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Bioconcentration of gaseous organic chemicals in plant leaves: Comparison of experimental data with model predictions

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Revised version: In this report some model values have been changed due to a more correct selection of some physical-chemical parameters compared to the former version. Therefore this report replaces the former version of March 1996.

This investigation has been performed in order and for the account of the Directorate General for Environmental Protection, Directorate for Chemicals, External Safety and Radiation Protection of the Ministry of Housing, Spatial Planning and Environment within the framework of project 679102: "Assessment Systems for Substances".

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SUMMARY

Chemical substances are distributed in the environment between compartments such as soil, water, air, and biota. Chemicals may be concentrated by plants from soil and air, and therefore plants may contribute substantially to the total daily intake of humans.

This study was performed to support the implementation of two models in USES 1.0 (RIVM et al. 1994) and in the European version EUSES, which will become available in 1997. The Uniform System for the Evaluation of Substances, USES 1.0, (RIVM et al., 1994) was developed to assess the lifetime risk of indirect exposure of man and top predators. One of the exposure pathways of plants included in USES 1.0 is the transfer of gaseous substances from air to plant leaves modeled by Riederer (1990). A model similar to that of Riederer (1990) but having a more refined approach is carried out by Trapp and Matthies (1995). The model of Trapp and Matthies (1995) takes the dynamics of the uptake processes into account, and is implemented in the new European version EUSES.

Purpose of this literature study is to evaluate the models of Riederer (1990) and Trapp and Matthies (1995) by comparing their results with experimental data on leaf-air partition coefficients ($K_{l/a}$) found in the literature. The data set was limited and therefore conclusions can only be drawn with reservations.

For herbaceous plants both models give good estimations for the leaf-air partition coefficient up to 10^7, with deviations for most substances within a factor of 5. For substances for which Riederer (1990) estimates a leaf-air partition coefficient above 10^7, the approach of Trapp and Matthies (1995) seems more adequate.

SAMENVATTING

Stoffen zijn in het milieu verdeeld over de compartimenten bodem, lucht, water en biota. Planten kunnen stoffen accumuleren na opname uit de bodem en de lucht. Planten vormen een belangrijk onderdeel van het dieet van zowel mensen als van vee en kunnen een substantiële bijdrage leveren aan de totale dagelijkse inname van een stof door de mens.

Deze studie is uitgevoerd ter onderbouwing van de implementatie van twee modellen in USES 1.0 (RIVM et al. 1994) en de Europese versie EUSES, die in 1997 beschikbaar wordt. Het Uniform Beoordelingssysteem Stoffen, USES 1.0 is ontwikkeld om het levenslang risico te schatten van indirecte blootstelling van de mens en van toppredatoren. Een van de in USES 1.0 ingebouwde blootstellingsroutes van planten is de overdracht van gasvormige stoffen uit de lucht aan bladeren van planten. Daartoe is het model van Riederer (1990) geïmplementeerd. De meer uitgewerkte benadering van Trapp en Matthies (1995) houdt rekening met de dynamiek van opnameprocessen, en is in de nieuwe Europese versie EUSES opgenomen.

In deze literatuurstudie zijn de modellen van Riederer (1990) en Trapp en Matthies (1995) geevalueerd door hun uitkomsten te vergelijken met experimenteel bepaalde blad-lucht partitiecoefficienten ($K_{l/a}$) die in de literatuur gevonden zijn. De gevonden experimentele gegevensset is beperkt, zodat conclusies alleen met de nodige voorzichtigheid getrokken mogen worden.

Voor kruidachtige planten geven beide modellen goede voorspellingen van de blad-lucht partitiecoefficienten tot een waarde van 10^7, met afwijkingen voor de meeste stoffen van maximaal een factor 5. Voor stoffen waarvoor Riederer (1990) een blad-lucht partitiecoefficient hoger dan 10^7 voorspelt, geeft de methode van Trapp en Matthies (1995) wellicht een realistischer schatting.

1. INTRODUCTION

Chemical substances are distributed in the environment between compartments such as soil, water, air and biota. Chemicals may be concentrated by plants from soil and air, and passed up the food chain via herbivores, omnivores and carnivores, and finally to man (McKone and Ryan 1989, McKone and Daniels 1991).
The Uniform System for the Evaluation of Substances, USES 1.0 (RIVM et al. 1994) was developed for a quantitative assessment of the risks posed by chemicals to man and the environment (Vermeire et al. 1994) . The system predicts the concentrations of organic substances in water, air and soil from estimated or measured emission rates. To assess the lifetime risk of indirect exposure of man and top predators, estimations are made of the concentrations in crops, meat, fish and milk. In this indirect exposure assessment, bioconcentration factors are applied to the concentrations in the environmental compartments. Subsequently, the concentrations in food products are combined with levels in other human intake media as well as dietary factors to estimate the total daily intake.

Plant products such as vegetables, grains and fruits form an important part of the human diet, as well as that of cattle. Therefore, the levels of a contaminant in plants or plant parts may contribute substantially to the total daily intake of humans. The exposure of plants can occur via different pathways, such as exposure of the roots via the soil, and exposure of the above ground plant parts to vapours and aerosoles in the air.

The above mentioned pathways have been included in USES 1.0 to predict the concentration of a substance in crops. The transfer of organic substances from soil to plant root and subsequent translocation to stem and leaf, are modelled in USES according to Briggs et al. (1982, 1983). The adequacy of these models was evaluated by Polder et al. (1995). To estimate the uptake of aerosoles the model of McKone and Ryan (1989) is implemented in USES 1.0. However, this pathway is not subject of this literature study.

For the uptake of gaseous organic substances by leaves the model of Riederer (1990) was implemented in USES 1.0 (Hulzebos 1994). Trapp and Matthies (1995) recently presented a model in which uptake from porewater and air are integrated. The transfer of gases from air to plant in their approach is similar to the model of Riederer (1990), extended with a term for growth dilution. The approach of Trapp and Matthies (1995) is proposed in the Technical Guidance Document for New and Existing Substances (EC 1995) and has been implemented in EUSES, the European version of USES, which will become available in 1997.

The adequacy of the models of Riederer (1990) and Trapp and Matthies (1995) is subject of this study. Experimental data on the leaf-air partition coefficients ($K_{l/a}$) for gaseous organic substances are collected from the literature. The results of the models of Riederer (1990) and Trapp and Matthies (1995) are compared to the experimental $K_{l/a}$ values in order to evaluate the application of these models in the existing and future versions of USES.

2. METHODOLOGY

The calculation of the leaf-air partition coefficient according to the models of Riederer (1990) and Trapp and Matthies (1995) is described in subsection 2.1. The collection of literature on experimental data on the bioconcentration of gaseous substances by plants, and the selection of physico-chemical data is dealt with in subsection 2.2. Subsection 2.3. explains the handling of the experimental data to make the comparison possible with the model values.

