Environment Agency

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Verification of bioaccumulation models for use in environmental standards. Part B: terrestrial models

Science Report – SC030197/SR3

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Steve Killeen

Head of Science

Executive summary

This report assesses two methods for predicting chemical exposure to terrestrial species. These are the Arctic Terrestrial Food-Chain model developed by Kelly and Gobas (2003), including the simplified steady-state wolf model developed by Gobas *et al.* (2003), and the earthworm accumulation model included in the EU Technical Guidance Document (TGD).

The Arctic Terrestrial Food-Chain model, and in particular the simplified steady-state wolf model, shows promise in being able to predict the accumulation of chemicals from food in terrestrial mammals. However, in this study it was possible to test the models only to a limited extent. It is recommended that the steady-state model described in Gobas *et al.* (2003) is parameterised for small plant-eating and worm-eating mammals, and is combined with the plant models described in Part C of this series of reports and the earthworm model discussed below. At present, such terrestrial mammal models will only provide reliable predictions for substances that do not undergo metabolism in the terrestrial mammal, and this is a major limitation to the general applicability of the model. Further work would be needed to determine if it is possible to reliably estimate the rates of metabolism of chemicals in terrestrial species from laboratory animal data or using other methods.

In this report, the TGD method was extensively tested against a large data set of experimental and field earthworm accumulation data. The analysis found that the TGD method consistently overpredicts the bioaccumulation factor in earthworms $BAF_{earthworm}$ (and hence the concentration in earthworms) at log K_{ow} values above four to five. However, it is possible to correct for this overprediction using the following equations:

For the TGD default QSAR for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.69 \times \log K_{ow}) + 2.72$$

For the QSAR for predominantly hydrophobic chemicals for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.39 \times \log K_{ow}) + 1.72$$

It is concluded that the TGD method, with these corrections, is sufficiently reliable for use in setting standards.

Contents

1 Introduction

This project forms part of a broader programme to support the Environment Agency's work in developing standards for the protection of the environment and human health from chemicals (P6-020/U, *A programme of work on environmental and human health standards for chemicals*).

The Environment Agency must derive standards to protect the environment and human health in order to fulfil its statutory pollution control role. This project is intended to help provide a sound scientific basis for setting such standards and to ensure a transparent and consistent approach to setting standards across different functions within the Environment Agency.

Bioaccumulative substances are of concern to the Environment Agency because they have the potential to biomagnify via the food chain and cause effects on organisms at higher trophic levels. Bioaccumulation is of particular concern when the chemical is toxic as well as persistent or continuously released to the environment.

The Environment Agency currently derives standards to protect the aquatic environment based on acute or chronic aquatic toxicity data divided by an extrapolation factor. This approach does not take into account possible effects on organisms higher in the food chain, nor does it consider routes of exposure other than direct contact with water. For highly lipophilic substances that bioaccumulate, water is unlikely to be the only route of exposure for aquatic organisms and top predators, and exposure via contaminated food or sediment may become important. The Environment Agency needs to consider these additional exposure routes when setting aquatic standards for bioaccumulative and persistent substances.

This project will help the Environment Agency's negotiating position at EU meetings to agree environmental quality standards for pollutants and priority substances listed in Annexes VIII to X to the Water Framework Directive (Directive 2000/60/EC).

When setting soil standards, the Environment Agency must consider indirect exposure routes for organisms at the top of the terrestrial food chain. The method used to derive soil standards will feed into the tiered terrestrial ecological risk assessment (ERA) framework that is being developed by the Environment Agency and the Department for Environment, Food and Rural Affairs (Defra). Once finalised, this framework will be used in Part 2A of the Environmental Protection Act 1990 to assess the impacts of soil contamination on wildlife top predators, and it is also likely to have other uses such as under the Habitats Directive.

In addition to aquatic and terrestrial organisms, bioaccumulation in or uptake through the food chain is also important when considering human exposure to contaminants. Methods for determining human exposure to chemicals from some types of soil contamination are already available in the Contaminated Land Exposure Assessment (CLEA) approach (Environment Agency and Defra, 2002). However, equivalent methods for determining exposure to chemicals from other types of soils, and from other routes such as the aquatic food chain, are not generally available.

This work was commissioned by the Environment Agency to validate models suitable for assessing the potential bioaccumulation of organic chemicals when setting environmental standards. The models selected for verification in this report are based on the results of an initial evaluation of a large number of possible models. The initial evaluation is covered in a separate report (Environment Agency, 2007).

