds can be clustered in two distinct groups on the basis of lipophilicity and metabolic fate the statistical validity of this correlation is doubtful.

Two other correlations were developed by Geyer et al. (1987) for 8 and 10 highly lipophilic compounds, respectively;

$$\log K_{ad} = 0.756\log (K_{ow}) - 1.415 \quad (r = 0.969) \qquad \text{Eq. 18}$$
$$\log K_{ad} = 2.56\log (K_{ow}) - 0.22(\log K_{ow})^2 - 4.82 \quad (r = 0.956) \qquad \text{Eq. 19}$$

In view of the high lipophilicity of the compounds used and the limited data set the applicability of these equations must be considered very restricted.

Travis & Arms (1988) reviewed biotransfer factors, defined as the steady-state concentration in a receiving medium (meat, milk) in mg/kg wet weight divided by the animals' daily contaminant intake in mg/day, for 36 compounds in meat and 28 compounds in milk. The compounds considered had log K_{ow}-values between 1.34 and 6.89. This concept is thought to be more useful for risk assessment

purposes, since chemical exposure to cattle may occur via different pathways. The biotransfer factors are related to K_{ad} and the bioconcentration factor BCF by the following expression:

$$BCF = B \cdot I_s = K_{ad} \cdot f_f \qquad \text{Eq. 20}$$

where B = biotransfer factor [(mg/kg wwt)/(mg/day)]

I_s = daily intake of source medium (soil, pasture crops, air) [kg dwt/day or m^3/day]

f_f = fraction of fat

The transfer factors for meat and milk appeared to be linearly related to the K_{ow}:

$$\log B_b = -7.6 + \log K_{ow} \quad (n = 36, \ r = 0.81) \quad \text{or} \quad B_b = 2.5 \cdot 10^{-8} \cdot K_{ow} \qquad \text{Eq. 21}$$

$$\log B_m = -8.1 + \log K_{ow} \quad (n = 28, \ r = 0.74) \quad \text{or} \quad B_m = 7.9 \cdot 10^{-9} \cdot K_{ow} \qquad \text{Eq. 22}$$

where B_b = biotransfer factor for meat (beef)

B_m = biotransfer factor for milk

The general validity of these equations remains to be proven. However, at present these transfer factors are the most reliable considering the number of compounds and the wide range of lipophilicity investigated.

It is noted here that, as the rate at which a pollutant is metabolized becomes important, the partitioning coefficient becomes less reliable as an indicator of the K_{ad}. Travis et al. (1988) have, however, also made clear that K_{ow} is the main parameter affecting biotransfer factors. Assuming Michaelis-Menten pharmacokinetics for the metabolic turnover of a substance it was shown that the biotransfer factors are related to metabolic parameters and K_{ow} as follows:

$$B = \alpha \cdot \frac{K_m}{V_{max}} \cdot K_{ow} \qquad \text{Eq. 23}$$

where α = a constant

K_m = Michaelis-Menten constant

V_{max} = maximum initial velocity of the reaction

Deviations from the linear relationship between biotransfer factors and the K_{ow} may occur because of variations in metabolic rates of individual substances. Realizing that metabolic rates within a given species differ by at most a few orders of magnitude, whereas K_{ow} values can differ by 6 to 8 orders of magnitude, it can be concluded that biotransfer factors are most sensitive to K_{ow}.

An approach that takes both metabolism and differences between species into account is that of Walker (1985) who proposed the following equation:

$$K_{ad} \cdot f_f = 2 \cdot t_{50} \cdot \frac{A}{T} \qquad\qquad \text{Eq. 24}$$

where f_f = fraction of fat of organism

t_{50} = half-life [days]

A = fraction of ingested compound that is absorbed

T = time for an organism to consume a weight of food equal to its own body weight [days]