2.1 Model predictions

The model of Riederer (1990)

Riederer (1990) developed a fugacity-based model to describe the partitioning of organic gases between the atmosphere and the leaf. In this theoretical approach the leaf is viewed as consisting of four well-mixed phases: an air phase, a liquid phase, a lipid phase, and a non-lipid solid phase which does not participate in the partitioning process. In the steady-state situation, a leaf-air partition coefficient can be defined on a volume basis as:

$$K_{l/a} = \frac{\text{concentration in leaf [ng/l fresh leaf]}}{\text{concentration in air [ng/l air]}}$$

This partition coefficient can be estimated with the octanol-water and air-water partition coefficients of the chemical (K_{ow} and K_{aw} respectively) and the volumes of the separate phases. K_{ow} is thought to be representative to describe the partition behaviour of chemicals with plant lipids. For the volume fractions of the phases in the leaf, the default values applied in USES 1.0 are given:

$$K_{l/a} = v_a + \frac{v_w}{K_{aw}} + \frac{v_{c+g} \cdot K_{ow}}{K_{aw}}$$

$K_{l/a}$	leaf-air partition coefficient	$[m^3.m^{-3}]$	
v_a	volume fraction of air in leaf	$[m^3.m^{-3}]$	0.5
v_w	volume fraction of water in leaf	$[m^3.m^{-3}]$	0.4
v_{c+g}	volume fraction of cuticula and glycerol in leaf	$[m^3.m^{-3}]$	0.01
K_{ow}	octanol/water partition coefficient	$[m^3.m^{-3}]$	
K_{aw}	air/water partition coefficient	$[m^3.m^{-3}]$	

The model of Trapp and Matthies (1995)

The modelling approach of Trapp and Matthies (1995) integrates uptake of organic substances from porewater in the soil and uptake from air into a simple, one-compartment model. This model is proposed in the Technical Guidance Document for New and Existing Substances (EC 1995) and will also be implemented in EUSES. For the purpose of this study, only uptake from air is described, the uptake and translocation from soil are not included here. In contrast with the steady-state approach of Riederer (1990), the model of Trapp and Matthies (1995) is a dynamic one. The leaf-air partition coefficient as defined by Riederer (1990) is included in this approach, but the kinetics of the uptake process are also taken into account. Furthermore, elimination processes and dilution by growth can be added.

Several plant-specific parameters are required for the model. As there are many different plant species acting as food crops for humans and cattle, an average or typical plant definition is not scientifically feasible. Therefore, the suggested defaults, mentioned with the parameters, should be regarded as 'typical' values (Trapp and Matthies 1995). The plant-specific parameters are referenced to 1 m^2 leaf area. The concentration in the leaf can be described with a differential equation:

$$\frac{dC_{leaf}}{dt} = -\alpha \cdot C_{leaf} + \beta$$

C_{leaf}	concentration in leaf tissue of plant	[$mg.m^{-3}$]
α	sink term	[d^{-1}]
β	source term	[$mg.m^{-3}.d^{-1}$]

The sink term is formed by diffusive transfer from leaf to air and dilution by growth:

$$\alpha = \frac{AREA_{leaf} \cdot g_{leaf}}{K_{l/a} \cdot V_{leaf}} + k_{growth\ plant}$$

$AREA_{leaf}$	leaf surface area	[m^2]	5
g_{leaf}	conductance (0.001 $m.s^{-1}$)	[$m.d^{-1}$]	86.4
$K_{l/a}$	leaf-air partition coefficient (Riederer 1990)	[-]	
V_{leaf}	leaf volume	[m^3]	0.002
$k_{growth\ plant}$	pseudo-first order rate constant for dilution by growth	[d^{-1}]	0.035

Naturally, the leaf surface area increases during growth, but the model is valid as long as the ratio area to volume remains the same. If relevant rate constants are known, any metabolism or other removal processes can be added to this term.

The source term in the differential equation is formed by the gaseous uptake from air:

$$\beta = C_{air} \cdot g_{leaf} \cdot \frac{AREA_{leaf}}{V_{leaf}}$$

C_{air}	concentration in air	[mg.m^{-3}]	
g_{leaf}	conductance (0.001 m.s^{-1})	[m.d^{-1}]	86.4
$AREA_{leaf}$	leaf surface area	[m^{2}]	5
V_{leaf}	leaf volume	[m^{3}]	0.002

The steady-state concentration in the leaf is now given by the ratio of the source and sink term:

$$C_{leaf}(\infty) = \frac{\beta}{\alpha}$$

C_{leaf}	concentration in leaf tissue	[mg.m^{-3}]

Comparison of the models of Riederer (1990) and Trapp and Matthies (1995)

The models of Riederer (1990) and Trapp and Matthies (1995) give identical results for the most relevant range of $K_{l/a}$ values (figure 1). Only for values of $K_{l/a}$ above 10^7 growth dilution starts to become a relevant process, and therefore Trapp and Matthies (1995) predict no further increase in leaf concentrations above that level. At lower values of $K_{l/a}$, kinetics of the uptake process are fast compared to the growth ratio of the plant, leading to rapid equilibration of leaf tissue with the air concentration.

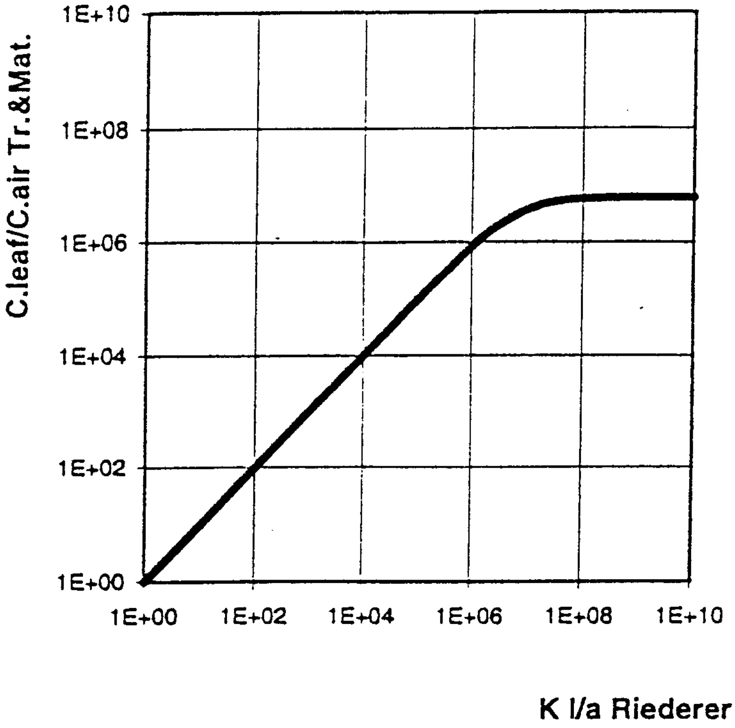

Figure 1. Model values of leaf-air partition coefficients: Riederer (1990) versus Trapp and Matthies (1995).

2.2 Selecting experimental data

An on-line research in TOXLINE and BIOSIS is performed using the search profile as given in Annex 1. Studies could not be used when the exposure duration was short, e.g. 4 hours, and an elimination phase was not included. The experimental design had to include continuous exposure via the vapour phase, with concentrations measured in the leaves immediately after the exposure period and reported units for the leaf-air partition coefficient. Data on concentrations in the whole plant or in the cuticle were not used. Field studies were not taken into account.

The log K_{ow}, vapour pressure and water solubility of the substances regarded are obtained in order of preference from Mackay et al. (1992a,b, 1993), the MEDCHEM database (1995), Howard (1991), British Crop Protection Council (1983, 1994) and Verschueren (1983). From Mackay et al. (1992a,b, 1993) the values selected by the authors are used. The K_{aw} values (dimensionless Henry coefficient) are calculated from the vapour pressure and the water solubility following the equation:

$$K_{aw} = \frac{P \cdot M}{S \cdot R \cdot T}$$

K_{aw}	Henry coefficient	[-]	
P	vapour pressure	[Pa]	
M	molecular weight	[g.mol^{-1}]	
S	water solubility	[g.m^{-3}]	
R	gas constant	[Pa.m^{3}.mol^{-1}.Kelvin^{-1}]	8.3
T	temperature	[Kelvin]	

2.3 Data handling

The plants in both human and cattle diets have all herbaceous features and the defaults set in USES 1.0 are representative for those plants.
Data were obtained for herbaceous plants but also for *Azalea* and *Picea* species. *Azalea* and *Picea* species have higher fractions of dry weight, lipid and cuticular wax than herbaceous plants (McCrady 1994, McCrady and Maggard 1993, Bacci et al. 1990a,b, Hauk et al. 1994, Schroll and Scheunert 1992). It can be expected that lipophilic substances (e.g. log K_{ow} above 5) reach higher concentrations in plants with these properties. Therefore, two plant groups are distinguished in this study: the herbaceous plants like vegetables and grass, and the more scleroforous *Azalea* and *Picea* species.
When concentrations in leaves were reported as dry weight (DW), they are recalculated to fresh weight (FW). For herbaceous species 15% DW was assumed (McCrady 1994, McCrady and Maggard 1993, Schroll and Scheunert 1992), when no percentage was determined by the authors. For recalculations in pine needle 40% DW and for *Azalea* species 30% DW is applied, similar to McCrady (1994) and Bacci et al. (1990a,b) respectively.