This report (Part B) outlines the verification of models and methods for the terrestrial environment. Verification of models for the aquatic environment and for the human food chain is considered in Parts A and C of this series of reports. The physico-chemical properties of chemicals used in this verification exercise are summarised in Part D.

For the terrestrial environment, the following two methods are considered for verification:

The Arctic Terrestrial Food-Chain Bioaccumulation model, which is presented in a paper by Kelly and Gobas (2003). A computerised version of the model is not yet available. A simplified, steady-state model for arctic wolf is also available (Gobas *et al*., 2003) based on similar principles.

The EU Technical Guidance Document (TGD) (European Commission, 2003). The TGD outlines the methods used for the risk assessment of new and existing chemicals and biocidal products in the EU. Methods in the TGD are implemented in a computer program called the European Union System for Evaluation of Substances, better known as EUSES (EUSES version 2.0.3 was used in this work). The TGD and the EUSES program are freely available from the European Chemicals Bureau website (http://ecb.jrc.it/).

2 Initial comparison of the models

2.1 Arctic Terrestrial Food-Chain model

The Arctic Terrestrial Food-Chain model is currently only available as a series of equations in a paper published by Kelly and Gobas (2003). These equations are included in Appendix A. The model is presented in two parts in Kelly and Gobas (2003). The first part is an air-to-vegetation distribution model which is not considered further in this report, although a similar model is considered as part of the ACC-HUMAN model in the Part C report. The second part of the Arctic model considers uptake into terrestrial herbivores (caribou) and carnivores (wolves).

No computerised or spreadsheet version of this model is available and so it was not possible to test this specific model as part of this work. However, Gobas *et al.* (2003) formulated a simplified, steady-state version of the model for accumulation in wolves via the diet as follows. This method is very similar in principle to that outlined in Kelly and Gobas (2003).

$$BMF = \frac{C_{Biota}}{C_{Diet}} = \frac{k_{Diet}}{\left(k_{Air} + k_{Urine} + k_{Bile} + k_{Faeces} + k_{Milk} + k_{Growth} + k_{Metab}\right)}$$

where BMF = biomagnification factor for uptake from food.

C_{Biota} = steady-state concentration in the animal (wolf) (mol m^{-3} or mg kg^{-1}).

C_{Diet} = concentration in diet (mol m^{-3} or mg kg^{-1}).

k_{Diet} = dietary uptake rate constant (day^{-1}).

k_{Air} = respiratory elimination rate constant (day^{-1}).

k_{Urine} = urinary excretion rate constant (day^{-1}).

k_{Bile} = bile excretion rate constant (day^{-1}).

k_{Faeces} = faecal excretion rate constant (day^{-1}).

k_{Milk} = milk excretion rate constant (day^{-1}).

k_{Growth} = growth rate constant for the organism (day^{-1}).

k_{Metab} = rate constant for metabolism of the substance (day^{-1}).

[It is not entirely clear if C_{Biota} and C_{Diet} are on a lipid volume/weight basis or a whole organism volume/weight basis; however, as the rate constants used do not depend on the lipid content of the food (prey), it is most likely that C_{Biota} and C_{Diet} (and hence BMF) are determined on a whole organism (or wet weight) basis.]

The value of k_{Growth} is an organism-specific property that is dependent to some extent on the age of the organism considered. For adults this can be set to zero. Similarly, the k_{Metab} is a chemical-specific property. A value of zero can be used for non-

metabolised substances. The other rate constants used in the model are estimated as follows.

$$k_{Diet} = \frac{E_{Diet} \times G_D}{V_B}$$

$$k_{Air} = \frac{E_{Air} \times G_A}{V_B \times L_B \times K_{OA}}$$

$$k_{Urine} = \frac{G_U}{V_B \times L_B \times P}$$

$$k_{Bile} = \frac{G_B}{V_B \times L_B \times K_{OB}} = \frac{G_B}{V_B \times L_B \times \left(Kow / \beta \right)}$$

$$k_{Faeces} = \frac{G_F}{V_B \times K_{BF}}$$

$$k_{Milk} = \frac{G_M}{V_B \times L_B \times K_{OM}}$$

where E_{Diet} = dietary uptake efficiency; a value of 0.9 (90%) is assumed for wolves.

E_{Air} = air uptake efficiency; a value of 0.3 (30%) is assumed for wolves.