4. CONCLUSIONS

Reviewing the state of knowledge at present, the estimation of human exposure through the food chain is still full of uncertainty because it is based on limited data and many assumptions. As outlined above, an approximation applying partitioning coefficients is the best possible at present. McKone & Ryan (1989) have assessed the amount and source of uncertainty in simple compartmental model predictions of human exposure. Their analysis revealed that much of the overall uncertainty is attributable to uncertainty in biotransfer factors and that uncertainties in the input data limit the precision of exposure predictions to a 90% confidence range of roughly 2 orders of magnitude. Being aware of this degree of uncertainty in our model estimates, it is recommended to use the biotransfer factor correlations with K_{ow} as determined by Travis & Arms (1988) to estimate the concentration of a substance in dairy products and meat. As is made clear in section 3.2, these correlations are thought to be more reliable than the correlation of Kenaga (1980) which was used so far in the RIVM Assessment System. Kinetic approaches such as that of Walker (1985) are promising but need be investigated further and are probably difficult to apply to new substances with a limited data set.

Concerning the uptake of chemicals in plants from soil, the method proposed by Ryan et al. (1988) is suggested for the estimation of plant concentrations, using the stem concentration factor based on the experimental work of Briggs et al. (1983). The correlation of the stem concentration factor with the physical properties of the soil and the substance itself more reliably describes reality than the mere assumption of a fixed soil-plant concentration factor of 10 as was made up to now in the RIVM Assessment System. The uptake from the air can be modelled conform McKone and Ryan (1989). In spite of the large uncertainties it is the only method available at the moment.

5. IMPLEMENTATION

Based on the above conclusions this section describes the implementation into the RIVM Assessment System for New Substances.

The total intake of a substance by man via food crops (vegetables, fruits grains), meat (beef, pork, poultry) and dairy products (milk, yoghurt, cheese) can be expressed by the following equation (Roghair et al.,1988):

$$D = \sum \frac{f_i \cdot DFI}{BW} \cdot C_i \cdot f_v \qquad \text{Eq. 25}$$

where D = the total daily dose [mg/kg bw/day]. Poultry and pork will be treated as having the same bioconcentrating properties as beef. Yoghurt and cheese will be treated as milk.

f_i = fraction of the total food intake which the medium of intake i represents

DFI = total daily food intake [kg/day]

C_i = concentration of the substance in medium of intake i [mg/kg wet weight]

f_v = fraction of the intake that comes from the contaminated area. This fraction is assumed to be the same for each medium of intake

BW = body weight.

The concentration of a substance in plants (C_p) is determined by the contribution from soil solution and the air. Foliar uptake from the air is considered to be of minor importance relative to the uptake from the soil solution, as concentrations of the substance in the air at production level 0 of the assessment system (1 - 100 tons/year) will be negligible.
The concentration of the soil solution can be calculated conform eq.4:

$$C_{liq} = \frac{\rho}{\rho \cdot K_{oc} \cdot f_{oc} + \theta} \cdot C_s \qquad \text{Eq. 4}$$

and the concentration in the plant C_p [mg/kg wwt] will be:

$$C_p = SCF_{liq} \cdot C_{liq} \qquad \text{Eq. 26}$$

in which SCF is the stem concentration factor (see eq. 10 and 11)

The concentration of a substance in meat C_b and dairy products C_m is the aggregate of the contributions from soil, pasture crops (plant), and air:

$$C_{b,m} = K_{ad_i} \cdot f_f \cdot (C_s \cdot a + C_p \cdot b + C_a) \qquad \text{Eq. 27}$$

where K_{ad_i} = animal fat/diet distribution factor [(mg/kg)/(mg/kg dwt) or (mg/kg)/(mg/m³)]; the subscript i refers to subsequently soil, pasture crops, and air

C_s = concentration of the substance in soil [mg/kg wet weight]

a = constant for conversion of C_s [wwt] to soil concentration [dwt] which is taken to be 1.4 (see Eq. 16)

C_p = concentration of the substance in pasture crops [mg/kg wet weight]

b = constant for conversion of C_p [wwt] to plant concentration [dwt] which is taken to be 4 (McKone & Ryan, 1989)

C_a = concentration of the substance as gas or particles in the atmosphere [mg/m³].