Experimental values for $K_{l/a}$ found in the literature were derived in several ways [9]. Some authors reported that equilibrium between leaf and air was reached and the $K_{l/a}$ was calculated as (concentration in leaf)/(concentration in air). In some experiments uptake and clearance were studied and the uptake rate constant (k_1) and the clearance rate constant (k_2) were calculated. The $K_{l/a}$ was calculated as k_1/k_2. In other studies it was not clear if equilibrium was reached and an elimination phase

was not performed. The $K_{l/a}$ was then calculated as (concentration in leaf) / (concentration in air). Reischl et al. (1989) calculated the $K_{l/a}$ with a two-compartment dynamic model, which was not described in their publication.
For the two plant groups the mean $K_{l/a}$ values are calculated for each substance over all experimental $K_{l/a}$ values available for that substance. Linear regression analysis is performed to compare the fitted lines to the 'ideal' line that is generated when model and experimental values are identical.
Plant and air concentrations expressed in mass units are recalculated to volume with a plant density of 1000 g/l (McKone and Daniels 1991) and an air density of 1.19 g/l.

3. RESULTS

Experimental leaf-air partition coefficients have been found for 24 substances with a log K_{ow} between 1.24 and 7.1 and a K_{aw} between $1.3.10^{6}$ and 5.6. A detailed overview of all experiments and their results as obtained from the literature is given in Annex 2. The physico-chemical parameters for all substances involved, calculated model $K_{l/a}$ values, and the (mean) experimental values are reported in Annex 3. Table 1 gives a summary of the physico-chemical parameters and the leaf-air partition coefficients calculated from the laboratory experiments.
Variation in the experimental data is reviewed in subsection 3.1, the comparison of the model predictions with the experimental values is made in subsection 3.2.

3.1 Variation in the experimental data

Variation within a substance

Scheunert et al. (1994) found for several chlorobenzenes $K_{l/a}$ values for *Hordeum vulgare* that were up to 4 times higher than for *Lepidium sativum*, except for 1,4-dichlorobenzene: for *H. vulgare* the $K_{l/a}$ was one order of magnitude higher than for *L. sativum*.
For DDT, γ-HCH and hexachlorobenzene similar experimental $K_{l/a}$ values were found for both *Azalea indica* (Bacci and Gaggi 1987, Bacci et al. 1990a) and *Picea omorika* (Reischl et al. 1989). For DDE the $K_{l/a}$ for *Picea abies* was 6 times higher than for *P. omorika* (Hauk et al. 1994) whereas *A. indica* showed much higher values (Bacci and Gaggi 1987): 50 times higher than for *P. omorika*, and eight-fold the value for *P. abies*.

Variation between the two plant groups

For DDE, DDT, α-HCH, γ-HCH, hexachlorobenzene, and pentachlorobenzene experimental data for both plant groups were available. For DDE and γ-HCH the mean value for Azalea/Pine was 3 times higher than for *Phaseolus vulgaris*, and for DDT it was 5 times higher. For α-HCH the $K_{l/a}$ for *A. indica* was one order of magnitude higher than for the herbaceous plants. For hexachlorobenzene the mean $K_{l/a}$ for Azalea/Pine was 20 times higher than for herbaceous plants. *P. omorika* showed for pentachlorobenzene a $K_{l/a}$ that was 60 times higher than the mean value for herbaceous plants.

Table 1. Experimental data on leaf-air partition coefficients.

Compound	K_{aw}	log K_{ow}	Species	ref	$K_{l/a}$	mean $K_{l/a}$
alachlor	$1.3 \text{x} 10^{-6}$	3.52	Azalea indica.	[1]	$2.85 \text{x} 10^{5}$	
p,p'-DDE	$8.1 \text{x} 10^{-4}$	6.96	Phaseolus vulgaris.	[2]	$4.56 \text{x} 10^{6}$	
			Azalea indica +	[3]	$3.38 \text{x} 10^{7}$	$1.48 \text{x} 10^{7}$
			Azalea indica +	[3]	$3.43 \text{x} 10^{7}$	
			Picea abies +	[4]	$4.6 \text{x} 10^{6}$	
			Picea omorika +	[4]	$6.54 \text{x} 10^{5}$	
			Picea omorika.	[4]	$9.33 \text{x} 10^{5}$	
p,p'-DDT	$1.2 \text{x} 10^{-3}$	6.91	Phaseolus vulgaris.	[2]	$6.74 \text{x} 10^{6}$	
			Azalea indica +	[3]	$4.85 \text{x} 10^{7}$	$3.65 \text{x} 10^{7}$
			Picea omorika.	[5]	$2.46 \text{x} 10^{7}$	
1,4-diCB	$6.5 \text{x} 10^{-2}$	3.4	Hordeum vulgare +	[6]	$1.34 \text{x} 10^{2}$	75.5
			Lepidium sativum.	[6]	17	
4,4'-diCBPh	$7.2 \text{x} 10^{-3}$	5.3	Picea omorika.	[5]	$2.34 \text{x} 10^{6}$	
dieldrin	$4.6 \text{x} 10^{-4}$	5.2	Azalea indica.	[1]	$1.08 \text{x} 10^{6}$	
α-HCH	$3.6 \text{x} 10^{-4}$	3.72	Phaseolus vulgaris.	[2]	$9.86 \text{x} 10^{4}$	
			Azalea indica.	[3]	$1.16 \text{x} 10^{6}$	
γ-HCH	$1.2 \text{x} 10^{-4}$	3.72	Phaseolus vulgaris.	[2]	$3.34 \text{x} 10^{5}$	
			Azalea indica +	[3]	$8.57 \text{x} 10^{5}$	$1.06 \text{x} 10^{6}$
			Picea omorika.	[5]	$1.25 \text{x} 10^{6}$	
heptaCBPh [1]	$2.2 \text{x} 10^{-3}$	7	Picea omorika.	[5]	$2.91 \text{x} 10^{6}$	
hexaCB	$5.3 \text{x} 10^{-2}$	5.5	Phaseolus vulgaris +	[2]	$3.39 \text{x} 10^{4}$	$1.98 \text{x} 10^{4}$
			Hordeum vulgare +	[6]	$1.13 \text{x} 10^{4}$	
			Lepidium sativum.	[6]	$1.44 \text{x} 10^{4}$	
			Azalea indica +	[7]	$4.69 \text{x} 10^{5}$	$4.49 \text{x} 10^{5}$
			Picea omorica.	[5]	$4.3 \text{x} 10^{5}$	
mirex	$4 \text{x} 10^{-5}$	5.28	Azalea indica.	[7]	$1.32 \text{x} 10^{7}$	
octaCBPh [1]	$1.5 \text{x} 10^{-2}$	7.1	Picea omorika.	[5]	$6.5 \text{x} 10^{6}$	
pentaCB	$3.4 \text{x} 10^{-2}$	5	Hordeum vulgare +	[6]	$2.36 \text{x} 10^{4}$	$1.49 \text{x} 10^{4}$
			Lepidium sativum.	[6]	$6.2 \text{x} 10^{3}$	
			Picea omorika.	[5]	$9.3 \text{x} 10^{5}$	
sulfotep	$1.9 \text{x} 10^{-4}$	3.99	Azalea indica.	[7]	$2.52 \text{x} 10^{4}$	
1,2,3,5-tetraCB	$2.4 \text{x} 10^{-1}$	4.5	Hordeum vulgare +	[6]	$3.67 \text{x} 10^{3}$	$2.38 \text{x} 10^{3}$
			Lepidium sativum.	[6]	$1.09 \text{x} 10^{3}$	
1,2,4,5-tetraCB	$5 \text{x} 10^{-2}$	4.5	Picea omorika.	[5]	$7.18 \text{x} 10^{4}$	
3,3',4,4'tetraCBPh	$6.9 \text{x} 10^{-3}$	6.5	Azalea indica.	[1]	$8.44 \text{x} 10^{7}$	
1,2,3,4-TCDD	$1.5 \text{x} 10^{-3}$	6.6	Azalea indica.	[8]	$9.1 \text{x} 10^{7}$	
2,3,7,8-TCDD	$1.4 \text{x} 10^{-3}$	6.8	Phalaris arundinacea.	[9]	$3.16 \text{x} 10^{7}$	

(to be continued)

Table 1. Experimental data on leaf-air partition coefficients (continued).