G_D = feeding rate (m^3 day^{-1} or kg day^{-1}); a value of 2.1 kg per day is assumed for wolves.

G_A = respiration rate (m^3 day^{-1} or l day^{-1}); a value of 20,000 l day^{-1} is assumed for wolves.

G_U = urinary excretion rate (m^3 day^{-1} or l day^{-1}); a value of 1.0 l day^{-1} is assumed for wolves.

G_B = bile excretion rate (m^3 day^{-1} or l day^{-1}); a value of 0.3 l day^{-1} is assumed for wolves.

G_F = faecal excretion rate (m^3 day^{-1} or kg day^{-1}); a value of 0.66 kg day^{-1} is assumed for wolves.

G_M = milk excretion rate (m^3 day^{-1} or l day^{-1}); a value of zero is assumed for males and non-lactating females.

V_B = volume or weight of the organism (m^3 or kg); a value of 80 kg is assumed for wolves.

L_B = lipid content of the organism; a value of 0.12 (12%) is assumed for wolves.

K_{ow} = octanol-water partition coefficient of the chemical.

K_{oa} = octanol-air partition coefficient of the chemical.

K_{OB} = octanol-bile partition coefficient.

β = a factor to account for differences in solubility of the substance between bile and water; a value of 10 is assumed in the model.

K_{BF} = organism-faeces partition coefficient; a value of 50 is assumed for persistent organic chemicals (POPs) in the model.

K_{OM} = octanol-milk partition coefficient; no information is given as to how this can be estimated, though this value is not needed for males and non-lactating females.

[The equations in Gobas *et al.* (2003) are formulated in terms of m^3 for volumes/weights. However, the model parameters given for wolves are formulated in kg or litres for weights/volumes. Care is needed in ensuring that units for the values used are internally consistent. This may require the use of corrections for the density of the different compartments (environmental and biota).]

Although the food chain included in this model is currently of limited relevance to the United Kingdom, this model is one of the few terrestrial models available to consider exposure of mammalian top predators, and the model would be adaptable to other terrestrial mammalian food chains.

2.2 TGD/EUSES

The TGD method for the terrestrial compartment uses an earthworm bioconcentration factor (BCF) that relates the concentration of a chemical in the worm to the concentration of the chemical in soil pore water. The method used to estimate the BCF uses the following equation developed by Jager (1998).

$$BCF_{earthworm} = (0.84 + 0.012 \times K_{ow})/RHO_{earthworm}$$

where $BCF_{earthworm}$ = earthworm bioconcentration factor (l kg^{-1} wet weight).

K_{ow} = octanol-water partition coefficient (note the actual octanol-water partition coefficient rather than the log K_{ow} [1] value is used in this equation).

$RHO_{earthworm}$ = density of the earthworm. A value of one kg fresh weight l^{-1} is assumed as default.

$BCF_{earthworm}$ relates the concentration in the earthworm to the concentration in pore water. In order to calculate the uptake from whole soil, the following equation is used:

$$C_{earthworm} = \frac{BCF_{earthworm} \times C_{porewater} + C_{soil} \times F_{gut} \times CONV_{soil}}{1 + F_{gut} \times CONV_{soil}}$$

where $C_{earthworm}$ = concentration in earthworm (mg kg^{-1} fresh weight).

$C_{pore\ water}$ = concentration in soil pore water (mg l^{-1}).

C_{soil} = total concentration in soil (mg kg^{-1} wet weight).

F_{gut} = fraction of gut loading of soil in worm = 0.1 kg^{-1} dry weight kg^{-1} wet weight.

$CONV_{soil}$ = conversion factor for soil concentration on wet-dry soil weight basis = 1.133 kg wet weight kg^{-1} dry weight.

[1] In this report, the term log K_{ow} is used to refer to the $\log_{10}$ of the octanol-water partition coefficient.

As can be seen from this equation, the final concentration in earthworm is a combination of the concentration resulting from bioconcentration from soil pore water plus the concentration resulting from the presence of contaminated soil in the gut. This approach is appropriate when considering the total concentration to which a predatory organism would be exposed via diet. However, when comparing the predictions against laboratory or field data, it is important to consider whether or not the gut contents of the earthworms have been voided prior to analysis. In cases where the gut contents have been voided, F_{gut} has been set to zero in the analysis in Section 3.

