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Validation of models on uptake of organic chemicals by plant roots

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SUMMARY

The fate of a substance is governed by the distribution of the substance between soil, water, air, and biota, and the concentration of the substance and its altered forms existing over time in these media.
As vegetable food forms a major part of the diet of human beings, and also of cattle, the contamination of plants will have a large influence on the total daily intake of a substance.

In this report the application of soil-plant transfer factors is investigated. The main goal was to find sufficient experimental data in the available literature, if possible adjusted for differences in experimental design, which could be used to evaluate the currently applied method in the Uniform System for the Evaluation of Substances (USES). In this method, concentrations in root and stem of the plant are estimated on the basis of an empirical relationship with the octanol-water partitioning coefficient.

It was concluded that the root concentration factor as applied in USES is an appropriate instrument for the estimation of residues in roots, whereas the application of the stem concentration factor is insufficient for the purpose set in USES. Consequently for above-ground plant parts other approaches need to be explored which can be applied in the general risk assessment of substances.

SAMENVATTING

Het lot van een stof wordt bepaald door de verdeling van de stof over bodem, water, lucht en biota, en de concentratie van de stof en zijn afgeleide producten in deze media.
Omdat zowel het menselijke dieet als dat van vee voor een belangrijk deel bestaat uit plantaardig voedsel, zal de verontreiniging van planten van grote invloed zijn op de totale dagelijkse inname van een stof.

In dit rapport is de toepassing van bodem-plant overdrachtsfactoren onderzocht. Hoofddoel was het vinden van voldoende experimentele gegevens op dit terrein, indien mogelijk gecorrigeerd voor verschillen in proefopzet, om de methode die nu in het Uniform Beoordelingssysteem Stoffen (USES) wordt toegepast, te evalueleren. Deze methode maakt een schatting van de concentraties in de wortel en stengel van de plant op basis van een empirische relatie met de octanol-water partitiecoëfficiënt.

De wortel concentratiefactor zoals die in USES wordt gebruikt, is een toereikend instrument voor het schatten van residuen in wortels, terwijl de toepassing van de stengel concentratiefactor niet voldoende geschikt is voor de doelstellingen van USES. Bijgevolg dienen voor de bovengrondse plantedelen andere methoden te worden onderzocht voor de toepassing in de algemene risicoschatting van stoffen.

1. INTRODUCTION

The fate of a substance is governed by the distribution of the substance between environmental media such as soil, water, air, and biota, and the concentration of the substance and its altered forms existing over time in these media. A substance may be taken up from soil by plants, then passed up the food chain via herbivores, omnivores, and carnivores, and, finally, to man. Such a food chain can be modelled as in the Uniform System for the Evaluaton of Substances, USES (RIVM et al., 1994; Vermeire et al., 1994; Jager et al., 1994) (Figure 1).

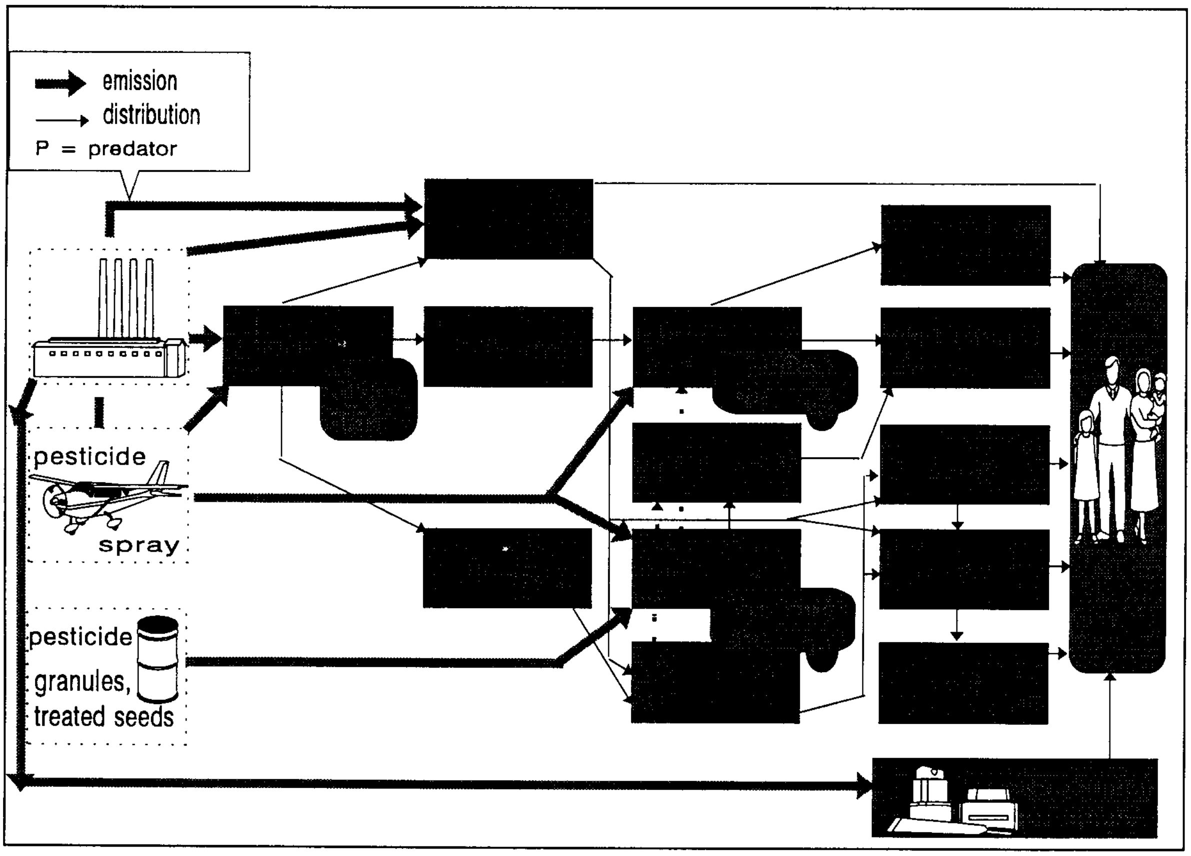

Figure 1. Exposure pathways in USES

USES was developed as a decision-support system to be applied by the government departments and institutes, by industry and institutes in the private sector and by international fora. USES is a tool that can be used for the rapid, quantitative assessment of the hazards and risks of organic substances, including new chemical substances, existing chemical substances, agricultural pesticides and biocides, to man and the environment. USES links emission quantities to concentrations in air, water and soil at a local and a regional scale. Based on these environmental concentrations, levels in crops, meat and milk are estimated by applying transfer factors. These are combined with levels in other human intake media and dietary factors to an estimate of the total daily intake.

Consumption of plants or plant products like vegetables, fruit and grains forms a major part of the food consumption of human beings, but also of the feed consumption of cattle. Contamination of plants therefore, will have a large influence on the total daily intake of a substance. When trying to predict concentrations in plant tissues, one will be confronted with several problems related to the variety of plant species, and the inhomogeneity in this group with regard to physiology, rooting depth, leaf area, growth period, and so on. Only a very rough approximation of concentrations in food crops seems feasible.

Plants can be exposed to contaminants in different ways (Topp et al., 1986):
- active or passive uptake by the roots and possibly subsequent transport by the transpiration stream;
- wet and/or dry deposition on the above ground parts and possibly absorption and translocation over the cuticula;
- uptake of vapours into the leaf through the stomata or the leaf surface;
- uptake and transport in oil cells which are found in oil containing plants like carrots and cress.

The transfer factors describing the transfer of organics from soil to plants are the subject of investigation in this report. Modelling the transfer of organic substances from air to plants has been the subject of another study within the framework of the USES-project (Hulzebos, 1994) and will not be discussed here.

Many processes play a role in the uptake of substances in plants from the soil. In general, this uptake is a passive process (Shone et al., 1973) governed by the transpiration stream of the plant, in case of accumulation in leaves, or physical sorption, in case of roots. The few methods available for the estimation of this transfer have been compared by De Nijs and Vermeire (1990). They concluded that the model of Briggs et al. (1982, 1983) offered the most appropriate description. In this method, concentrations in root and stem of the plant are estimated on the basis of an empirical relationship with the octanol-water partitioning coefficient. It was recognized though, that the relations derived are based on experiments with barley only and used a relatively small range of non-ionised substances (RIVM et al., 1994).

The main assumptions of De Nijs and Vermeire (1990) for the route of organics from soil to plant were:

1. With regard to the fate of substances in soil:
   - organic compounds are primarily sorbed by the organic fraction of the soil.
   - the concentration in the soil pore water is determined by the partitioning between solids and soil solution and the uptake of substances in plants from soil is dependent on the concentration in the soil pore water.
2. With regard to uptake processes:
   Plant uptake from soil can be described by concentration factors such as the ratio of the concentration in the plant (mg/kg fresh weight) and the concentration in the external solution (mg/l). The use of fixed concentration factors assumes that a steady state between plant and external solution occurs.

In this report the application of soil-plant transfer factors is further investigated. The main goal was to find sufficient experimental data in this area, if possible adjusted for differences in experimental design, which could be used to evaluate the currently applied method in USES (i.e. the concentration factors of Briggs et al., 1982, 1983) or to adapt it.

2. METHODOLOGY

Predictions of concentration factors for plants are calculated according to the model of Briggs and coworkers (1982, 1983), as described in subsection 2.1. Literature on accumulation experiments with plants is collected and selected according to the criteria, given in subsection 2.2. The adaptations of the selected data that are necessary to make the comparison with the model predictions possible, are described in subsection 2.3.

2.1. Model concentration factors

Concentration factors for root (RCF), transpiration stream (TSCF) and stem (SCF) are calculated according to the empirically derived models of Briggs et al. (1982, 1983).
Shone & Wood (1974) defined the RCF for the uptake and sorption of a chemical by plant roots as:

$$\text{RCF [l/kg root ww]} = \frac{\text{concentration in root [mg/kg ww]}}{\text{concentration in external solution [mg/l]}}$$

with the concentration in root expressed in tissue wet weight (ww). Briggs et al. (1982) related experimental RCF values with the log K_{ow} values of the tested substances according to the following equitation:

$$\log(RCF_{Briggs} - 0.82) = 0.77 \log(K_{ow}) - 1.52$$

The TSCF according to Shone & Wood (1974) is defined as:

$$\text{TSCF [-]} = \frac{\text{concentration in transpired water [mg/l]}}{\text{concentration in external solution [mg/l]}}$$

and is related by Briggs et al. (1982) with the log K_{ow} values of the tested substances as:

$$TSCF_{Briggs} = 0.748\ e^{-[(\log(K_{ow}) - 1.78)^2 / 2.44]}$$

Briggs et al. (1983) defined the SCF_{liq}, which is the stem/external solution partition coefficient and the SCF_{tss}, being the stem/xylem sap partition coefficient:

$$SCF_{liq}\ \text{[l/kg stem ww]} = \frac{\text{concentration in stem [mg/kg ww]}}{\text{concentration in external solution [mg/l]}}$$

and

$$SCF_{tss}\ [l/kg\ stem\ ww] = \frac{\text{concentration in stem [mg/kg ww]}}{\text{concentration in transpired water [mg/l]}}$$

The SCF_{liq} can be calculated from the SCF_{tss} and TSCF as follows:

$$SCF_{tss}\ .\ TSCF_{Briggs} = (0.82 + 10^{[0.95\log(K_{ow}) - 2.05]})\ .\ (0.748e^{-[(\log(K_{ow}) - 1.78)^2 / 2.44]})$$

2.2. Data selection

Literature on experimental concentration factors for plants is collected from local databases at the RIVM and by on-line research in BIOSIS. The search profile is given in Annex 1. Laboratory studies with plants grown in soil and nutrient medium as well as field studies are included.