Compound	K_{aw}	log K_{ow}	Species	ref	$K_{l/a}$	mean $K_{l/a}$
tetrachloroethene	1.1	2.88	Picea abies excelsa +	[10]	85.3	74.9
			Picea abies excelsa.	[10]	64.4	
thionazin	$3.6x10^{-5}$	1.24	Azalea indica.	[7]	$3.05x10^{4}$	
1,2,4-triCB	$1.1x10^{-1}$	4.1	Hordeum vulgare +	[6]	$1.13x10^{3}$	$1.05x10^{3}$
			Lepidium sativum.	[6]	$9.66x10^{2}$	
2,2 ,5-triCBPh	$3.7x10^{-2}$	5.6	Picea omorika.	[5]	$7.06x10^{5}$	
trifluralin	$6.0x10^{-3}$	5.34	Azalea indica.	[7]	$1.17x10^{5}$	

Plants contributing to one mean $K_{l/a}$ value, are connected with '+', the series ends with '.'

CB = chlorobenzene
CBPh = chlorobiphenyl
[1] data from another congener

1 = Bacci et al. 1990b
2 = Bacci and Gaggi 1986
3 = Bacci and Gaggi 1987
4 = Hauk et al. 1994
5 = Reischl et al. 1989
6 = Scheunert et al. 1994
7 = Bacci et al. 1990a
8 = Bacci et al. 1992
9 = McCrady and Maggard 1993
10 = Frank and Frank 1989

3.2 Comparison of model and experimental values.

Herbaceous species

To quantify the agreement between the model $K_{l/a}$ values and the experimental data for herbaceous plants linear regression was conducted. The comparison with the model of Riederer (1990) resulted in the following regression equation:

$$\log(\text{experimental } K_{l/a}) = 0.87 \log(\text{model } K_{l/a}) + 0.29$$ (n=10, r^2=0.95, S.E.=0.44)

The regression line comparing the model values calculated according to Trapp and Matthies (1995) and the experimental data followed the equation:

$$\log(\text{experimental } K_{l/a}) = 1.12 \log(\text{model } C_{leaf}/C_{air}) - 0.65$$ (n=10, r^2=0.96, S.E.=0.38)

Mean experimental data for $K_{l/a}$ of herbaceous plants and model values calculated according to Riederer (1990) and Trapp and Matthies (1995) are plotted in figure 2 and 3, respectively. The solid lines in these figures represent full agreement (slope = 1 and intercept = 0), as the deviations of the experimental data from these lines are important for the risk assessment purpose of this study.

When $K_{l/a}$ values according to Riederer (1990) are higher than 10^7 growth dilution becomes a relevant process (figure 1), which is accounted for in the model of Trapp and Matthies (1995). This occurred for 2,3,7,8-TCDD, DDE and DDT in this data set. The estimated values from Trapp and Matthies (1995) for DDE and DDT are similar to the mean experimental values (figure 3), whereas those from Riederer [5] are a factor 25 and 10, respectively, higher (figure 2). For 2,3,7,8-TCDD the $K_{l/a}$ of Riederer (1990) is similar to the experimental value, while the estimated value from Trapp and Matthies (1995) is a factor 6 lower than the experimental value.

Azalea/Pine

The data on *Picea* and *Azalea* are more scattered as can be seen in Figures 4 and 5. Regression analysis on the data for this plant group showed for both models less similarity between experimental and model values than was found for herbaceous species. The comparison of the experimental data with the model values of Riederer (1990) is described by the following regression equation:

$$\log(\text{experimental } K_{l/a}) = 0.68 \log(\text{model } K_{l/a}) + 1.98$$ (n=20, r^2=0.70, S.E.=0.80)

Regression analysis comparing the experimental data with the model values according to Trapp and Matthies (1995) resulted in the equation:

$$\log(\text{experimental } K_{l/a}) = 0.83 \log(\text{model } C_{leaf}/C_{air}) + 1.39 \quad (n=20,\ r^2=0.71,\ S.E.=0.79)$$

As can be seen from the figures 4 and 5 the model of Trapp and Matthies (1995) did not provide better estimates for the substances for which Riederer (1990) estimated $K_{l/a}$ values of 10^7 and higher.

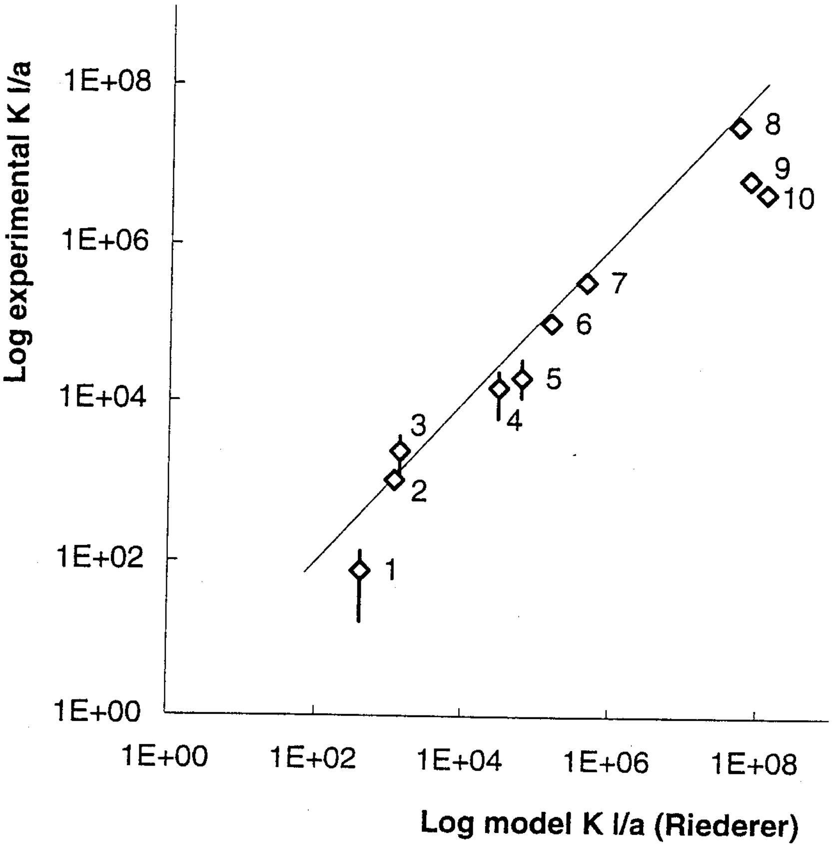

Figure 2. Herbaceous plants: model predictions (Riederer 1990) versus mean experimental leaf-air partition coefficients.

Error bars show the minimum and maximum, when more than one experimental $K_{l/a}$ was found. The solid line represents full agreement between model estimations and experimental values.