The concentration in soil pore water is related to the total concentration in soil by the following equation:

$$C_{porewater} = \frac{C_{soil} \times RHO_{soil}}{K_{soil-water} \times 1{,}000}$$

where RHO_{soil} = bulk density of wet soil = 1,700 kg m^{-3} as a default.

$K_{soil\text{-}water}$ = solids-water partitioning coefficient for bulk soil ($m^3\ m^{-3}$).

$K_{soil\text{-}water}$ can be estimated from basic physico-chemical properties of the substance using the following methods:

$$K_{soil-water} = (F_{air} \times Kaw) + F_{water} + \left(F_{solid} \times \frac{Kp_{soil}}{1{,}000} \times 2{,}500 \right)$$

where F_{air} = volume fraction of air in soil; default is 0.2 $m^3\ m^{-3}$.

F_{water} = volume fraction of water in soil; default is 0.2 $m^3\ m^{-3}$.

F_{solid} = volume fraction of solid in soil; default is 0.6 $m^3\ m^{-3}$.

K_{aw} = air-water partition coefficient (also known as the dimensionless Henry's law constant).

Kp_{soil} = soil-water partition coefficient (l kg^{-1}).

The value of K_{aw} can be estimated from Henry's law constant using the following equation:

$$K_{aw} = \frac{H}{R \times T}$$

where H = Henry's law constant (Pa $m^3\ mol^{-1}$).

R = gas constant = 8.314 Pa $m^3\ mol^{-1}\ K^{-1}$

T = absolute temperature; the default is 285 K.

The soil-water partition coefficient can be estimated using the following equation:

$$Kp_{soil} = F_{oc} \times Koc$$

where F_{oc} = fraction organic carbon in soil; the default is 0.02.

K_{oc} = organic carbon-water partition coefficient (l kg^{-1}).

Combining the above equations, the concentration in earthworms can be estimated using the following equation:

$$C_{earthworm} = C_{soil} \times \frac{\left[\frac{\left(\frac{(0.84 + 0.012 \times 10^{logKow})}{RHO_{earthworm}} \times RHO_{soil} \right)}{1{,}000 \times \left((F_{air} \times K_{aw}) + F_{water} + \left(F_{solid} \times \left(\frac{Koc \times F_{oc}}{1{,}000} \right) \times 2{,}500 \right) \right)} + (F_{gut} \times CONV_{soil}) \right]}{1 + (F_{gut} \times CONV_{soil})}$$

Using the default values in the TGD, this can be simplified to the following equation:

$$C_{earthworm} = C_{soil} \times \frac{\left[\left(\frac{1.7 \times (0.84 + 0.012 \times 10^{logKow})}{(0.2 \times Kaw) + 0.2 + (0.03 \times Koc)} \right) + 0.1133 \right]}{1.1133}$$

For substances of low volatility (where K_{aw} is much smaller than K_{oc}, as is the case for the majority of chemicals considered in Section 3 of this report), the equation can be further simplified as follows:

$$C_{earthworm} = C_{soil} \times \frac{\left[\left(\frac{1.7 \times (0.84 + 0.012 \times 10^{logKow})}{0.2 + (0.03 \times Koc)} \right) + 0.1133 \right]}{1.1133}$$

If needed, an earthworm bioaccumulation factor ($BAF_{earthworm}$) on a wet weight earthworm/wet weight soil basis can be estimated from the above equation as $C_{earthworm}/C_{soil}$.

$$BAF_{earthworm} = \frac{C_{earthworm}}{C_{soil}} = \frac{\left[\left(\frac{1.7 \times (0.84 + 0.012 \times 10^{logKow})}{0.2 + (0.03 \times Koc)} \right) + 0.1133 \right]}{1.1133}$$

where $BAF_{earthworm}$ is on a mg kg^{-1} wet weight worm/mg kg^{-1} wet weight soil basis.

$BAF_{earthworm}$ therefore relates the concentration in earthworms directly to a concentration in soil. This form could readily be used in a back-calculation from a concentration in worms that is thought to be protective of predatory wildlife to the

equivalent concentration in soil (as outlined in Environment Agency, 2007), thereby allowing standards for soil to be set that would protect wildlife. For the exposure of worm-eating predators, the concentration in earthworm on a wet weight basis should be calculated (as the whole worm is eaten). However, concentrations in soil are more normally determined on a dry weight than wet weight basis, and it may be more relevant to consider soil concentrations on a dry weight basis when setting standards. In order to convert $BAF_{earthworm}$ to a dry weight soil basis, the following conversion can be used:

$$BAF_{earthworm}\frac{(\text{mg kg}^{-1}\text{ wet worm})}{(\text{mg kg}^{-1}\text{ dry soil})} = BAF_{earthworm}\frac{(\text{mg kg}^{-1}\text{ wet worm})}{(\text{mg kg}^{-1}\text{ wet soil})} \times \left(\frac{100 - \text{water}}{100}\right)$$

where 'water' is the percentage water content of the wet soil (percentage by weight). The default water content of soil in the TGD is approximately 12 per cent by weight.