Data selection is carried out according to the following criteria:

- The Henry coefficient (dimensionless) of the tested substance is $< 3.10^{-2}$, to limit errors on concentration factors due to decreasing exposure concentrations in soil caused by volatilization.
- The % organic matter (o.m.) of the test soil is between 0 and 30, in view of the fact that the linear relation between organic fraction and the adsorption on soil does not hold with larger organic fractions.
- At least the initial nominal concentration in the soil is reported.
- Calculated concentrations in soil pore water (see 2.3.) and concentrations in nutrient medium are not above the water solubility.
- Calculated concentrations in the soil pore water lower than 0.00005 mg/l are excluded as these concentrations are considered insignificant, and because calculation errors are expected to become relative large compared to the values calculated. The value of 0.00005 mg/l is chosen arbitrarily.
- If it is obvious from the literature that the residues found in shoots are caused mainly by foliar uptake from the air, the shoot concentration factor is not included.

Data on log K_{ow}, water solubility and Henry coefficient of the substances regarded are collected from Mackay et al. (1992), the MEDCHEM database, Howard (1989, 1991) and the Agrochemicals Handbook (1994).

Experimental K_{oc} values are collected for the substances tested in soil (see 2.3). From Mackay et al. (1992) the soil, HPLC-determined values are selected, and if such value is not available, the values recommended by Bockting et al. (1993) are chosen. If not present in these public sources, values are obtained from confidential RIVM databases.

The following choices are made:

- When it is not reported whether a concentration is expressed in wet or dry weight, for plants wet weight (ww) and for soil dry weight (dw) is assumed, being the most common way of expression.
- The concentration factors from studies with radio-active labeled test compounds are based on total ^{14}C content of the plant tissue. So, metabolites formed in the plant tissue are included.

2.3. Data handling

When the exposure concentrations have been analysed, the geometric mean of the sample results at the end of the test and the initial (nominal) concentration is used for further calculations.
Concentrations in soil are recalculated to concentrations in the soil pore water according to the approach applied in USES (RIVM et al., 1994):

$$Cpore\ water_{soil} = \frac{Ctot_{soil} \cdot RHO_{soil}}{Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHO_{solid}}$$

with:

$Cpore\ water_{soil}$	: concentration in the pore water of the soil $[kg_{chem}/m_{water}^3]$
$Ctot_{soil}$	: total concentration in soil $[kg_{chem}/kg_{wet\ soil}]$
RHO_{soil}	: bulk density of the soil $[kg_{wet\ soil}/m_{wet\ soil}^3]$
$Fwater_{soil}$	: volume fraction of water in soil $[m^3/m^3]$
$Fsolid_{soil}$	: volume fraction of solids in soil $[m^3/m^3]$
Kp_{soil}	: solids-water partition coefficient $[m^3_{water}/kg_{solids}]$
RHO_{solid}	: density of the solid phase in the soil $[kg_{solids}/m_{wet\ soil}^3]$

The Kp_{soil} is calculated as:

$$Kp_{soil} = \frac{Foc_{soil} \cdot K_{oc}}{1000} \quad \text{or} \quad \frac{a \cdot Foc_{soil} \cdot K_{ow}}{1000}$$

with:

Kp_{soil}	: solids-water partition coefficient $[m^3_{water}/kg_{solids}]$
Foc_{soil}	: weight fraction organic carbon $[kg_{oc}/kg_{solid}]$
K_{oc}	: organic carbon-water partition coefficient $[l_{water}/kg_{solid}]$
a	: 0.411 as given by Karickhoff (1981)
K_{ow}	: octanol-water partition coefficient

If no experimental K_{oc} is found, the K_{oc} is replaced by: a . K_{ow} (see Annex 3). For RHO_{soil} and

RHO_{solid} values of 1400 kg/m^3 and 2500 kg/m^3 respectively are assumed (Koorevaar et al., 1983); for both $Fwater_{soil}$ and $Fsolid_{soil}$, 0.4 is used (default values in USES (RIVM et al., 1994)) unless these data have been reported.

Residues expressed in plant dry weight are recalculated to wet weight with the assumption of 15% plant dry weight.

As many authors have reported residues in whole shoots, we have compared the SCF_{liq}, which is the concentration factor for stems, with the experimental SCF for above ground plant parts (stem and leaves). When concentrations in leaves, stem and grow tip are given, the mean of these values is used to calculate the SCF. Whole plant concentration factors are included in this report, but are not used in any further action.

For all compounds the mean RCF, TSCF and SCF are calculated based on all exposure concentrations and plant species.

3. RESULTS

3.1. General remarks

An overview of all evaluated studies with relevant data is presented in Annex 2. Data on the physico-chemical properties of the tested substances are given in Annex 3. Latin names of the tested plant species, and the calculations of the concentrations in the soil pore water are given in Annex 4 and 5, respectively.

For mirex no reliable data on the water solubility have been found. The results from exposure to mirex up to 8.7 µg/l calculated soil pore water are included. When the calculated concentrations of mirex in soil pore water raise above 8.7 µg/l, concentration factors in plants decrease proportionally, which indicates that these higher concentrations may not be reached in the soil pore water.

3.2. Root concentration factor

Mean experimental data selected from the literature are summarized in Table 1, the comparison with the calculated RCFs according to Briggs et al. (1982) is shown in Figure 2.

Most of the 27 compounds involved are deviating less than a factor 5 from the model prediction. More than 5 times lower than the RCF_{Briggs} are the mean RCFs of endrin, ethirimol, mirex, phenanthrene, tetrachloroazobenzene and TCDD. These compounds have a log Kow ≥ 4.32. The mean RCFs of 2,4-dichlorophenol and pentachlorophenol are more than 5 times higher than the RCF_{Briggs}.

From the pesticides regarded, 12 out of 17 experimental RCFs are lower than the model values; the RCFs for the 5 PAHs involved are all below the RCF_{Briggs}.

The mean RCF of Aroclor 1248 (O'Connor et al, 1990) is based on residues in root peel only; residues in root core were below the detection limit of 20 µg/kg, indicating a mean concentration factor of below 110. DDT residues in potato and carrot roots as well as endrin levels in sugar beet and potatoe roots were below the detection limit, which was not reported (Harris & Sans, 1969). These data are not included in Table 1 and Figure 2.

3.3. Transpiration stream concentration factor

Table 2 and Figure 3 show the mean TSCF values found in the literature, and the comparison of these values with the model of Briggs et al. (1982). Three studies with TSCFs are available, all performed with plants exposed via nutrient medium. TSCF values more than 5 times below the $TSCF_{Briggs}$ are not found. More than 5 times higher are the experimental TSCFs of three of the oxabicycloalkanes: SD204328, SD204690 and SD208586, all with log Kow ≥ 4.2.

TABLE 1. Experimental data on root concentration factors.

compound	log K_{ow}	plant species	ref[1]	mean expos. conc in µg/l (S.D., n)[2]	mean RCF (S.D., n)[2]
acenaphthene/fluorene	3.92	carrot	1	0.14 (0.072 n=4)	23 (8.3 n=4)
Aroclor 1248	6.3	carrot	2	0.38 (0.33 n=4)	1500 (1400 n=4)
atratone	2.69	barley	3	100	1.3
atrazine	2.75	barley	3	100	1.9
benfluralin	5.29	carrot	4	1.1 (0.35 n=2)	230 (57 n=2)
bromacil	2.11	soybean	5	58000	6
carbofuran	2.32	garden bean	6	100	1.3
2,4-D	2.81	barley	3	200	8.1
DDT	6.91	sugar beet	7	3.8 (5.3 n=2)	4100 (5000 n=2)
		ryegrass	8		
2,4-dichlorophenol	3.06	soybean	9	110 (7.1 n=2)	130 (5.5 n=2)
		oat	9		
dieldrin	4.32	potatoe	7	21 (25 n=3)	43 (90 n=6)
		carrot	7		
		sugar beet	7		
		ryegrass	8		
diuron	2.68	barley	3	200	3.1
endrin	4.32	carrot	7	0.82	12
ethirimol	4.39	barley	3	200	0.66
ethofumesate	2.16	sugar beet	10	160	8.3
fluoranthene	5.22	carrot	1	0.066 (0.011 n=4)	65 (40 n=4)
haloxyfop	4.63	soybean	11	-	50 (47 n=3)
		red fescue	11		
		tall fescue	11		
lindane	3.61	ryegrass	8	19	17
mirex	5.28	garden bean	12	3.8 (4.3 n=3)	30 (11 n=12)
		soybean	12		
		sorghum	12		
		wheat	12		
naphthalene	3.37	carrot	1	0.37 (0.35 n=5)	5.8 (3.9 n=5)

(TABLE 1. continued)

compound	log K_{ow}	plant species	ref[1]	mean expos. conc in µg/l (S.D., n)[2]	mean RCF (S.D., n)[2]
nitrobenzene	1.85	soybean	13	8000	1.2 (0.45 n=8)
		barley	13		
		lettuce	13		
		russian olive	13		
		autumn olive	13		
		green ash	13		
		hybrid poplar	13		
		honeysuckle	13		
pentachlorophenol	5.24	soybean	14	12 (2.6 n=2)	2700 (1700 n=2)
		spinach	14		
phenanthrene	4.57	carrot	1	0.14 (0.053 n=7)	11 (7.6 n=7)
pyrene	5.18	carrot	1	0.069 (0.017 n=4)	77 (43 n=4)
simazine	2.18	barley	3	200	4.5
TCDD	6.8	soybean	15	0.15 (0.033 n=2)	780 (180 n=2)
		maize	15		
tetrachloro-azobenzene	6.46	carrot	16	0.39	490 (660 n=2)

[1] List of authors, mentioned in Table 1, 2 or 3:

1 Wild & Jones, 1992	11 Aguero-Alvarado et al., 1991
2 O'Connor et al., 1990	12 De la Cruz et al., 1975
3 Shone & Wood, 1974	13 McFarlane et al., 1990
4 Businelli et al., 1975	14 Casterline et al., 1985
5 Boersma et al., 1991	15 McCrady et al., 1990
6 Trapp et al., 1991	16 Worobey, 1988
7 Harris & Sans, 1969	17 Hsu et al., 1990
8 Voerman et al., 1975	18 Pylypiw et al., 1993
9 Isensee & Jones, 1971	19 Tafuri et al., 1977
10 Eshel et al., 1978	20 Beall & Nash, 1971

[2] S.D.: standard deviation; n: number of measurements

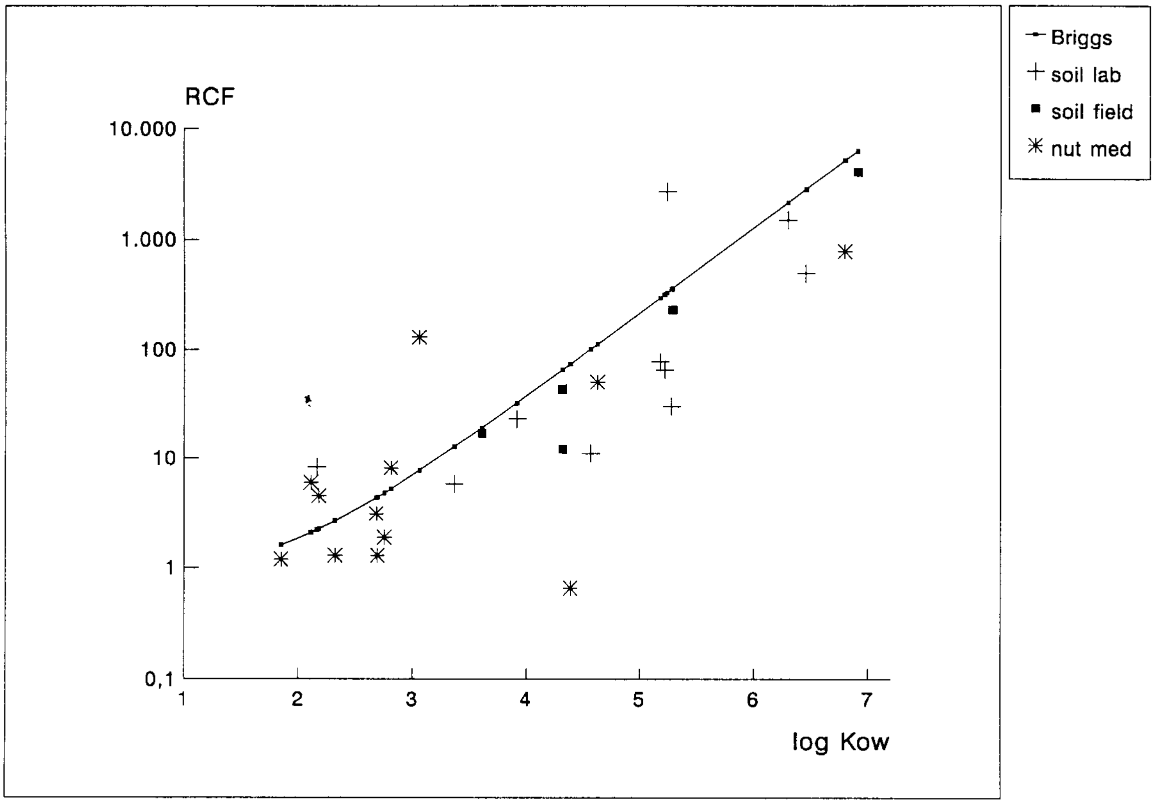

FIGURE 2. RCF: Comparison of the model of Briggs et al. (1982) and mean experimental values.

(Briggs: RCF calculated according to Briggs et al. (1982); soil lab: RCF from laboratory experiment(s), exposure via soil pore water; soil field: RCF from field experiment(s), exposure via soil pore water; nut med: experimental RCF, exposure via nutrient medium.)

TABLE 2. Experimental data on transpiration stream concentration factors.

compound	log K_{ow}	plant species	ref[1]	mean expos. conc in µg/l (S.D., n)[2]	mean TSCF (S.D., n)[2]
atratone	2.69	barley	3	100	0.78
atrazine	2.75	barley	3	100	0.75
cinmethylin (SD95481)	4.62	soybean	17	-	0.08
2,4-D	2.81	barley	3	200	0.14
diuron	2.68	barley	3	200	0.81
ethirimol	4.39	barley	3	200	0.09
nitrobenzene	1.85	soybean	13	8000	0.74 (0.067 n=8)
		barley	13		
		lettuce	13		
		russian olive	13		
		autumn olive	13		
		green ash	13		
		hybrid poplar	13		
		honeysuckle	13		
SD96638	4.1	soybean	17	-	0.35
SD98319	2.73	soybean	17	-	0.58
SD204328	4.59	soybean	17	-	0.5
SD204689	3.68	soybean	17	-	0.47
SD204690	4.2	soybean	17	-	0.52
SD204691	3.53	soybean	17	-	0.72
SD205857	3.55	soybean	17	-	0.51
SD207573	0.96	soybean	17	-	0.22
SD208213	2.52	soybean	17	-	0.55
SD208380	1.82	soybean	17	-	0.24
SD208586	5.29	soybean	17	-	0.19
simazine	2.18	barley	3	200	0.9

[1] See legenda to Table 1.

[2] S.D.: standard deviation; n: number of measurements

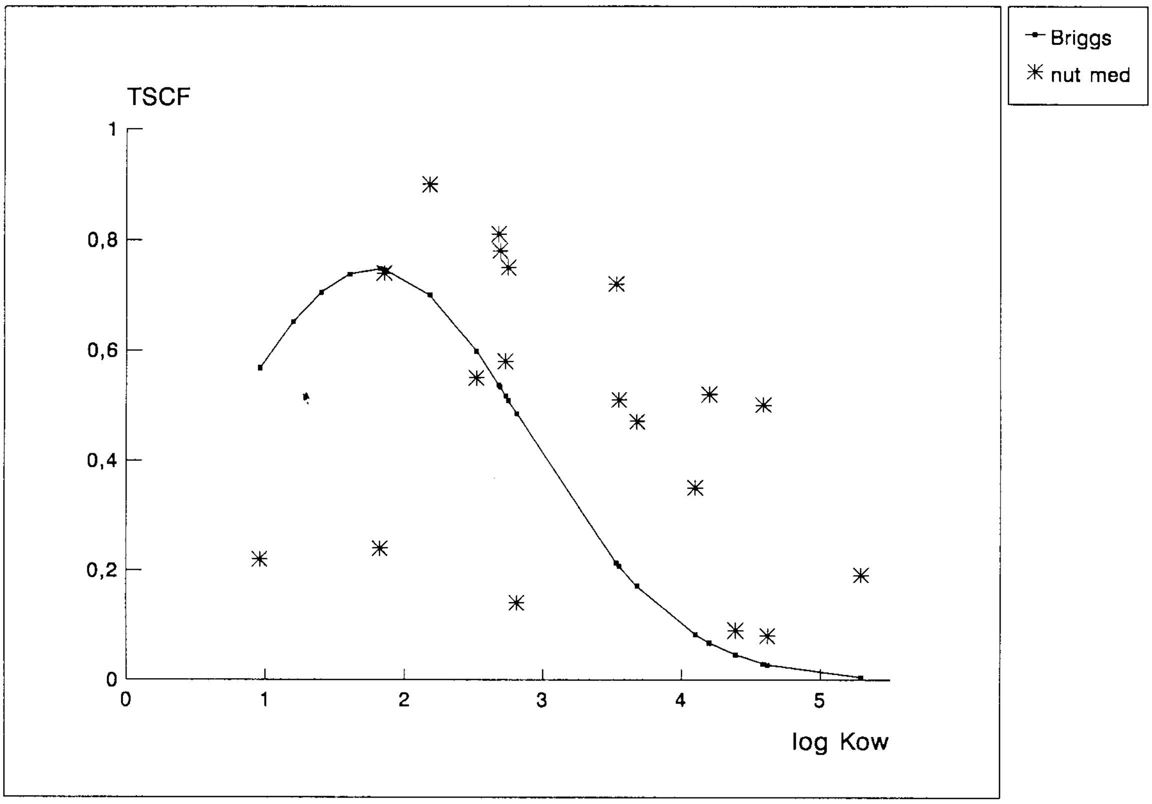

FIGURE 3. TSCF: Comparison of the model of Briggs et al. (1982) and mean experimental values.
(Briggs: TSCF calculated according to Briggs et al. (1982); nut med: experimental TSCF, exposure via nutrient medium.)

3.4. Shoot concentration factor

Mean concentration factors for whole shoots are given in Table 3, and are compared to the model values of Briggs et al. (1983) in Figure 4. For 9 of the 16 substances involved, the mean SCF values deviate more than a factor 5 of the SCF_{Briggs}.
More than 5 times lower than the model prediction are the SCFs found for atrazine, metolachlor, alachlor and lindane. The SCFs of DDT, ethofumesate, pentachlorophenol and tetrachloroazobenzene (510, 74, 620, and 77, respectively) are more than 50 times higher. They are excluded from Figure 4, because otherwise the values more close to the model become invisible. The SCF of bromacil is 13 times higher than could be expected from the model of Briggs et al. (1983).
Residues of Aroclor 1248 in shoots were below the detection limit of 20 µg/kg (O'Connor et al., 1990), which would give a mean SCF of lower than 110. The levels of benfluralin in carrot foliage were below the detection limit of 5 µg/kg (Businelli et al., 1975), so a mean SCF should be below 5. Endrin levels in alfalfa, oat and sugar beet (Harris & Sans, 1969) were also below the detection limit, which was not reported. These data are not included in Table 3 and Figure 4.