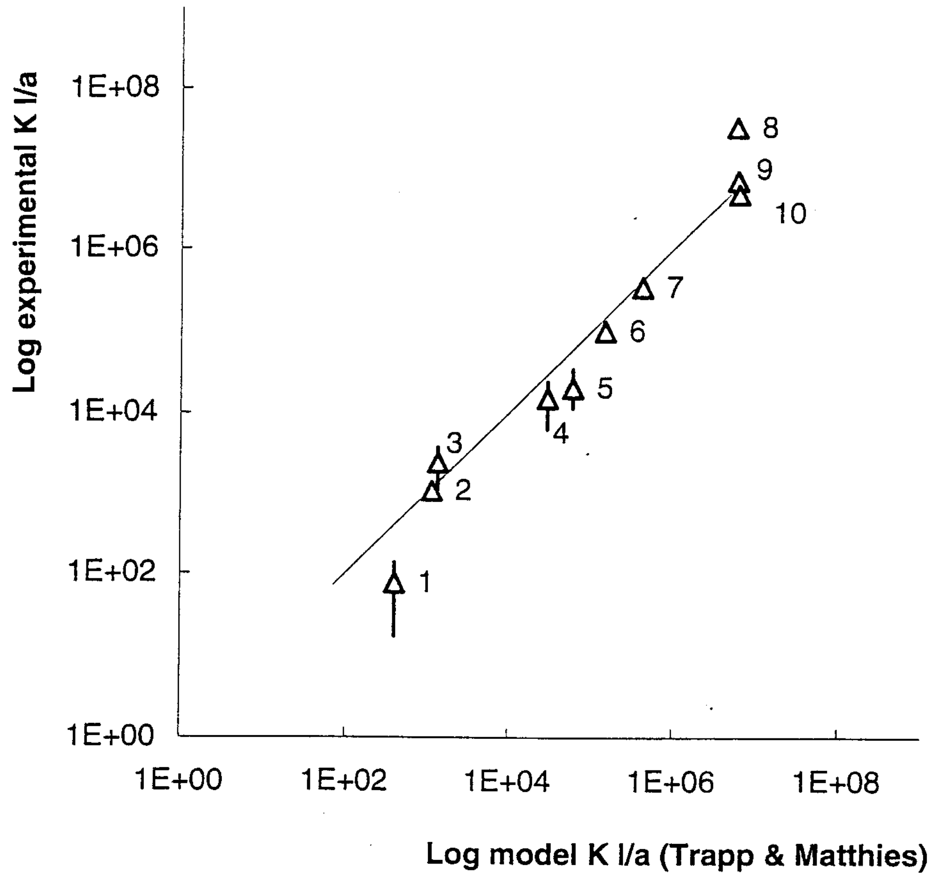

Figure 3. Herbaceous plants: model predictions (Trapp and Matthies 1995) versus mean experimental leaf-air partition coefficients.

Error bars show the minimum and maximum, when more than one experimental $K_{l/a}$ was found. The solid line represents full agreement between model estimations and experimental values.

Substances in Figure 2 and 3:

1 = 1,4-dichlorobenzene
2 = 1,2,4-trichlorobenzene
3 = 1,2,3,5-tetrachlorobenzene
4 = pentachlorobenzene
5 = hexachlorobenzene

7 = α-HCH
7 = γ-HCH
8 = 2,3,7,8-TCDD
19 = DDE
10 = DDT

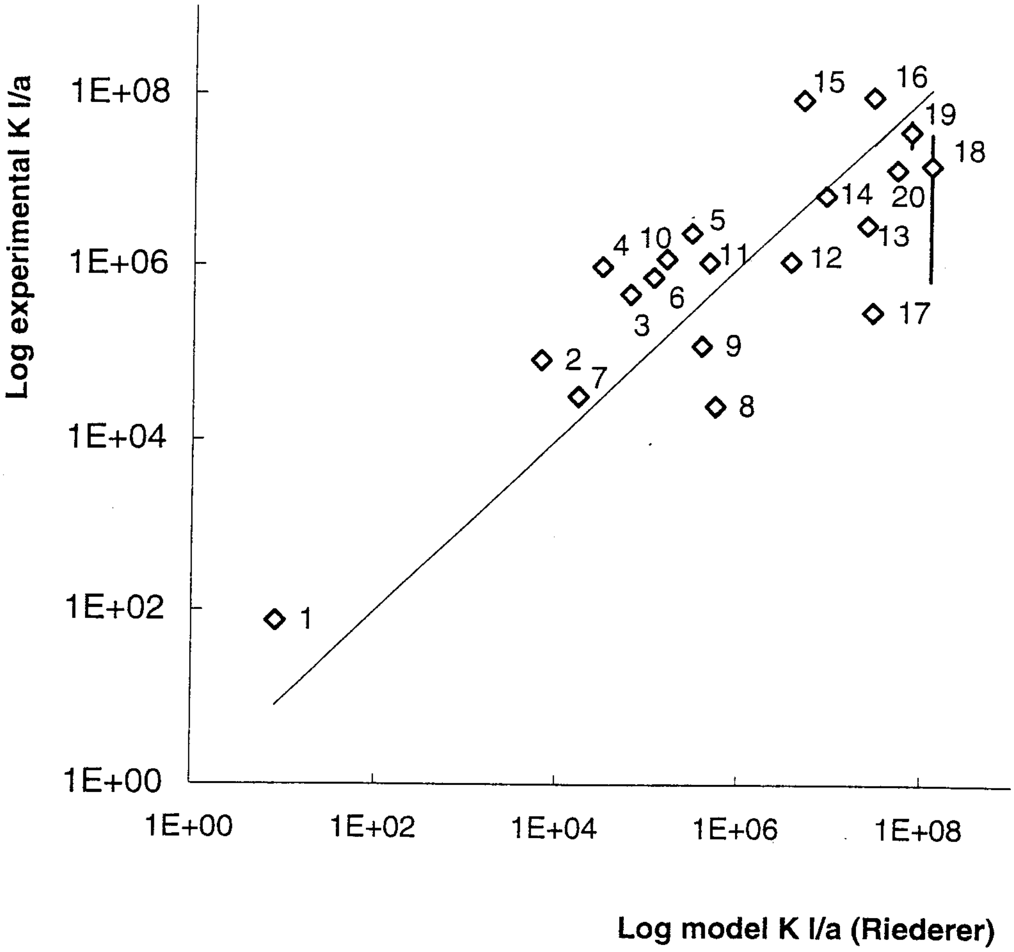

Figure 4. Azalea and Pinus: model predictions (Riederer 1990) versus mean experimental leaf-air partition coefficients.

Error bars show the minimum and maximum when more than one experimental $K_{l/a}$ was found. The solid line represents full agreement between model estimations and experimental values.