$BAF_{earthworm}$ is also dependent on the soil-water partitioning properties of the chemical, which in turn are dependent on the K_{oc} value and the soil organic carbon content. The TGD gives several quantitative structure activity relationships (QSARs) for estimating the K_{oc} of a substance from the log K_{ow} for a range of chemical types. The TGD also gives a default organic carbon content of two per cent by weight for soil; however, in practice the organic carbon content can vary from soil to soil, and different values of $BAF_{earthworm}$ would be estimated for the same chemical in soils of differing organic carbon contents.

The TGD suggests that the method for estimating uptake into earthworms is applicable to chemicals with a log K_{ow} in the range one to eight, and that it is reasonable to assume that the method would also be applicable to chemicals with a log K_{ow} of less than one.

The equation to estimate $BCF_{earthworm}$ was generated from a theoretical mechanistic model developed by Jager (1998). The model assumed that the bioconcentration in the earthworm can be described by thermodynamic partitioning equilibrium between the soil solids, soil pore water and the worm tissue. Jager (1998) tested the model against a data set consisting of bioconcentration factors for a series of chemicals determined using water-only exposures or whole soil exposures. Jager (1998) reported that the model was able to estimate correctly the $BCF_{earthworm}$ from the experiments using water-only exposure, but the values of $BCF_{earthworm}$ from experiments in soil were consistently overestimated (the average overestimate was by a factor of 5.6). One possible explanation for the poor performance of the model for soil experiments was thought to be a lack of true equilibrium in the soil-pore water-earthworm system in these experiments.

The method used by Jager (1998) to estimate soil pore water concentrations of the chemicals in the test set is slightly different to that used in the TGD method, and so this study set out to verify the TGD method against the test set used by Jager (1998). This test set was supplemented by a significant amount of new data that became available after the Jager (1998) study. The results of this verification are summarised in Section 3.

The TGD method also calculates concentrations in plants (root crops, grass and leaf crops), mainly in relation to human exposure. However, these aspects of the model may also be relevant to the exposure of herbivorous species in the environment. This part of the model has been tested in Part C of this report series.

2.3 Comparison of predictions using a hypothetical test set

As the methods under consideration are concerned with different food chains, it is not relevant to compare predictions obtained for a hypothetical test set using the two methods. Instead, the two methods are considered separately.

2.3.1 Arctic Terrestrial Food-Chain model

As discussed earlier, a computerised or spreadsheet version of the Arctic Terrestrial Food-Chain model described in Kelly and Gobas (2003) is not yet available. However, a slightly simplified, steady-state version of the model for uptake in wolves via food has been reported by Gobas *et al.* (2003), and this was used here to estimate the BMF (concentration in wolf (mg kg^{-1} wet weight)/concentration in food (mg kg^{-1} wet weight)) for a series of hypothetical test chemicals. The two key physico-chemical properties used by the model are the log K_{ow} and the octanol-air partition coefficient (K_{oa}).

Measured values of K_{oa} are available only for a limited number of substances; however, the value can be estimated for organic chemicals from relatively simple physico-chemical properties such as log K_{ow}, vapour pressure and solubility as shown below.

Defining the equilibrium partition coefficients K_{oa}, K_{ow}, and K_{aw} as follows:

$$K_{oa} = \frac{C_{Oct}}{C_{Air}} \qquad Kow = \frac{C_{Oct}}{C_{Water}}$$

$$K_{aw} = \frac{C_{Air}}{C_{Water}}$$

where K_{oa} = octanol-air partition coefficient.

K_{ow} = octanol-water partition coefficient.

K_{aw} = air-water partition coefficient (dimensionless Henry's law constant).

C_{air} = concentration in air (mol m^{-3}).

$C_{octanol}$ = concentration in octanol (mol m^{-3}).