TABLE 3. Experimental data on shoot concentration factors.

compound	log K_{ow}	plant species	ref[1]	mean expos. conc in μg/l (S.D., n)[2]	mean SCF (S.D., n)[2]
alachlor	3.52	corn	18	110	0.42
atrazine	2.75	corn	18	380	0.084
bromacil	2.11	soybean	5	58000	16 (7.8 n=2)
carbofuran	2.32	garden bean	6	100	1.6
chlordane	5.54	alfalfa	19	1.6 (1 n=2)	7.8 (5.3 n=2)
DDT	6.91	alfalfa	7	4.1 (4.7 n=4)	510 (550 n=8)
		oat	7		
		corn	7		
		sugar beet	7		
		ryegrass	8		
		soybean	20		
2,4-dichlorophenol	3.06	soybean	9	110 (7.1 n=2)	1.4 (1.7 n=2)
		oat	9		
dieldrin	4.32	alfalfa	7	130 (210 n=4)	3.0 (1.3 n=7)
		oat	7		
		corn	7		
		sugar beet	7		
		ryegrass	8		
		soybean	20		
endrin	4.32	soybean	20	110 (150 n=2)	20 (11 n=2)
		corn	7		
ethofumesate	2.16	sugar beet	10	160	74
haloxyfop	4.63	soybean	11	-	6.6 (3.4 n=3)
		red fescue	11	-	
		tall fescue	11	-	
lindane	3.61	ryegrass	8	19	0.79
metolachlor	3.13	corn	18	600	0.046
mirex	5.28	garden bean	12	3.8 (4.3 n=3)	13 (8.6 n=12)
		soybean	12		
		sorghum	12		
		wheat	12		

(TABLE 3, continued)

compound	log K_{ow}	plant species	ref[1]	expos. conc in µg/l (S.D., n)[2]	mean SCF (S.D., n)[2]
pentachlorophenol	5.24	soybean	14	12 (2.6 n=2)	620 (55 n=2)
		spinach	14		
tetrachloroazobenzene	6.46	carrot	16	0.39	77

[1] See legenda to Table 1.

[2] S.D.: standard deviation; n: number of measurements

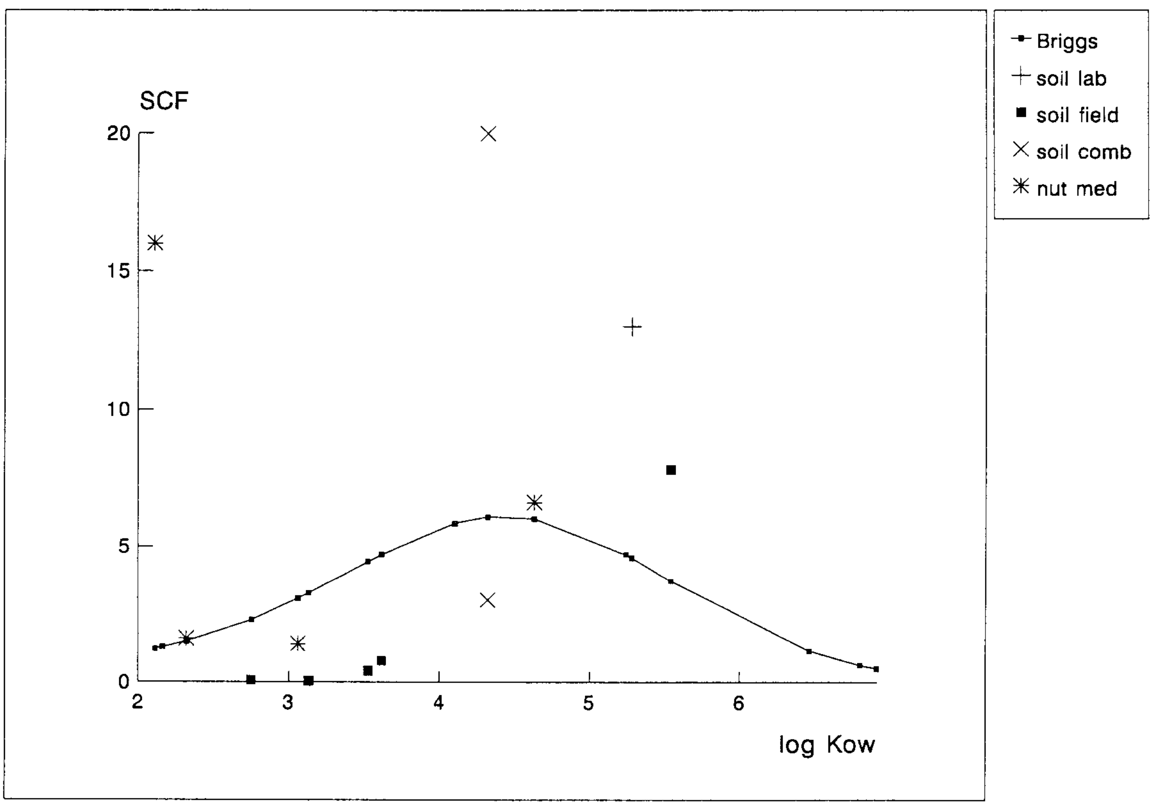

FIGURE 4. SCF: Comparison of the model of Briggs et al. (1983) and mean experimental values.
(Briggs: SCF calculated by Briggs et al. (1983); soil lab: SCF from laboratory experiment(s), exposure via soil pore water; soil field: SCF from field experiment(s), exposure via soil pore water; soil comb: SCF from laboratory and field experiments, exposure via soil pore water; nut med: experimental SCF, exposure via nutrient medium.)

4. DISCUSSION

4.1. General remarks

Briggs et al. (1982, 1983) derived the relations between log K_{ow} and plant concentration factors from experiments using young soybean plants grown in nutrient medium for compounds with log K_{ow} values in the range of -0.57 to 3.7. The experimental data set collected in this report, contains data on compounds with a log K_{ow} between 0.96 and 6.91 and a variety of plant species at different growth stages. A huge diversity of exposure methods and duration was also observed. Variation in extraction methods for plant and soil samples will have influenced the comparison between the data. From studies with radio-labeled substances the concentrations of the substance and metabolites were used for the calculation of the concentration factors. Metabolites formed in soil or in plants may have higher water solubilities and therefore move upwards more than expected on the basis of the log K_{ow} value of the parent compound. For example, the formation and translocation of metabolites may have caused the high SCF value of radio-labeled ethofumesate (Eshel et al., 1978).

Biodegradation of the tested compound in the soil can lead to an underestimation of the concentration factors in studies where soil concentrations were not analysed.

The uptake and transport will be influenced for substances (mainly pesticides, e.g. ethirimol, 2,4-D with pKa values close to the pH of the soil, nutrient solution or xylem fluid (Shone & Wood, 1974). These substances will partly be dissociated and therefore may be translocated more easily. For this type of compounds a direct relation between log K_{ow} (at a certain pH) and concentration factors in root and stem is not clear.

Several sources of uncertainty have been introduced by calculating the concentration in soil pore water from the concentration in soil. For RHO_{soil} a value of 1400 kg/m^3 was assumed, where this parameter may vary substantially in different soil types, probably from 800 to 3400 kg/m^3. In most cases the default values from USES (RIVM et al., 1994) had to be used for RHO_{solid}, $Fwater_{soil}$ and $Fsolid_{soil}$. The constant a in the calculated Kp values is considered 0.411 according to Karickhoff (1981), but will differ for various compounds.

We selected studies carried out in test soils with a percentage organic matter below 30. However, in soils with less than 2% o.m. the adsorption might not be linear with the organic fraction (Denneman & van Gestel, 1990). For example, O'Connor et al. (1990) exposed carrots to Aroclor 1248 in two test soils with organic fractions of 1.1 and 0.2%. In the soil with 1.1% o.m. the RCF values for root peel were 222 and 379, whereas RCFs of 2452 and 2885 were found after exposure in soil with 0.2% o.m.

The recalculation from plant dry weight to wet weight is based on an assumed dry weight of 15%. This can lead to an underestimation of the concentration factors of a factor 1.5 to 3 in studies with young plants without well developed energy-storing organs like seeds or tubers, having 5 to 10% dry weight (see Bockting & Van den Berg, 1992).

4.2. Root concentraton factor

The experimental values for the RCF are in reasonable good agreement with the relation proposed by Briggs et al. (1982), and certainly adequate for general risk assessment purposes (Fig. 2). This is even more remarkable when viewing the diversity of plant species and substances for which the experimental data were derived.

It is striking that the experimental data are generally lower than the regression of Briggs and coworkers (1982) predicts. This may be explained by the fact that the barley plants of Briggs and coworkers were grown in nutrient solution and that there was evidence that an equilibrium between roots and solution was reached within 24 hours. For many of the experimental results collected here, it remains unclear if an equilibrium was actually achieved. Results of Boersma et al. (1991) and Trapp et al. (1994) showed that for soybean there was no equilibrium reached with bromacil after 8 days.

Furthermore, observed RCF values in soil may be lower than expected because the plant is diminishing the concentration in the vicinity of the roots due to uptake, i.e., a gradient is formed in the soil. However, differences between studies in soil vs. nutrient medium were not obvious (Fig. 2 and Annex 2). Results of field and laboratory studies were also similar.

For several compounds high standard deviations were calculated (see Table 1). For haloxyfop (Aguero-Alvarado et al., 1991), DDT and dieldrin (Harris & Sans, 1969; Voerman et al., 1975) the high variation can be clearly attributed to the different plant species tested: grass species showed RCF values 10 or more times higher than crop species such as carrot, potatoe and soybean. For pentachlorophenol the RCF of soybean was 2.5 times higher than of spinach (Casterline et al. 1985).

The high variation in the RCF values of Aroclor 1248 (O'Connor et al., 1990) is probably related to the low percentage organic matter in the test soils (see 4.1.).

In several studies with carrots the residues in root peel and root core were analysed seperately. For Aroclor 1248 only residues in root peel could be determined, residues in core were not found (O'Connor et al., 1990). The concentration of tetrachloroazobenzene in root peel was ca. 40 times higher than in root core (Worobey, 1988). The residues of PAHs in root peel of carrots were always higher than in core, with some variation between the different compounds (Wild & Jones, 1992). However, the differences were never more than a factor of 6. It has to be noted that the exposure to a mixture of PAHs in sewage sludge mixed with soil might have influenced the accumulation of the individual compounds, although the mechanism is not known.

4.3. Transpiration stream concentration factor

Data on experimental TSCFs are more or less in agreement with the predictions of Briggs et al. (1982) although the variation is large. The contribution of this plant compartment to the assessments made in USES is less important than that from the root and shoot.

4.4. Shoot concentration factor

For the SCF, the agreement between expected values and experimental data is not satisfactory (Fig. 4). This may sometimes be due to the experimental situation, where volatilization and subsequent uptake by the leaf could not be avoided. It is clear that this pathway exists (see e.g. Bacci & Gaggi, 1985; Schroll et al., 1994), but its contribution in the laboratory and the field remains unclear. In contrast with the laboratory situation, air concentrations in the field will not build up rapidly.

It has to be kept in mind that the SCF of Briggs et al. (1983) describes the partitioning between exposure medium and *stems* of plants. Stems may equilibrate with the transpiration stream. In our study the concentration in the leaves is also included. Substances with low log K_{ow} values may accumulate in the leaf, as they move upwards in the transpiration stream. In the leaf the water is transpired, leaving the substance in the leaf tissue. An indication can be retrieved from the experiments of Trapp et al. (1994), where concentrations in leaves were higher than in stems when the transpiration rate was high. The authors concluded that the leaves become a sink for bromacil and its metabolites. The results of Boersma et al. (1991) support this view. This implies that the SCF as derived by Briggs and coworkers (1983) is not an appropriate relationship when predicting concentrations in food crops for human exposure.