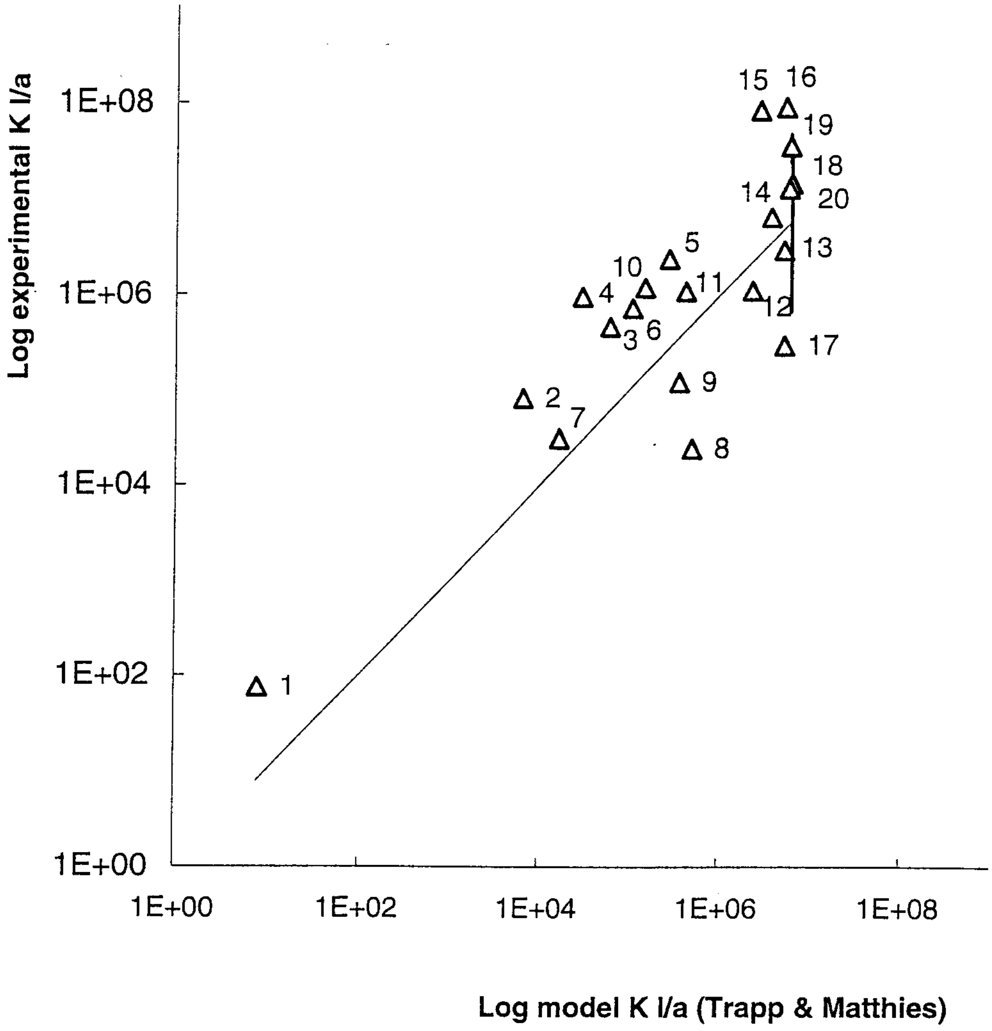

Figure 5. Azalea and Pinus: model predictions (Trapp and Matthies 1995) versus mean experimental leaf-air partition coefficients.

Error bars show the minimum and maximum when more than one experimental $K_{l/a}$ was found. The solid line represents full agreement between model estimations and experimental values.

Substances Figure 4 and 5:

1 = tetrachloroethene
2 = 1,2,4,5-tetrachlorobenzene
3 = hexachlorobenzene
4 = pentachlorobenzene
5 = 4,4'-dichlorobiphenyl
6 = 2,2',5-trichlorobiphenyl
7 = thionazin
8 = sulfotep
9 = trifluralin
10 = α-HCH
11 = γ-HCH
12 = dieldrin
13 = heptachlorobiphenyl
14 = octachlorobiphenyl
15 = 3,3',4,4'-tetrachlorobiphenyl
16 = 1,2,3,4-TCDD
17 = alachlor
18 = DDE
19 = DDT
20 = mirex

4. DISCUSSION

4.1 General remarks

The variation in experimental $K_{l/a}$ values for a certain substance between the herbaceous species is within a factor 5. In the Azalea/Pine group the experimental $K_{l/a}$ values for a substance for different species are similar, except for DDE. The $K_{l/a}$ values in Azalea and Pine species are always higher than in herbaceous plants for the same substances tested in both groups of plants.
Differences in test circumstances may have been contributed to the variation in the experimental data. Other factors of uncertainty in the experimental $K_{l/a}$ values could have been the mobilisation and metabolism of the substances in the plants. The experiments reviewed here did not include analyses of metabolites, nor research on mobility in the plants.

The field measurements of Keymeulen et al. (1993) for ethylbenzene, toluene and m,p- and o-xylene in Pseudotsuga are 10^4 or more times higher than the model of Riederer (1990) estimates (see Annex 3). No results from laboratory experiments are available for these compounds. Frank and Frank (1989) reported that the values for $K_{l/a}$ for tetrachloroethene are higher in the field, where the conifer needles were exposed to substantially lower air concentrations than in their laboratory experiments. Reischl et al. (1989), however, refer to similar values for laboratory and field studies. Under field conditions bioaccumulation occurs over a long period with exposure to lower gaseous air concentrations, combined with exposure to aerosoles and molecules dissolved in precipitation forms (e.g. rain or snow). Based on the data gathered here no conclusions can be drawn from the comparison of the results from laboratory and field experiments.

4.2 Comparison of model and experimental values

Herbaceous species

Both the models of Riederer (1990) and Trapp and Matthies (1995) predict $K_{l/a}$ values fairly well for the herbaceous species as can be seen in the regression equations and figures 2 and 3. Variation between experimental and calculated values for a substance is within a factor of 5 for most chemicals, which is similar to the variation in $K_{l/a}$ values between the different herbaceous species exposed to the same substance (see 4.1). We consider this initial amount of uncertainty acceptable for risk assessment purposes.

For DDE and DDT the $K_{l/a}$ values predicted by Riederer (1990) are too high when compared to the $K_{l/a}$ measured in *P. vulgaris* (figure 2). The model of Trapp and Matthies (1995) seems more adequate for these two compounds (figure 3). This may be expected in view of the high $K_{l/a}$, the exposure duration of 60 days, and the growth of these plants in that span of time (Bacci and Gaggi 1986). For 2,3,7,8-TCDD the estimation of Riederer (1990) is more adequate than that of Trapp and Matthies (1995). The short duration of the experiment with 2,3,7,8-TCDD (McCrady and Maggard 1993) may have excluded the influence of growth dilution.
For substances with log K_{ow} below 3.4 no data on experimental $K_{l/a}$ values have been found.

Azalea/Pine

For the *Azalea* and *Pinus* species both models of Riederer (1990) and Trapp and Matthies (1995) estimate the accumulation in leaves less adequately than for herbaceous plants. Partly this will be caused by the higher lipid content for these species. However, when the volume fractions applied in the model are corrected, based on an assumed volume fraction of cuticula and glycerol in leaf of 0.05, the agreement between model and experimental values for $K_{l/a}$ increases only slightly (data not shown).
For substances for which Riederer (1990) predicts $K_{l/a}$ values above 10^7, the $K_{l/a}$ values calculated by Trapp and Matthies (1995) are better nor worse. This is also expected as the growth dilution factor included in the model of Trapp and Matthies (1995) will not have played a role in the hardly growing Azalea leaves (e.g. Bacci and Gaggi 1987) and Pine needles (e.g. Frank and Frank 1989).

4.3 Conclusions

The experimental data on herbaceous plants fit well with the models of Riederer (1990) and Trapp and Matthies (1995). Based on these data the implementation of these models for risk assessment purposes has been correct. For more thorough validation of the models more high-quality experimental data are needed. The model of Trapp and Matthies (1995) might be more adequate for $K_{l/a}$ values above 10^7, however too few data are available to draw a conclusion in favour of this model. The prediction of bioconcentration in herbaceous plants under field conditions can not be evaluated with this data set.
The bioconcentration in Pine needles and Azalea leaves is estimated less accurately with the models of Riederer (1990) and Trapp and Matthies (1995) with the parameter settings used here.

4.3 Recommendations

A useful supplement of the data set gathered here will improve this evaluation. It has to include experimental research in the laboratory exposing herbaceous plants to substances for which model predictions for $K_{l/a}$ are lower than 10^3.