C_{water} = concentration in water (mole m^{-3}).

Therefore,

$$K_{oa} = \frac{Kow}{K_{aw}}$$ (or log K_{oa} = log K_{ow} – log K_{aw}).

The value of K_{aw} can be estimated from Henry's law constant (and hence water solubility and vapour pressure) as follows:

$$K_{aw} = \frac{H}{R \times T} = \frac{VP}{Sol_{water} \times R \times T}$$

where H = Henry's law constant (Pa m^3 mol^{-1}).

R = gas constant = 8.314 J K^{-1} mol^{-1}.

T = absolute temperature (K).

VP = vapour pressure at temperature T (Pa).

Sol_{water} = water solubility (mol m^{-3}).

Therefore,

$$K_{oa} = \frac{Kow \times Sol_{water} \times R \times T}{VP}.$$

From this it can be seen that K_{oa} also has some dependence on K_{ow}, but also takes into account the solubility and vapour pressure of the substance.

For the hypothetical test set, both log K_{ow} and log K_{oa} were varied between zero and 10. No metabolism was assumed to be occurring. The resulting BMFs (defined as the concentration in the organism/concentration in food) are plotted in **Error! Reference source not found.** (showing the variation with log K_{ow} at a constant log K_{oa}) and **Error! Reference source not found.**.2 (showing the variation with log K_{oa} at a constant log K_{ow}).

As can be seen from the plots, the predicted BMF depends crucially on the log K_{oa} as well as log K_{ow}. Indeed, it is apparent that no significant uptake from food (BMF < 0.1) occurs for any chemical (regardless of the log K_{ow} value) when the log K_{oa} is below 3.5 (log K_{ow} – log K_{aw} < 3.5).