For lipophilic substances, e.g. mirex and pentachlorophenol (log K_{ow} > 5) concentrations found in leaves were lower than in stems, as one would expect. However, levels in both plant parts were significantly higher than predicted by Briggs and coworkers (1983) (see Annex 2.) On the contrary, the residues of mirex in roots were considerably lower than predicted by Briggs et al. (1982). The concentration factors of mirex decreased with increasing soil concentrations or decreasing soil organic matter content for all plant species tested (De la Cruz et al., 1975). The water solubility of mirex varies highly in the different handbooks (between 'practically insoluble' and a calculated value of 6.4 mg/l). The maximum concentration possible in the soil pore water is therefore hard to estimate and might have influenced the concentration factors. The low contents of organic matter of the two test soils (0.87 and 0.04% o.m., respectively) used in the study of De la Cruz et al. (1975) may also have influenced the results (see 4.1).

Differences between plant species may have played a role in the high standard deviations calculated for the mean SCF of 2,4-dichlorophenol and DDT (see Table 3.) The SCF value of 2,4-dichlorophenol for soybean and oat were 0.2 and 2.5, respectively (Isensee & Jones, 1971). A SCF of DDT of 93 was found in ryegrass (Voerman & Besemer, 1975) and in soybean of 14 (Beall & Nash, 1971). The high SCF values for DDT (166 - 1700) obtained from Harris & Sans (1969) were probably the result of drift from the treatment of adjacent fields, as these authors stated.

For haloxyfop the SCF values found for two grasses were higher than for soybean, but less obvious than was seen with the RCF values (Aguero-Alvarado et al., 1991).

4.5. Conclusions

It can be concluded that the root concentration factors as derived by Briggs et al. (1982), are satisfactory for the purpose set in USES (see Vermeire et al., 1994; Jager et al., 1994). It seems likely that this RCF is a maximum value especially for substances with log $K_{ow} > 4$.

The transpiration stream concentration factors found in the literature are more or less in agreement with the values calculated by Briggs et al. (1982).

Several shoot concentration factors found in the literature are much higher than the values calculated by Briggs et al. (1983). This might be due to uptake from air, non-equilibrium situations and in case of radio-labeled substances, the SCF might be based on metabolites instead of the parent compound. In addition Briggs et al. (1983) uses stem concentrations; leaves were excluded, whereas in this study the SCF was based on shoots. For the SCF used in USES major adaptations are necessary.

4.6. Recommendations

It is clear that the inability to predict shoot concentration factors requires further research.

Research on the applicability of other existing models for estimating concentrations in shoots (e.g. Trapp et al. 1994) can be performed with the data set collected for this report.

Further refinement of the data on SCF values gathered in this study with regard to exposure methods, plant species, and specific physico-chemical properties of the tested substances is also possible.

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ANNEXES

ANNEX 1

SEARCH PROFILE FOR ON-LINE RESEARCH IN BIOSIS, APRIL 1993

f (bioaccumulat? or bioconcentrat? or accumulat?)/(ti;ut)

f (biotransfer or transfer or uptake or translocation or stem#)/ (ti;ut)

f (transpiration stream or root# or distribution or disposition)/(ti;ut)

f bcf or baf or tscf or rcf or scf

f 1 to 4

f (soil# or nutrient solution or hydroponic? or terrestri?)/(ti;ab)

f 5 and 6

f 7 and sc=51520

f (selenium or aluminium or cadmium or coppper or iron)/(ti;ut)

f (manganese or zinc or lead or mercury or tin or phosphorus)/(ti;ut)

f (sulphur or phosphate# or sodium or potassium or metal#)/(ti;ut)

f (arsenic or magnesium or calcium or nitrogen or ammonium)/(ti;ut)

f (nitrification or nitrifying or nitrate# or nitrite#)/(ti;ut)

f 9 to 13

f 8 not 14

f 15 not la=(bu or ch or cz or hu or it or ja or po or ru or sp)

ANNEX 2

ACCUMULATION FACTORS FOR PLANTS

Exposure duration:

d: days, w: weeks, m: months, gr se: growing season

Nutrient medium:

Hoagl sol: Hoagland solution, nutr sol: nutrient solution,
modif Hoagl sol: modified Hoagland solution,
half str Hogl sol: half strength Hoagland solution

Concentrations reported as:

- soil: mg/kg dry weight
- plant tissue: mg/kg wet weight
- soil liq (calculated concentration in soil pore water): mg/l
- nutrient medium: mg/l

If otherwise, it is mentioned in the column 'comment".

BCF: bioconcentration factor for the plant part(s), mentioned in the column 'exposure period and plant part(s)'

compound	species	% OM	exposure period and plant part(s)	soil conc in mg/kg dw	tissue conc in mg/kg ww	BCF plant/ soil	conc in soil liq in mg/l	BCF plant/ soil liq	reference	comment
FIELD STUDIES:										
DDT	alfalfa	3.6%	1 gr se shoot	0.57	0.01	0.018	0.00006	166.66	Harris & Sans 1969	DDT was not detected in carrot and potatoe.
	oat		1 gr se shoot	0.57	0.03	0.053	0.00006	500		Residues in aerial plant parts
	corn		1 gr se shoot	0.57	0.04	0.07	0.00006	666.66		were probably the result of
	sugar beet		1 gr se shoot	0.57	0.04	0.07	0.00006	666.66		drift from treatment to
	sugar beet		1 gr se tuber	0.57	0.03	0.05	0.00006	500		adjacent fields.
	alfalfa	1.4%	1 gr se shoot	0.23	0.02	0.089	0.00007	285.71		
	corn		1 gr se shoot	0.23	0.12	0.533	0.00007	1714.2		
Dieldrin	alfalfa	3.6%	1 gr se shoot	1.12	0.02	0.018	0.0061	3.2786		
	oat		1 gr se shoot	1.12	0.02	0.018	0.0061	3.2786		
	corn		1 gr se shoot	1.12	0.02	0.018	0.0061	3.2786		
	sugar beet		1 gr se shoot	1.12	0.03	0.027	0.0061	4.9180		
	potato		1 gr se tuber	1.12	0.03	0.027	0.0061	4.9180		
	carrot		1 gr se tuber	1.12	0.04	0.036	0.0061	6.5573		
	sugar beet		1 gr se tuber	1.12	0.07	0.063	0.0061	11.475		
	corn	1.4%	1 gr se shoot	0.57	0.01	0.018	0.008	1.25		
	potato		1 gr se tuber	0.57	0.03	0.053	0.008	3.75		
	carrot		1 gr se tuber	0.57	0.05	0.088	0.008	6.25		
endrin	corn	1.4%	1 gr se shoot	0.12	0.01	0.083	0.00082	12.195		
	carrot		1 gr se tuber	0.12	0.01	0.083	0.00082	12.195		
alachlor	corn	3–5%	14 d shoot	0.52	0.047	0.09	0.112	0.4196	Pylypiw et al. 1993	Soil samples were taken from a depth of 0–15 cm.
atrazine	corn	3–5%	14 d shoot	1.50	0.032	0.021	0.382	0.0837		
metolachlor	corn	3–5%	14 d shoot	2.63	0.028	0.011	0.604	0.0463		
DDT	ryegrass	3%	6 m shoot	56.50	0.7	0.0124	0.0075	93.333	Voerman et al. 1975	Conc's in plant reported in DW recalculated to WW.
			6 m root	56.50	57.21	1.0126	0.0075	7628		DDT: DDT + DDE residues in
dieldrin	ryegrass	3%	6 m shoot	7.64	0.06	0.0079	0.05	1.2		soil and plant were summed.
			6 m root	7.64	11.33	1.483	0.05	226.6		The grass was mown 2 times
lindane	ryegrass	3%	6 m shoot	0.33	0.015	0.04545	0.019	0.7894		during the growing season.
			6 m root	0.33	0.33	1	0.019	17.368		

compound	species	% OM	exposure period and plant part(s)	soil conc in mg/kg dw	tissue conc in mg/kg ww	BCF plant/ soil	conc in soil liq in mg/l	BCF plant/ soil liq	reference	comment
chlordane	alfalfa	1.7%	79 d shoot	1.24	0.01	0.008064	0.00087	11.494	Tafuri et al. 1977	10% granules. Soil concs based on 0–10cm layer. Shoots washed with 1% lauryl suphate.
			79 d shoot	3.30	0.0093	0.002818	0.0023	4.0434		
benfluralin	carrot	1.2%	106 d root	0.46	0.214	0.465217	0.0008	267.5	Businelli et al. 1975	Residues in foliage were *always below detection limit of 5 ng/g.
			106 d root	0.76	0.243	0.319736	0.0013	186.92		
			106 d peeled root	0.46	0.017	0.036956	0.0008	21.25		
				0.76	0.019	0.025	0.0013	14.615		
LABORATORY STUDIES:										
DDT	soybean	0.9%	53 d shoot	20.00	0.12	0.006	0.00885	13.559	Beall & Nash 1971	14C labeled test compounds. Initial nominal soil concs, volatilization prohibited. Concs in plant dw reported, converted to ww.
dieldrin			53 d shoot	20.00	1.62	0.081	0.4361	3.7147		
endrin			53 d shoot	20.00	5.72	0.286	0.2115	27.044		
Aroclor 1248	carrot	1.1%	75 d root peel	0.50	0.020	0.04	0.00009	222.22	O'Connor et al. 1990	Conc's in all plant parts except root peel were below detection limits (0.02 mg/kg). BCF based on initial soil concentration in dw.
			75 d root peel	0.75	0.053	0.07	0.00014	378.57		
		0.2%	75 d root peel	0.50	1.275	2.55	0.00052	2451.9		
			75 d root peel	0.75	2.250	3.00	0.00078	2884.6		
DDT	barley	3.5%	7 d whole pl	2.16	0.87	0.41	0.00022	3954.5	Trapp et al. 1990	Test substance mixed with soil; soil not covered, so volatilization could occur.
dieldrin			7 d whole pl	2.08	1.24	0.60				
atrazine			7 d whole pl	0.98	2.53	2.58	0.332	7.6204		
naphtalene	carrot	2.1%	82 d root peel	1.88	1.58	0.84	0.8127	1.9441	Wild & Jones 1992	Sewage sludge contaminated with PAH's was mixed with soil at three rates (6.1, 18.6 and 62.1 g/kg dry weight giving 2.9, 3.9 and
		2.1%	82 d root core	1.59	0.62	0.39	0.09746	6.3615		
		2.9%	82 d root core	1.47	0.78	0.53	0.0657	11.872		
		3.9%	82 d root core	6.58	1.25	0.19	0.2197	5.6895		
		7.6%	82 d root core	39.40	1.97	0.05	0.6794	2.8996		