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ANNEXES

Annex 1

SEARCH PROFILE ON-LINE RESEARCH IN BIOSIS, 1970-JUNE 1995

1. find bioaccumulat? or accumulat? or bioconcentrat? or biotransfer?
2. find transfer? or uptake or translocat? or transport? or mobilit? or sorption
3. find retention or partition? or kinetic? or transpirat? or penetrat? or permea?
4. find partition?
5. find distribution/ti or response/ti
6. find gaseous or gas or gases or vapour? or vapor or air or airborne
7. find atmospher? or volatil? or aerosol or aerial or semivolatil or evapor?
8. find plant or plants or crop# or vegetation or leaf or leaves
9. find needle# or foliar
10. find (1 to 4)/(ti;ut) and (8 or 9)/ti and (6 or 7)
11. find 10 and pps=plantae
12. find 11 and sc=225?
13. find 12 not la=(bu;ch;cz;hu;it;ja;po;ru;sp)
14. find 13 and (6 or 7)/(ti;ut)
15. find 13 not 14

SEARCH PROFILE ON-LINE RESEARCH IN TOXLINE PLUS, 1987-JUNE 1994

#1 bioaccumulat* or accumulat* or bioconcentrat* or biotransfer*
#2 transfer or uptake or translocat* or transport* or mobilit*
#3 sorption or retention or partition* or kinetic*
#4 distribution
#5 plant? or crop? or vegetation or leaf or leaves or foliage or foliar or needle?
#6 gas or gases or vapour* or vapor* or air or airborne
#7 aerosol? or atmospher* or volatile? or aerial
#8 (#1 or #2 or #3 or #4) and #5 and (#6 or #7)
#9 #5 in ti
#10 #8 and #9

#11 #10 and ((#1 or #2 or #3 or #4) in ti)
#12 #10 and ((#6 or #7) in ti)
#13 #11 or #12

Annex 2

Basic data on experimental K l/a values

Compound	Plant species	Expos. dur.	Air conc ng/l	Conc in plantDW ug/kg	Conc in ng/l fresh leaf	K l/a in ng/l fresh leaf/ ng/l air	Reference	Comment
alpha-HCH	Phaseolus vulgaris	60 d	7.3	4800	720000	9.86E+04	Bacci & Gaggi 1986	Concs. in leaf DW after 60 d, recalculated to FW, assuming 15% DW. Mean air concs. are reported. Plants were 1-2 weeks old at the start of the experiment. K l/a calculated as conc. leaf/conc. air.
gamma-HCH	Phaseolus vulgaris	60 d	19.2	42700	6405000	3.34E+05		
hexachlorobenzene	Phaseolus vulgaris	60 d	3.1	700	105000	3.39E+04		
p,p'-DDE	Phaseolus vulgaris	60 d	0.93	28300	4245000	4.56E+06		
p,p'-DDT	Phaseolus vulgaris	60 d	0.089	4000	600000	6.74E+06		
p,p'-DDT	Azalea indica	34 d	0.032			4.85E+07	Bacci & Gaggi 1987	Old, hardly growing leaves, 30% DW. Test conducted in 200 l greenhouses. K l/a calculated by the authors as k1/k2.
p,p'-DDE	Azalea indica	34 d	0.45			3.38E+07		
p,p'-DDE	Azalea indica	34 d	0.061			3.43E+07		
alpha-HCH	Azalea indica	34 d	3.49			1.16E+06		
gamma-HCH	Azalea indica	34 d	4.94			8.57E+05		
trifluralin	Azalea indica	18 d	29.6			1.17E+05	Bacci et al. 1990a	Old, hardly growning leaves, 30% DW. Equilibrium possibly not reached for trifluralin, mirex, and thionazin. K l/a calculated by the authors as k1/k2.
hexachlorobenzene	Azalea indica	18 d	4.9			4.69E+05		
mirex	Azalea indica	18 d	0.027			1.32E+07		
thionazin	Azalea indica	14 d	19.2			3.05E+04		
sulfotep	Azalea indica	14 d	20.47			2.52E+04		
alachlor	Azalea indica	15 d	1.1		320000	2.85E+05	Bacci et al. 1990b	Old, hardly growing leaves were used. Mean air concs. Leaf concs. read from graph. K l/a calculated by the authors as k1/k2. K l/a of alachlor is probably low due to mobility and degradability in the plants.
dieldrin	Azalea indica	15 d	1.46		1200000	1.08E+06		
3,3',4,4'-tetrachlorobiphenyl	Azalea indica	15 d	0.017		140000	8.44E+07		
1,2,3,4-TCDD	Azalea indica	15 d	0.0062		43000	9.10E+07	Bacci et al. 1992	Old, hardly growing leaves were used. Mean air concs. Leaf concs. from graph; K l/a calculated by the authors as k1/k2.

Annex 2

Basic data on experimental K l/a values

Compound	Plant species	Expos. dur.	Air conc ng/l	Conc in plantDW ug/kg	Conc in ng/l fresh leaf	K l/a in ng/l fresh leaf/ ng/l air	Reference	Comment
tetrachloroethene	Picea abies excelsa		75		6400	8.53E+01	Frank & Frank 1989	Lab experiment, equilibrium is reached within 6 h. Field: K l/a ca. f. 10 higher, at f. 20 or more lower air concs. One-year old needles were analysed. K l/a calculated as conc. leaf/conc. air.
tetrachloroethene	Picea abies excelsa		180		11600	6.44E+01		
DDE	Picea omorika	13 d	0.02	32.7	13080	6.54E+05	Hauk et al. 1994	Exposure in 700 l glass chambers. From P. omorika 6-month-old needles were analysed, and from P.abies 12-month-old. K l/a calculated as conc. leaf/conc./air.
DDE	Picea omorika	7 d	0.006	14	5600	9.33E+05		
DDE	Picea abies	15 d	0.01	115	46000	4.60E+06		
1,2,4,5'-tetrachlorobenzene	Picea omorika					7.18E+04	Reischl et al. 1989	Data originate from doctoral thesis. K l/a calculated by the authors with a two-compartment kinetic model.
pentachlorobenzene	Picea omorika					9.30E+05		
hexachlorobenzene	Picea omorika					4.30E+05		
gamma-HCH	Picea omorika					1.25E+06		
p,p'-DDT	Picea omorika					2.46E+07		
4,4'-dichlorobiphenyl	Picea omorika					2.34E+06		
2,2'5-trichlorobiphenyl	Picea omorika					7.06E+05		
2,2',3,4,5,5',6-heptachlorobiph.	Picea omorika					2.91E+06		
2,2',3,4,4',5,6,6'-octachlorobiph.	Picea omorika					6.50E+06		
1,4-dichlorobenzene	Hordeum vulgare	7 d				1.34E+02	Scheunert et al. 1994	14C-labeled testcompounds, concs. in air and shoots were measured but not reported by the authors. Growing seedlings were used in this test. Seeds in clean and contaminated soil, placed in a 10 L dessicator,. Plants from clean soil, exposed only via the air, are included in this table.K l/a calculated by the authors as conc. leaf/conc. air. NB. concs. in shoots.
1,4-dichlorobenzene	Lepidium sativum	7 d				1.68E+01		
1,2,4-trichlorobenzene	Hordeum vulgare	7 d				1.13E+03		
1,2,4-trichlorobenzene	Lepidium sativum	7 d				9.66E+02		
1,2,3,5-tetrachlorobenzene	Hordeum vulgare	7 d				3.67E+03		
1,2,3,5-tetrachlorobenzene	Lepidium sativum	7 d				1.09E+03		
pentachlorobenzene	Hordeum vulgare	7 d				2.36E+04		
pentachlorobenzene	Lepidium sativum	7 d				6.20E+03		
hexachlorobenzene	Hordeum vulgare	7 d				1.13E+04		
hexachlorobenzene	Lepidium sativum	7 d				1.44E+04		