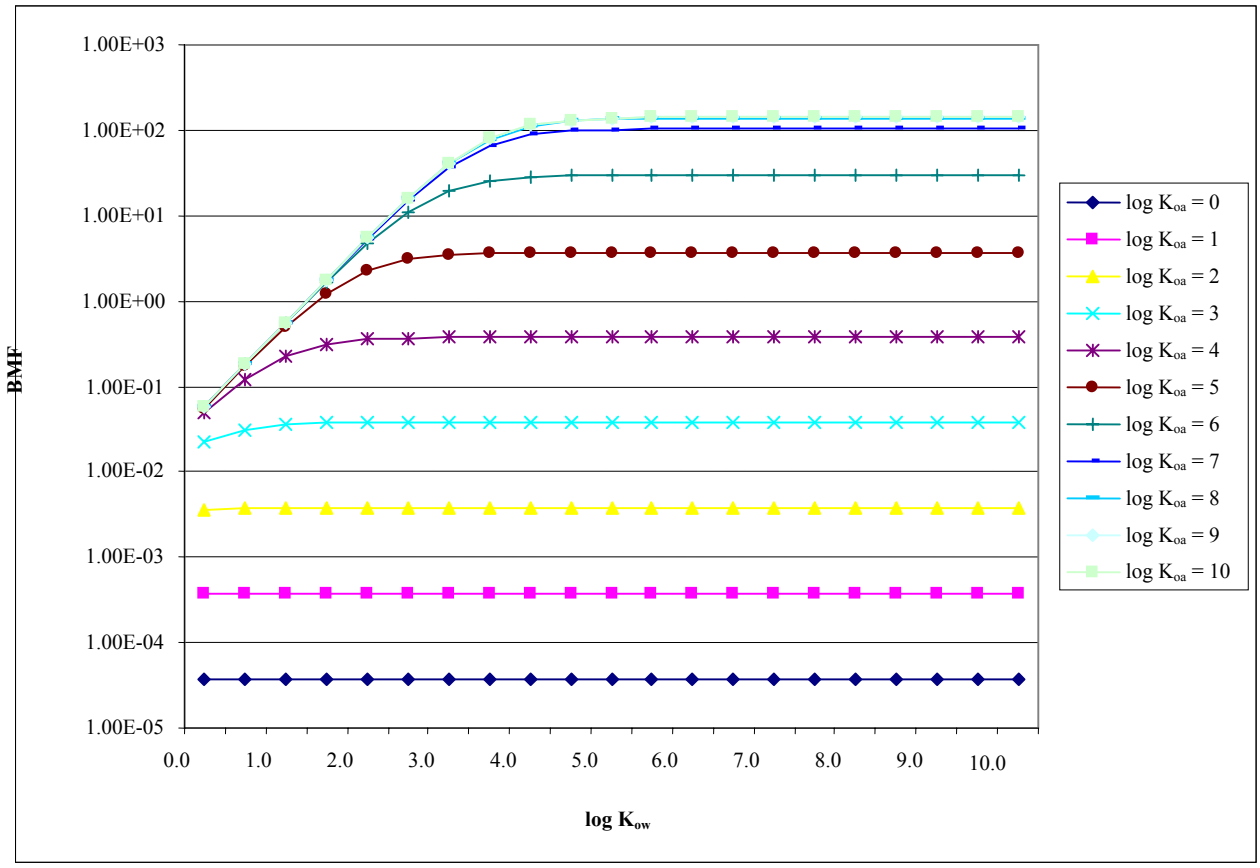

Figure 2.1 Variation of predicted BMF with log K_{ow} for wolves

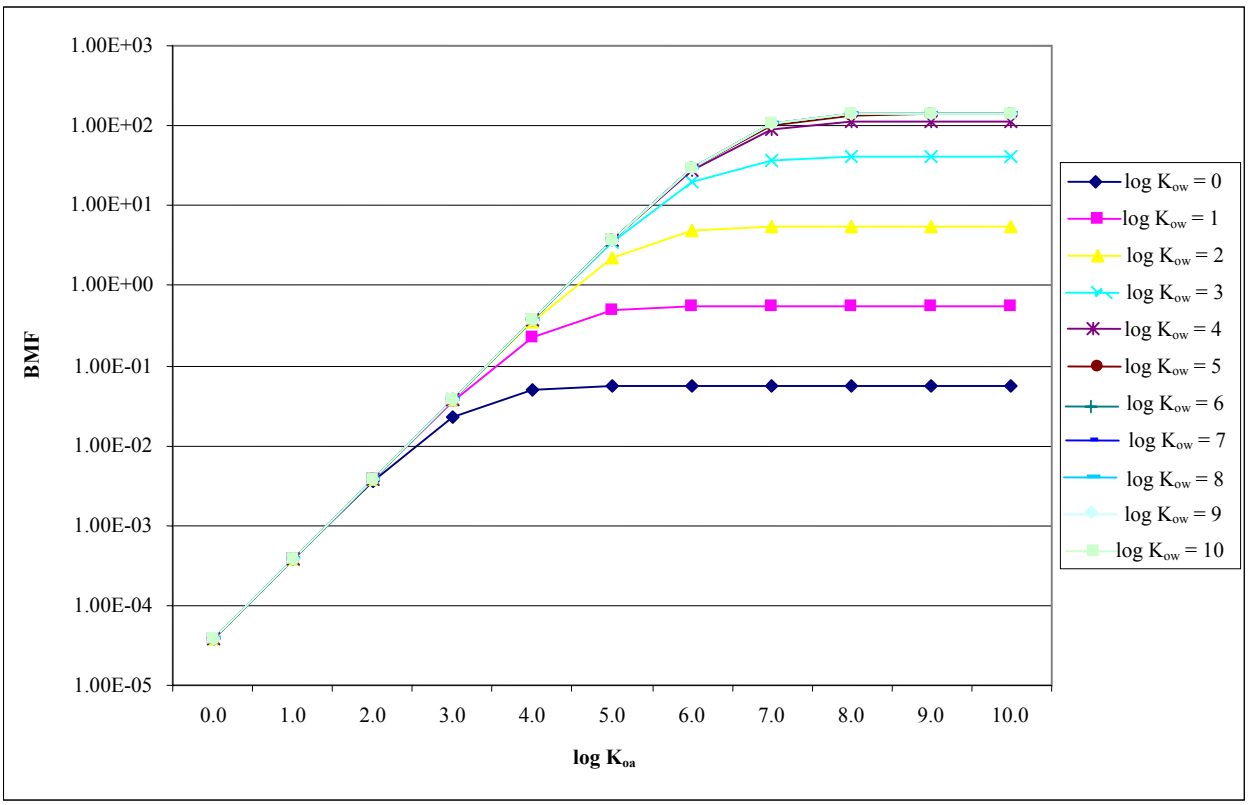

Figure 2.2 Variation of predicted BMF with log K_{oa} for wolves

The model also predicts a maximum value for the BMF of around 100 (as indicated earlier, it is not entirely clear if this value is a whole body wet weight value or a lipid-normalised value). This occurs for substances with log K_{ow} values of around four, provided they also have a log K_{oa} of seven or greater.