compound	species	% OM	exposure period and plant part(s)	soil conc in mg/kg dw	tissue conc in mg/kg ww	BCF plant/ soil	conc in soil liq in mg/l	BCF plant/ soil liq	reference	comment
acenaphthene/ fluorene	carrot	2.1%	82 d root peel	4.06	2.19	0.54	0.0667	32.833		Concentrations of 12 PAH's
		2.9%	82 d root peel	8.38	3.27	0.39	0.0998	32.765		were measured at start and
		3.9%	82 d root peel	17.74	4.08	0.23	0.1573	25.937		end of test in the treat–
		7.6%	82 d root peel	51.00	3.57	0.07	0.2325	15.354		ments and the control
		2.1%	82 d root core	3.57	1.25	0.35	0.0586	21.331		(2.1% om). The BCF values
		2.9%	82 d root core	7.09	2.27	0.32	0.08445	26.879		are based on average soil
		3.9%	82 d root core	16.53	3.14	0.19	0.1466	21.418		concs. Concs in plant dw
		7.6%	82 d root core	53.00	2.12	0.04	0.2416	8.7748		reported, converted to ww.
										Soil concs not reported by
phenanthrene	carrot	2.1%	82 d root peel	16.27	1.79	0.11	0.07393	24.212		the authors, calculated as
		2.9%	82 d root peel	48.67	1.46	0.03	0.1602	9.1136		tissue conc/BCF.
		3.9%	82 d root peel	74.25	2.97	0.04	0.1818	16.336		Concentration factors
		7.6%	82 d root peel	130.00	2.6	0.02	0.1634	15.911		reported as 0 by the
		2.1%	82 d root core	15.00	0.3	0.02	0.0682	4.3988		authors were not included
		2.9%	82 d root core	36.00	0.72	0.02	0.1185	6.0759		in this table.
		3.9%	82 d root core	83.00	0.83	0.01	0.2033	4.0826		Compounds with soil liq concs
										< 0.05 ug/l are excluded.
fluoranthene	carrot	2.1%	82 d root peel	47.00	0.47	0.01	0.0794	5.9193		
		2.9%	82 d root peel	42.90	4.29	0.1	0.0525	81.714		
		3.9%	82 d root peel	72.00	5.76	0.08	0.0655	87.938		NB SOIL AND TISSUE CONC'S
		7.6%	82 d root peel	140.25	5.61	0.04	0.0655	85.648		IN UG/KG AND UG/L!!!!!
pyrene	carrot	2.1%	82 d root peel	41.50	0.83	0.02	0.052	15.961		
		2.9%	82 d root peel	63.63	5.09	0.08	0.0578	88.062		
		3.9%	82 d root peel	111.83	6.71	0.06	0.07548	88.897		
		7.6%	82 d root peel	258.75	10.35	0.04	0.0896	115.51		
3,4,3',4'– tetrachloro– azobenzene	carrot	3%	4 m root peel	0.02	0.0019	0.095	0		Worobey 1988	Soil conc's not analysed;
			4 m root peel	10.00	0.375	0.038	0.00039	961.53		plant residues likely in WW.
			4 m root pulp	0.02	0.0011	0.055	0			
			4 m root pulp	10.00	0.01	0.001	0.00039	25.641		
			4 m tops	0.02	0.00005	0.0025	0			
			4 m tops	10.00	0.03	0.003	0.00039	76.923		

compound	species	% OM	exposure period and plant part(s)	soil conc in mg/kg dw	tissue conc in mg/kg ww	BCF plant/ soil	conc in soil liq in mg/l	BCF plant/ soil liq	reference	comment
mirex	garden bean	0.87%	4 w grow tip	3.50	0.018	0.005142	0.0087	2.0689	De la Cruz et al 1975	Concs in plant dw reported, converted to ww.
			4 w leaves	3.50	0.03	0.008571	0.0087	3.4482		
			4 w stem	3.50	0.0705	0.020142	0.0087	8.1034		
			4 w root	3.50	0.177	0.050571	0.0087	20.344		
		0.04%	4 w grow tip	3.40	0.0405	0.011911	0.1806	0.2242		
			4 w leaves	3.40	0.06	0.017647	0.1806	0.3322		
			4 w stem	3.40	0.0825	0.024264	0.1806	0.4568		
			4 w root	3.40	0.252	0.074117	0.1806	1.3953		
mirex	garden bean	0.87%	4 w grow tip	0.80	0.009	0.01125	0.002	4.5		
			4 w leaves	0.80	0.0165	0.020625	0.002	8.25		
			4 w stem	0.80	0.0353	0.044125	0.002	17.65		
			4 w root	0.80	0.0735	0.091875	0.002	36.75		
		0.04%	4 w grow tip	0.80	0.0135	0.016875	0.0425	0.3176		
			4 w leaves	0.80	0.0285	0.035625	0.0425	0.6705		
			4 w stem	0.80	0.0495	0.061875	0.0425	1.1647		
			4 w root	0.80	0.1035	0.129375	0.0425	2.4352		
mirex	garden bean	0.87%	4 w grow tip	0.30	0.003	0.01	0.00075	4		
			4 w leaves	0.30	0.0015	0.005	0.00075	2		
			4 w stem	0.30	0.009	0.03	0.00075	12		
			4 w root	0.30	0.0315	0.105	0.00075	42		
		0.04%	4 w grow tip	0.31	0.006	0.019354	0.0165	0.3636		
			4 w leaves	0.31	0.0015	0.004838	0.0165	0.0909		
			4 w stem	0.31	0.0278	0.089677	0.0165	1.6848		
			4 w root	0.31	0.0345	0.111290	0.0165	2.0909		
mirex	soybean	0.87%	4 w grow tip	3.50	0.0135	0.003857	0.0087	1.5517		
			4 w leaves	3.50	0.0315	0.009	0.0087	3.6206		
			4 w stem	3.50	0.0833	0.0238	0.0087	9.5747		
			4 w root	3.50	0.1875	0.053571	0.0087	21.551		
		0.04%	4 w grow tip	3.40	0.0465	0.013676	0.1806	0.2574		
			4 w leaves	3.40	0.054	0.015882	0.1806	0.2990		
			4 w stem	3.40	0.1238	0.036411	0.1806	0.6854		
			4 w root	3.40	0.2205	0.064852	0.1806	1.2209		
mirex	soybean	0.87%	4 w grow tip	0.80	0.009	0.01125	0.002	4.5		
			4 w leaves	0.80	0.018	0.0225	0.002	9		
			4 w stem	0.80	0.0338	0.04225	0.002	16.9		
			4 w root	0.80	0.0735	0.091875	0.002	36.75		
		0.04%	4 w grow tip	0.80	0.012	0.015	0.0425	0.2823		
			4 w leaves	0.80	0.027	0.03375	0.0425	0.6352		
			4 w stem	0.80	0.045	0.05625	0.0425	1.0588		
			4 w root	0.80	0.0735	0.091875	0.0425	1.7294		

compound	species	% OM	exposure period and plant part(s)	soil conc in mg/kg dw	tissue conc in mg/kg ww	BCF plant/ soil	conc in soil liq in mg/l	BCF plant/ soil liq	reference	comment
mirex	soybean	0.87%	4 w grow tip	0.30	0.0015	0.005	0.00075	2	De la Cruz et al 1975	
			4 w leaves	0.30	0.015	0.05	0.00075	20		
			4 w stem	0.30	0.0173	0.057666	0.00075	23.066		
			4 w root	0.30	0.0255	0.085	0.00075	34		
		0.04%	4 w grow tip	0.31	0.0075	0.024193	0.0165	0.4545		*
			4 w leaves	0.31	0.0045	0.014516	0.0165	0.2727		
			4 w stem	0.31	0.03	0.096774	0.0165	1.8181		
			4 w root	0.31	0.048	0.154838	0.0165	2.9090		
mirex	sorghum	0.87%	4 w leaves	3.50	0.033	0.009428	0.0087	3.7931		
			4 w stem	3.50	0.0765	0.021857	0.0087	8.7931		
			4 w root	3.50	0.1215	0.034714	0.0087	13.965		
		0.04%	4 w leaves	3.50	0.06	0.017142	0.1806	0.3322		
			4 w stem	3.50	0.24	0.068571	0.1806	1.3289		
			4 w root	3.50	0.2565	0.073285	0.1806	1.4202		
mirex	sorghum	0.87%	4 w leaves	0.80	0.03	0.0375	0.002	15		
			4 w stem	0.80	0.0465	0.058125	0.002	23.25		
			4 w root	0.80	0.066	0.0825	0.002	33		
		0.04%	4 w leaves	0.80	0.0495	0.061875	0.0425	1.1647		
			4 w stem	0.80	0.069	0.08625	0.0425	1.6235		
			4 w root	0.80	0.1005	0.125625	0.0425	2.3647		
mirex	sorghum	0.87%	4 w leaves	0.30	0.0165	0.055	0.00075	22		
			4 w stem	0.30	0.0255	0.085	0.00075	34		
			4 w root	0.30	0.03	0.1	0.00075	40		
		0.04%	4 w leaves	0.31	0.027	0.087096	0.0165	1.6363		
			4 w stem	0.31	0.0315	0.101612	0.0165	1.9090		
			4 w root	0.31	0.042	0.135483	0.0165	2.5454		
mirex	wheat	0.87%	4 w leaves	3.50	0.0255	0.007285	0.0087	2.9310		
			4 w stem	3.50	0.084	0.024	0.0087	9.6551		
			4 w root	3.50	0.1755	0.050142	0.0087	20.172		
		0.04%	4 w leaves	3.40	0.0315	0.009264	0.1806	0.1744		
			4 w stem	3.40	0.1425	0.041911	0.1806	0.7890		
			4 w root	3.40	0.1995	0.058676	0.1806	1.1046		
mirex	wheat	0.87%	4 w leaves	0.80	0.027	0.03375	0.002	13.5		
			4 w stem	0.80	0.03	0.0375	0.002	15		
			4 w root	0.80	0.0405	0.050625	0.002	20.25		
		0.04%	4 w leaves	0.80	0.0285	0.035625	0.0425	0.6705		
			4 w stem	0.80	0.048	0.06	0.0425	1.1294		
			4 w root	0.80	0.0825	0.103125	0.0425	1.9411		

compound	species	% OM	exposure period and plant part(s)	soil conc in mg/kg dw	tissue conc in mg/kg ww	BCF plant/ soil	conc in soil liq in mg/l	BCF plant/ soil liq	reference	comment
mirex	wheat	0.87%	4 w leaves	0.30	0.0135	0.045	0.00075	18	De la Cruz et al 1975	
			4 w stem	0.30	0.03	0.1	0.00075	40		
			4 w root	0.30	0.0345	0.115	0.00075	46		
		0.04%	4 w leaves	0.31	0.006	0.019354	0.0165	0.3636		
			4 w stem	0.31	0.0315	0.101612	0.0165	1.9090		
			4 w root	0.31	0.054	0.174193	0.0165	3.2727		
pentachloro–phenol	soybean	2%	90 d root	4.00	40.5	10.125	0.0105	3857.1	Casterline et al 1985	Soil was sterilized to pro–
			90 d shoot	4.00	6.1	1.525	0.0105	580.95		hibit microbial degradation.
			90 d stem	4.00	11.8	2.95	0.0105	1123.8		Soil conc for soybean as geom.
			90 d leaf	4.00	5.54	1.385	0.0105	527.61		mean of measured concs on day
			90 d pod	4.00	0.75	0.1875	0.0105	71.428		0, 8, 32, and 90. For spinach
			90 d seed	4.00	0.2	0.05	0.0105	19.047		conc on day 64 estimated, geom
	spinach	2%	64 d root	5.40	20.57	3.809259	0.0142	1448.5		mean of day 0, 8, 32 and 64.
			64 d shoot	5.40	9.35	1.731481	0.0142	658.45		
ethofumesate	sugar beet	2.9%	20 d root	1.00	1.34	1.34	0.162	8.2716	Eshel et al. 1978	14C ring–labeled compound.
			20 d hypocotyl	1.00	1.46	1.46	0.162	9.0123		Activated charcoal on soil to
			20 d cotyledon	1.00	40.12	40.12	0.162	247.65		prevent movement of ethofume–
			20 d leave	1.00	11.96	11.96	0.162	73.827		sate. Plant conc measured at d
										3, 5, 10, 15, 20, highest at d
										20. Soil conc not measured.