Combining equations 20 and 27 results in:

$$C_b = B_b \cdot (I_s \cdot C_s \cdot 1.4 + I_p \cdot C_p \cdot 4 + I_a \cdot C_a) \qquad \text{Eq. 28}$$

$$C_m = B_m \cdot (I_s \cdot C_s \cdot 1.4 + I_p \cdot C_p \cdot 4 + I_a \cdot C_a) \qquad \text{Eq. 29}$$

for the concentration of a substance in meat and dairy products, respectively, where I_s = daily intake by cattle of soil [kg dwt/day]

I_p = daily intake by cattle of pasture crops [kg dwt/day]

I_a = daily intake by cattle of air = inhalation rate [m³/day]

B_b = biotransfer factor for meat (beef) [(mg/kg wwt)/(mg/day)]

B_m = biotransfer factor for milk [(mg/kg wwt)/(mg/day)].

McKone & Ryan (1989) have searched the literature available for the estimated intake by cattle of the source media soil (I_s), pasture crops (I_p), and air (I_a). They have proposed the mean values and standard deviations

(based on a uniform distribution of each parameter) as shown in Table 1, which were obtained from eight papers. These values can be adopted for the RIVM Assessment System. It should be noted that soil ingestion by grazing cattle may range from 0.09 to as high as 1.6 kg/day, as reviewed by McDowell (1985) and is subject to, among others, climatic and seasonal variations and differences in soil type, pasture management, and individual animal differences.

Table 1: Estimated intakes of source media for cattle (McKone & Ryan, 1989)

Property	Beef cattle			Dairy cattle		
	mean	n	σ	mean	n	σ
I_s [kg dwt/day]	0.39	4	0.27	0.41	5	0.24
I_p [kg dwt/day]	12.2	7	4.4	16.9	7	3.7
I_a [m³/day]	122	3	33	122	3	33

For the mean estimated total daily intake by adults (f * DFI), food (wwt) intake data for The Netherlands had been obtained from the Food Inspectorate (Roghair et al., 1988). More recently, a survey, funded by the Ministry of Welfare, Health and Cultural Affairs and the Ministry of Agriculture and Fisheries, was carried out from April 1987 till March 1988. This survey included 5898 persons constituting a representative sample of the Dutch population within the age of 1 to 75 years old (WVC, 1988). Annex I shows these data as pertaining to daily intakes of both children (1 - 3 and 1 -15 years old) and adults (16 - 75 years old). Taking into account the large uncertainties involved in the intake assessment, the difference between the intake of adults and that of children can be disregarded, resulting in the model parameters for the Assessment System as shown in Table 2.

Table 2: Daily intakes of food in The Netherlands (WVC, 1988)

Food type	Intake [kg wwt/day] Adults 16-75 y
Food crops	0.558
Meat	0.126
Dairy products	0.371
Fish	0.010

These data compare well with those of McKone & Ryan (1989) for the US.

The mean body weight (BW) can be assumed to be 71 kg for adults over 15 years old and 29 kg for children from 1 to 15 years old (CBS, 1986). Finally, it is assumed that the fraction of the intake that comes from the contaminated area (f_v) is 1.

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DAILY INTAKES OF FOOD IN THE NETHERLANDS

FOOD ITEM	INTAKE [G/DAG][1]		
	children		adults
	1-3y	1-15	16-75y
	(n=231)	(n=1300)	(n=4598)
* potatoes, tuberous plants	64	105	139
* vegetables	67	98	156
* leguminous plants	4	4	7
* fruits	98	116	128
* grains, bindings agents	22	32	40
* bread (60% grains)	67	120	147
* milk, milk-products	502	477	339
* cheese	8	15	32
eggs	8	12	18
* meat, meat-products, poultry	48	81	126
* fish, shell-fish	3	3	10
fats, oils, mayonaise, hearty sauces	22	39	51
soup	23	44	81
compound dishes	11	12	23
cakes	23	33	44
sugar, sweets, sweet sauces	29	50	49
nuts, seeds, snacks	9	20	23
hearty bread-spreads	4	5	3
non-alcoholic drinks	361	502	1129
alcoholic drinks	0	2	221
herbs, spices	0	0	0
preparations	0	0	1
others	1	1	1
TOTAL	1372	1772	2768

[1] Adapted from: WVC (1988); figures have been rounded off to whole numbers and pertain to both sexes combined with a nearly equal distribution into males and females. The food items marked by an asterix were used for determination of the daily intake per category (food crops, dairy products, meat, and fish)