Annex 2

Basic data on experimental K l/a values

Compound	Plant species	Expos. dur.	Air conc ng/l	Conc in plantDW ug/kg	Conc in ng/l fresh leaf	K l/a in ng/l fresh leaf/ ng/l air	Reference	Comment
2,3,7,8-TCDD	Phalaris arundinacea	96 h	4.0E-05	5	750	3.16E+07	McCrady & Maggard , 1993	Vapor-phase [1,6-3H] labeled TCDD was applied. Plants were ca. 3 w. old. K l/a calculated as conc. leaf/conc./air.
FIELD MEASUREMENTS								
DDE	Picea abies	164 d	1.4E-05	1	400	2.86E+07	Hauk et al. 1994	K l/a calculated as conc. leaf/conc./air. Air conc. was measured continuously. Analysed needles were 3-8.5 months old.
ethylbenzene+A4	Pseudotsuga menziesii	1 year	8			3.26E+05	Keymeulen et al. 1993	Mean air concs. at two sites, measured regularly during the test year. K l/a calculated as ZL/ZA, presuming 26.7% DW and a water content of 70%. One year old leaves were analysed.
ethylbenzene		1 year	1.6			3.93E+05		
toluene	Pseudotsuga menziesii	1 year	35.5			3.60E+04		
toluene		1 year	7.2			3.03E+04		
m,p-xylene	Pseudotsuga menziesii	1 year	25.1			3.48E+05		
m,p-xylene		1 year	3.7			5.28E+05		
o-xylene	Pseudotsuga menziesii	1 year	10.1			4.04E+05		
o-xylene		1 year	1.7			4.49E+05		

Annex 3

Physico-chemical properties, and K l/a from models and experiments

Compound	Log Kow	ref	S in mg/l	ref	vap.press. in Pa	ref	M.W. g/mol	H dim. less	K l/a Riederer	K l/a Tr&Mat	K l/a exp herbs	Ried/ exp	T&M/ exp	K l/a exp azal./pine	Ried/ exp	T&M/ exp
alachlor	3.52	ME	242	PM	2.90E-03	PM	269.8	1.31E-06	2.6E+07	5.0E+06				2.85E+05	89.97	17.45
p,p'-DDE	6.96	ME	0.065	Ve	4.00E-04	Ca	319.1	8.07E-04	1.1E+08	5.9E+06	4.56E+06	24.74	1.28	1.48E+07	7.61	0.39
p,p'-DDT	6.91	ME	0.003	ME	2.50E-05	PM	354.5	1.21E-03	6.7E+07	5.7E+06	6.74E+06	9.93	0.84	3.65E+07	1.83	0.15
1,4-dichlorobenzene	3.4	Ma	83	Ma	9.02E+01	Ma	147.1	6.46E-02	4.0E+02	4.0E+02	7.55E+01	5.24	5.24			
4,4'-dichlorobiphenyl	5.3	Ma	0.06	Ma	4.80E-03	Ma	223.1	7.22E-03	2.8E+05	2.6E+05				2.34E+06	0.12	0.11
dieldrin	5.2	ME	0.17	Ho	5.00E-04	Ho	380.9	4.61E-04	3.4E+06	2.2E+06				1.08E+06	3.19	2.05
alpha-HCH	3.72	ME	2	Ho	6.00E-03	Ho	290.9	3.53E-04	1.5E+05	1.5E+05	9.86E+04	1.52	1.48	1.16E+06	0.13	0.13
gamma-HCH (lindane)	3.72	ME	7.3	Ho	7.40E-03	Ho	290.9	1.19E-04	4.4E+05	4.1E+05	3.34E+05	1.33	1.24	1.06E+06	0.42	0.39
*2,2'3,4,5,5',6-heptaCB	6.7	Ma	0.002	Ma	2.73E-05	Ma	395.3	2.18E-03	2.3E+07	4.9E+06				2.91E+06	7.89	1.67
hexachlorobenzene	5.5	Ma	0.005	Ma	2.30E-03	Ma	284.8	5.30E-02	6.0E+04	5.9E+04	1.98E+04	3.01	2.98	4.49E+05	0.13	0.13
mirex	5.28	ME	pract.insol.		1.00E-04	Ba	545.6	4.00E-05	4.8E+07	5.5E+06				1.32E+07	3.60	0.41
*2,2',3,4,4',5,6,6'-octaCB	7.1	Ma	0.0003	Ma	2.66E-05	Ma	429.7	1.54E-02	8.2E+06	3.5E+06				6.50E+06	1.26	0.54
pentachlorobenzene	5	Ma	0.65	Ma	2.20E-01	Ma	250.3	3.43E-02	2.9E+04	2.9E+04	1.49E+04	1.96	1.95	9.30E+05	0.03	0.03
sulfotep	3.99	PM	10	PM	1.40E-02	PM	322.3	1.86E-04	5.3E+05	4.9E+05				2.52E+04	20.98	19.32
1,2,3,5-tetrachlorobenzene	4.5	Ma	3.6	Ma	9.80E+00	Ma	215.9	2.38E-01	1.3E+03	1.3E+03	2.38E+03	0.56	0.56			
1,2,4,5-tetrachlorobenzene	4.5	Ma	1.27	Ma	7.20E-01	Ma	215.9	4.95E-02	6.4E+03	6.4E+03				7.18E+04	0.09	0.09
3,3'4,4'-tetrachlorobiphenyl	6.5	Ma	0.001	Ma	5.88E-05	Ma	292	6.94E-03	4.6E+06	2.6E+06				8.44E+07	0.05	0.03
1,2,3,4-TCDD	6.6	Ma	0.00055	Ma	6.40E-06	Ma	322	1.51E-03	2.6E+07	5.0E+06				9.10E+07	0.29	0.05
2,3,7,8-TCDD	6.8	Ma	0.0000193	Ma	2.00E-07	Ma	322	1.35E-03	4.7E+07	5.5E+06	3.16E+07	1.48	0.17			
tetrachloroethene	2.88	Ma	150	Ma	2.42E+03	Ma	165.8	1.08E+00	7.9E+00	7.9E+00				7.49E+01	0.11	0.11
thionazin	1.24	PM	1140	PM	4.00E-01	PM	248.2	3.50E-05	1.6E+04	1.6E+04				3.05E+04	0.54	0.54
1,2,4-trichlorobenzene	4.1	Ma	40	Ma	6.10E+01	Ma	181.5	1.12E-01	1.1E+03	1.1E+03	1.05E+03	1.08	1.08			
2,2'5-trichlorobiphenyl	5.6	Ma	0.4	Ma	1.43E-01	Ma	257.5	3.72E-02	1.1E+05	1.1E+05				7.06E+05	0.15	0.15
trifluralin	5.34	ME	0.22	PM	9.50E-03	PM	335.3	5.95E-03	3.7E+05	3.5E+05				1.17E+05	3.14	2.96

=mean value used $=lowest value used

*=data from other congener, CB=chlorobiphenyl

ME=Medchem, Ma=Mackay et al.1992; Ho=Howard et al.1991; PM=Pesticide Manual 1983,1994;

Ve=Verschueren 1983; Ba=Bacci et al.1990a; Ca=Calamari et al.1985

Annex 3

Physico-chemical properties, and K l/a from models and experiments

Compound	Log Kow	ref	S in mg/l	ref	vap.press. in Pa	ref	M.W. g/mol	H dim. less	K l/a Riederer	K l/a Tr&Mat	K l/a exp herbs	Ried/ exp	T&M/ exp	K l/a exp azal./pine	Ried/ exp	T&M/ exp
FIELD MEASUREMENTS																
p,p'-DDE	6.96	ME	0.065	Ve	4.00E-04	Ca	319.1	8.07E-04	1.1E+08	5.9E+06				2.86E+07	3.95	0.20
ethylbenzene	3.13	Ma	152	Ma	1.27E+03	Ma	106.2	3.59E-01	3.9E+01	3.9E+01				3.60E+05	0.00	0.00
toluene	2.69	Ma	515	Ma	3.80E+03	Ma	92.13	2.75E-01	2.0E+01	2.0E+01				3.31E+04	0.00	0.00
m,p-xylene	3.19	Ma	187.5	Ma	1.14E+03	Ma	106.2	2.60E-01	6.2E+01	6.2E+01				4.38E+05	0.00	0.00
o-xylene	3.15	Ma	220	Ma	1.17E+03	Ma	106.2	2.28E-01	6.4E+01	6.4E+01				4.27E+05	0.00	0.00