compound	species	nutrient solution	exposure period plant part(s)	medium conc in mg/l	tissue conc in mg/kg wet weight	BCF	reference	comment
TCDD	soybean	nutr sol	5 d root	0.00013	0.117	900	McCrady et al. 1990	TCDD conc in shoot was insignificant so translocation from root to shoot does not occur.
	maize	nutr sol	5 d root	0.000177	0.115	650		
bromacil	soybean	modif Hoagl sol	8 d root	58.00	345.8	6	Boersma et al. 1991	14C–labeled bromacil; shorter exposure durations with higher concs not included because equilibr. after 8 d not reached.
			8 d stem	58.00	601	10.36		
			8 d leaves	58.00	1237.6	21.34		
nitrobenzene	soybean	N.R.	3 d root	8.00		1.1	McFarlane et al 1990	RCF = (dpm/g fresh root) / (dpm/ml solution). TSCF = (dpm/ml stem sap) / (dpm/ml nutrient medium)
			3 d transp str	8.00		0.77		
	barley		3 d root	8.00		0.57		
			3 d transp str	8.00		0.77		
	lettuce		3 d root	8.00		0.92		
			3 d transp str	8.00		0.7		
	russian olive		3 d root	8.00		1.5		
			3 d transp str	8.00		0.59		
	autumn olive		3 d root	8.00		0.9		
			3 d transp str	8.00		0.77		
	green ash		3 d root	8.00		1.4		
			3 d transp str	8.00		0.81		
	hybrid poplar		3 d root	8.00		0.9		
			3 d transp str	8.00		0.75		
	honeysuckle		3 d root	8.00		2		
			3 d transp str	8.00		0.75		

compound	species	nutrient solution	exposure period plant part(s)	medium conc in mg/l	tissue conc in mg/kg wet weight	BCF	reference	comment
cinmethylin	soybean	half str.	1 d transp str			0.08	Hsu et al. (1990)	High pressure chamber techn–
SD207573		Hoagl				0.218		nique; decapitated plants.
SD208380		sol				0.243		Steady state reached in 0–24 h
SD208213						0.552		TSCF based on conc in plant
SD98319						0.582		sap at steady state and conc
SD204691						0.723		in nutrient medium after 24 h.
SD205857						0.513		All substances tested are
SD204689						0.466		oxabicycloalkane compounds.
SD96638						0.349		
SD204690						0.52		
SD204328						0.498		
SD208586						0.192		
haloxyfop	soybean	half str.	4 d root			6.86	Aguero–Alvarado 1991	14C activity reported as
		Hoagl	4 d leaves			3.57		dpm/g DW, converted to WW
	red fescue	sol	4 d root			100		Initial conc 10.85 ug/l; BCF
			4 d shoot			10.29		calculated as
	tall fescue		4 d root			43.19		(dpm/g WW) / (dpm/ml).
			4 d shoot			5.81		
carbofuran	garden bean	N.R.	3 d root	0.10	130.00	1.3	Trapp et al. 1991	Conc factors given by the
			3 d stem	0.10	91.40	0.91		authors were 1000 x lower than
			3 d leaves	0.10	224.00	2.24		the values calculated by the
								evaluators. Conc in nutrient
								medium of 100 ug/l was repor–
								ted; it could have been
								100 mg/l. Conc factors given
								as reported by the authors.
2,4–dichloro–phenol	soybean	nutr	14 d root	0.10	13.05	130.5	Isensee & Jones 1971	Conc in plants in DW, conver–
		sol	14 d shoot	0.10	0.02	0.195		ted to WW. Conc in nutrient
	oat		14 d root	0.11	13.50	122.7272		medium as geom. mean of init.
			14 d shoot	0.11	0.28	2.545454		nominal and calculated final
								conc. 14C ring–labeld compound
								tested.

compound	species	nutrient solution	exposure period plant part(s)	medium conc in mg/l	tissue conc in mg/kg wet weight	BCF	reference	comment
atrazine	barley	nutr	1 d root	0.10		1.85	Shone & Wood 1974	14C ring-labeled compounds
		sol	1 d transp str	0.10		0.753		tested. 1 week old plants.
		pH 6.5						
atratone	barley		1 d root	0.10		1.28		
			1 d transp str	0.10		0.783		
simazine	barley		1 d root	0.20		4.54		
			1 d transp str	0.20		0.902		
diuron	barley		1 d root	0.20		3.1		
			1 d transp str	0.20		0.814		
ethirimol	barley		1 d root	0.20		0.661		
			1 d transp str	0.20		0.09		
2,4-D	barley		1 d root	0.20		8.07		
			1 d transp str	0.20		0.142		

compound	species	nutrient solution	exposure period plant part(s)	medium conc in mg/l	tissue conc in mg/kg wet weight	BCF	reference	comment
diflufenican	wheat	Hoagl sol	7 d whole plant	0.24	6.60	27.84810	Haynes et al. 1992	Water solubility 0.05 mg/l. Concs in plant tissue reported in DW, converted to WW.
				0.25	4.50	18.14516		
				0.35	5.55	15.99423		
				1.34	11.70	8.731343		
				11.28	131.10	11.62234		
	barley	Hoagl sol	7 d whole plant	0.24	4.35	18.35443		
				0.25	4.35	17.54032		
				0.35	3.45	9.942363		
				1.34	9.75	7.276119		
				11.28	126.15	11.18351		
	Galium aparine	Hoagl sol	7 d whole plant	0.24	7.95	33.54430		
				0.25	7.35	29.63709		
				0.35	6.30	18.15561		
				1.34	5.70	4.253731		
				11.28	601.20	53.29787		
	Setaria viridis	Hoagl sol	7 d whole plant	0.24	18.60	78.48101		
				0.25	18.90	76.20967		
				0.35	23.10	66.57060		
				1.34	25.50	19.02985		
				11.28	670.05	59.40159		
	Stellaria media	Hoagl sol	7 d whole plant	0.24	21.15	89.24050		
				0.25	16.2	65.32258		
				0.35	23.25	67.00288		
				1.34	233.25	174.0671		
				11.28	1242.9	110.1861		
	Viola arvensis	Hoagl sol	7 d whole plant	0.24	24.15	101.8987		
				0.25	19.35	78.02419		
				0.35	29.1	83.86167		
				1.34	324.6	242.2388		
				11.28	1336.35	118.4707		

ANNEX 3

PHYSICO-CHEMICAL PROPERTIES

compound	log K_{ow}	water sol. in mg/l	Henry coeff.	log K_{oc}
acenaphthene/fluorene	3.92[a]	3.8	5.10^{-3}	3.69
alachlor	3.52[b]	242[d]	$1.3.10^{-6}$	2.27[g]
anthracene	4.54[a]	0.0045	$1.6.x10^{-3}$	4.44
Aroclor 1248	5.8-6.3[a]	0.1-0.5	2.10^{-3}-0.12	-
atratone	2.69[b]	-	-	
atrazine	2.75[c]	30	$1.1.10^{-7}$	2.19[g]
benfluralin	5.29[b]	1.1	$4.6.10^{-4}$	-
bromacil	2.11[b]	815	$4.3.10^{-9}$	
carbofuran	2.32[c]	700	$1.6.10^{-7}$	
chlordane	5.54[c]	0.1	2.10^{-3}	-
cinmethylin (SD95481)	4.62[e]	63[d]	$1.8.10^{-5}$	
2,4-D	2.81[c]	682	$7.8.10^{-9}$	
DDT	6.91[b]	0.003	$1.2.10^{-3}$	5.63[f]
2,4-dichlorophenol	3.06[b]	146	$6.1.10^{-3}$	
dieldrin	4.32[c]	0.17	$2.4.10^{-3}$	-
diflufenican	5.42[b] (est)	0.05[d]	$9.7.10^{-5}$	
diuron	2.68[b]	37[c]	$2.7.10^{-6}$	
endrin	4.32[b]	$2.5.10^{-4}$ [c]	$3.1.10^{-4}$	4.25[f]
ethirimol	4.39[b] (est)	200[d]	$1.2.10^{-7}$	
ethofumesate	2.16[b] (est)	110[d]	$6.9.10^{-8}$	2.53[g]
fluoranthene	5.22[a]	0.26	$4.3.10^{-4}$	4.68
haloxyfop	4.63[b] (est)	2.7[d]	$8.6.10^{-8}$	
lindane	3.61[c]	7.3	$1.2.10^{-4}$	2.98[f]
metolachlor	3.13[b]	530[d]	$3.7.10^{-7}$	2.24[g]
mirex	5.28[b]	pract. insol.	4.10^{-5}	-
naphthalene	3.37[a]	31	$1.8.10^{-2}$	3.11
nitrobenzene	1.85[c]	1900	10^{-3}	
pentachlorophenol	5.24[b]	14[c]	$1.1.10^{-4}$	4.51[g]
phenanthrene	4.57[a]	1.1	$1.3.10^{-3}$	4.25

compound	log K_{ow}	water sol. in mg/l	Henry coeff.	log K_{oc}
pyrene	5.18[a]	0.13	$3.8.10^{-4}$	4.81
SD96638	4.1[e]	15.7[b] (est)	$2.9.10^{-6}$ (est)	
SD98319	2.73[e]	765[b] (est)	$1.3.10^{-9}$ (est)	
SD204328	4.59[e]	4[b] (est)	$7.9.10^{-7}$ (est)	
SD204689	3.68[e]	49[b] (est)	$1.7.10^{-5}$ (est)	
SD204690	4.2[e]	11[b] (est)	$2.1.10^{-6}$ (est)	
SD204691	3.53[e]	69[b] (est)	$2.8.10^{-7}$ (est)	
SD205857	3.55[e]	70[b] (est)	$1.3.10^{-5}$ (est)	
SD207573	0.96[e]	128 g/l[b] (est)	$2.7.10^{-13}$ (est)	
SD208213	2.52[e]	1320[b] (est)	$2.2.10^{-9}$ (est)	
SD208380	1.82[e]	10 g/l[b] (est)	8.10^{-11} (est)	
SD208586	5.29[e]	0.79[b] (est)	$1.3.10^{-11}$ (est)	
simazine	2.18[b]	3.5[d]	$1.9.10^{-8}$ (est)	
TCDD	6.8[a]	$1.9.10^{-5}$	$1.4.10^{-3}$	
tetrachloroazobenzene	6.46[b] (est)	0.011	$7.1.10^{-6}$	-

a Mackay et al. 1992

b MEDCHEM database

c Howard, 1989, 1991

d Agrochemicals Handbook, 1994

e MEDCHEM database as consulted by Hsu et al., 1990

f Bockting et al., 1993

g confidential RIVM database

ANNEX 4

SCIENTIFIC PLANT NAMES

Common name	Scientific name
Alfalfa	Medicago sativa L.
Autumn olive	Eleagnus umbellata Thun.
Barley	Hordeum vulgare L.
Carrot	Daucus carota Sorte
Corn	Zea mays L.
Garden bean	Phaseolus vulgaris L.
Green ash	Fraxinus pennsylvanica Marsh.
Green bean	Phaseolus vulgaris L.
Honeysuckle	Lonicera tatarica L.
Hybrid poplar	Populus x robusta C.K. Schneid.
Lettuce	Lactuca sativa L.
Maize	Zea mays L.
Oat	Avena sativa L.
Potato	Solanum tuberosum L.
Red fescue	Festuca rubra
Russian olive	Eleagnus angustifolia L.
Ryegrass	Lolium perenne L.
Sorghum	Sorghum vulgare Pers.
Soybean	Glycine max Merr.
Sugar beet	Beta vulgaris L.
Tall fescue	Festuca arundinacea
Wheat	Triticum aestivum L.

ANNEX 5

CALCULATION OF CONCENTRATIONS IN THE SOIL PORE WATER

compound	log Kow	Kow	% OM	foc	log Koc exp.	Kp	water content in soil	conc soil DW mg/kg	conc soil WW mg/kg	conc liq in mg/l	reference
ethofumesate	2.16	144.544	2.90	0.01706	2.53	0.00578	0.40	1.00	0.714	0.16180	Eshel et al. 1978
atrazine	2.75	562.341	3.87	0.02276	2.19	0.00353	0.40	1.50	1.071	0.38208	Pylypiw et al. 1993
	2.75	562.341	3.50	0.02059	2.06	0.00236	0.30	0.98	0.632	0.33229	Trapp et al. 1990
lindane	3.61	4073.803	3.00	0.01765	2.98	0.01685	0.40	0.33	0.236	0.01913	Voerman et al 1975
alachlor	3.52	3311.311	3.87	0.02276	2.27	0.00424	0.40	0.52	0.371	0.11209	Pylypiw et al. 1993
metolachlor	3.13	1348.963	3.87	0.02276	2.24	0.00396	0.40	2.63	1.879	0.60376	
naphtalene	3.37	2344.229	2.10	0.01235	3.11	0.00191	0.40	1.88	1.343	0.81271	Wild & Jones (1992)
	3.37	2344.229	2.10	0.01235	3.11	0.01591	0.40	1.59	1.136	0.09746	CONC'C in UG/L
	3.37	2344.229	2.90	0.01706	3.11	0.02198	0.40	1.47	1.050	0.06570	
	3.37	2344.229	3.90	0.02294	3.11	0.02955	0.40	6.58	4.700	0.21967	
	3.37	2344.229	7.60	0.04471	3.11	0.05759	0.40	39.40	28.143	0.67940	
acenaphthene/fluorene	3.92	8317.638	2.10	0.01235	3.69	0.06050	0.40	4.06	2.900	0.06666	Wild & Jones 1992
	3.92	8317.638	2.90	0.01706	3.69	0.08355	0.40	8.38	5.986	0.09982	CONC'C in UG/L
	3.92	8317.638	3.90	0.02294	3.69	0.11236	0.40	17.74	12.671	0.15732	
	3.92	8317.638	7.60	0.04471	3.69	0.21896	0.40	51.00	36.429	0.23249	
	3.92	8317.638	2.10	0.01235	3.69	0.06050	0.40	3.57	2.550	0.05862	
	3.92	8317.638	2.90	0.01706	3.69	0.08355	0.40	7.09	5.064	0.08445	
	3.92	8317.638	3.90	0.02294	3.69	0.11236	0.40	16.53	11.807	0.14659	
	3.92	8317.638	7.60	0.04471	3.69	0.21896	0.40	53.00	37.857	0.24161	
dieldrin	4.32	20892.961	3.60	0.02118		0.18184	0.40	1.12	0.800	0.00615	Harris et al. 1969
	4.32	20892.961	1.40	0.00824		0.07072	0.40	0.57	0.407	0.00802	
	4.32	20892.961	3.00	0.01765		0.15154	0.40	7.64	5.457	0.05028	Voerman et al 1975
	4.32	20892.961	0.90	0.00529		0.04546	0.40	20.00	14.286	0.43610	Beall & Nash 1971
endrin	4.32	20892.961	0.90	0.00529	4.25	0.09414	0.40	20.00	14.286	0.21154	
	4.32	20892.961	1.40	0.00824	4.25	0.14645	0.40	0.12	0.086	0.00082	Harris et al. 1969
phenanthrene	4.57	37153.523	2.10	0.01235	4.25	0.21967	0.40	16.27	11.621	0.07393	Wild & Jones 1992
	4.57	37153.523	2.90	0.01706	4.25	0.30335	0.40	48.67	34.764	0.16023	CONC'C in UG/L
	4.57	37153.523	3.90	0.02294	4.25	0.40796	0.40	74.25	53.036	0.18183	
	4.57	37153.523	7.60	0.04471	4.25	0.79500	0.40	130.00	92.857	0.16344	
	4.57	37153.523	2.10	0.01235	4.25	0.21967	0.40	15.00	10.714	0.06816	
	4.57	37153.523	2.90	0.01706	4.25	0.30335	0.40	36.00	25.714	0.11852	
	4.57	37153.523	3.90	0.02294	4.25	0.40796	0.40	83.00	59.286	0.20325	

compound	log Kow	Kow	% OM	foc	log Koc exp.	Kp	water content in soil	conc soil DW mg/kg	conc soil WW mg/kg	conc liq in mg/l	reference
pentachlorophenol	5.24	173780.083	2.00	0.01176	4.51	0.38070	0.40	4.00	2.857	0.01050	Casterline et al. 1985
	5.24	173780.083	2.00	0.01176	4.51	0.38070	0.40	5.40	3.857	0.01417	
pyrene	5.18	151356.125	2.10	0.01235	4.81	0.79757	0.40	41.50	29.643	0.05201	Wild & Jones 1992
	5.18	151356.125	2.90	0.01706	4.81	1.10141	0.40	63.63	45.450	0.05775	CONC'C in UG/L
	5.18	151356.125	3.90	0.02294	4.81	1.48121	0.40	111.83	79.879	0.07548	
	5.18	151356.125	7.60	0.04471	4.81	2.88645	0.40	258.75	184.821	0.08963	
fluoranthene	5.22	165958.691	2.10	0.01235	4.68	0.59125	0.40	47.00	33.571	0.07944	Wild & Jones 1992
	5.22	165958.691	2.90	0.01706	4.68	0.81649	0.40	42.90	30.643	0.05252	CONC'C in UG/L
	5.22	165958.691	3.90	0.02294	4.68	1.09803	0.40	72.00	51.429	0.06555	
	5.22	165958.691	7.60	0.04471	4.68	2.13976	0.40	140.25	100.179	0.06553	
mirex	5.28	190546.072	0.87	0.00512		0.40079	0.40	3.50	2.500	0.00872	De la Cruz et al. 1975
	5.28	190546.072	0.87	0.00512		0.40079	0.40	0.80	0.571	0.00199	
	5.28	190546.072	0.87	0.00512		0.40079	0.40	0.30	0.214	0.00075	
	5.28	190546.072	0.04	0.00024		0.01843	0.40	3.40	2.429	0.18059	
	5.28	190546.072	0.04	0.00024		0.01843	0.40	0.80	0.571	0.04249	
	5.28	190546.072	0.04	0.00024		0.01843	0.40	0.31	0.221	0.01647	
benfluralin	5.29	194984.460	1.20	0.00706		0.56568	0.40	0.46	0.329	0.00081	Businelli et al. 1975
	5.29	194984.460	1.20	0.00706		0.56568	0.40	0.76	0.543	0.00134	
chlordane	5.54	346736.850	1.70	0.01000		1.42509	0.40	1.24	0.886	0.00087	Tafuri et al. 1977
	5.54	346736.850	1.70	0.01000		1.42509	0.40	3.30	2.357	0.00231	
DDT	6.91	8128305.162	3.50	0.02059	5.63	8.78252	0.30	2.16	1.394	0.00022	Trapp et al. 1990
	6.91	8128305.162	3.60	0.02118	5.63	9.03345	0.40	0.57	0.407	0.00006	Harris et al. 1969
	6.91	8128305.162	1.40	0.00824	5.63	3.51301	0.40	0.23	0.164	0.00007	
	6.91	8128305.162	3.00	0.01765	5.63	7.52787	0.40	56.50	40.357	0.00751	Voerman et al 1975
	6.91	8128305.162	0.90	0.00529	5.63	2.25836	0.40	20.00	14.286	0.00885	Beall & Nash 1971
tetrachloroazobenzene	6.46	2884031.503	3.00	0.01765		20.91771	0.20	10.00	5.882	0.00039	Woroby 1988
	6.46	2884031.503	3.00	0.01765		20.91771	0.20	0.02	0.012	0.00000	
Aroclor 1248	6.30	1995262.315	1.10	0.00647		5.30622	0.40	0.50	0.357	0.00009	O'Connor et al. 1990
	6.30	1995262.315	1.10	0.00647		5.30622	0.40	0.75	0.536	0.00014	
	6.30	1995262.315	0.20	0.00118		0.96477	0.40	0.50	0.357	0.00052	
	6.30	1995262.315	0.20	0.00118		0.96477	0.40	0.75	0.536	0.00078	