An interesting finding from the model is that BMFs greater than one are predicted for substances of only moderate log K_{ow} values of two to four, if they also have log K_{oa} values of around five or above. This implies that log K_{ow} may not be sufficiently robust on its own to determine the accumulation potential of chemicals in higher mammals.

The dependence of the predicted BMF on both the log K_{oa} and log K_{ow} value (Kelly and Gobas, 2003; Gobas *et al*., 2003) appears to be reasonable, as for air-breathing organisms the log K_{oa} essentially describes the partitioning behaviour of a chemical between lipid and air, and log K_{ow} essentially describes the partitioning behaviour between lipid and water. These two partitioning processes can be visualised as representing the main routes of transfer of a chemical in mammals; that is, transfer across the lungs to and from blood, transfer across the gut to and from blood and transfer from blood to lipid in the organism.

There are some parallels between this model and the cattle/milk parts of the ACC-HUMAN model considered in Part C of the report series. Both models follow broadly similar principles, along with patterns of uptake predicted using the hypothetical test set.

2.3.2 TGD method

The TGD method was tested using a hypothetical test set of chemicals with log K_{ow} values ranging from zero to 10. For the calculations, a nominal soil concentration of one mg kg^{-1} wet weight was assumed, and the K_{oc} value was estimated using the recommended default QSAR equation for non-hydrophobic chemicals[2] and also the QSAR for predominantly hydrophobic chemicals[3]. The chemicals were all assumed to be essentially non-volatile (and hence have a low Henry's law constant). The resulting concentrations predicted in earthworms are summarised in Table 2.1 and are shown graphically in **Error! Reference source not found.**. As the soil concentration in this case was one mg kg^{-1} wet weight, the overall $BAF_{earthworm}$ (concentration in earthworm (mg kg^{-1} wet weight)/concentration in soil (mg kg^{-1} wet weight)) is numerically equivalent to the predicted concentration in the earthworm.

Table 2.1 Predicted concentrations in earthworms and overall bioaccumulation factor for a hypothetical test set

Log K_{ow}	Assumed soil concentration (mg kg^{-1} wet weight)	Log BCF earthworm (l kg^{-1})	Estimated log K_{oc} (l kg^{-1})		Estimated concentration in earthworm (mg kg^{-1} wet weight)[c]	
			a	b	a	b
0.0	1	-0.07	1.00	0.00	2.6	5.6
0.5	1	-0.06	1.28	0.48	1.8	4.6
1.0	1	-0.02	1.54	0.90	1.3	3.4
1.5	1	0.08	1.80	1.32	1.0	2.4
2.0	1	0.30	2.06	1.72	1.0	1.9
2.5	1	0.66	2.32	2.12	1.2	1.8
3.0	1	1.11	2.58	2.53	1.8	2.0
3.5	1	1.59	2.84	2.94	2.9	2.4
4.0	1	2.08	3.10	3.34	5.0	2.9
4.5	1	2.58	3.36	3.74	8.5	3.6
5.0	1	3.08	3.62	4.15	15	4.4
5.5	1	3.58	3.88	4.55	26	5.5
6.0	1	4.08	4.14	4.96	44	6.8
6.5	1	4.58	4.40	5.36	77	8.4
7.0	1	5.08	4.66	5.77	134	10
7.5	1	5.58	4.92	6.18	232	13
8.0	1	6.08	5.18	6.58	404	16
8.5	1	6.58	5.44	6.99	701	20
9.0	1	7.08	5.70	7.39	1,219	25
9.5	1	7.58	5.96	7.80	2,118	31
10.0	1	8.08	6.22	8.20	3,681	39

a) Calculations using the estimated K_{oc} value based on the QSAR for non-hydrophobic chemicals.
b) Calculations using the estimated K_{oc} value based on the QSAR for predominantly hydrophobic chemicals.
c) The value is numerically equivalent to the $BAF_{earthworm}$ in these calculations.

[2] This QSAR is log K_{oc} = (0.52 × log K_{ow}) + 1.02. The QSAR is derived for a log K_{ow} range of -2.0 to 8.0.
[3] This QSAR is log K_{oc} = (0.81 × log K_{ow}) + 0.10. The QSAR is derived for halogenated organic chemicals with a log K_{ow} value in the range 1.0 to 7.5.

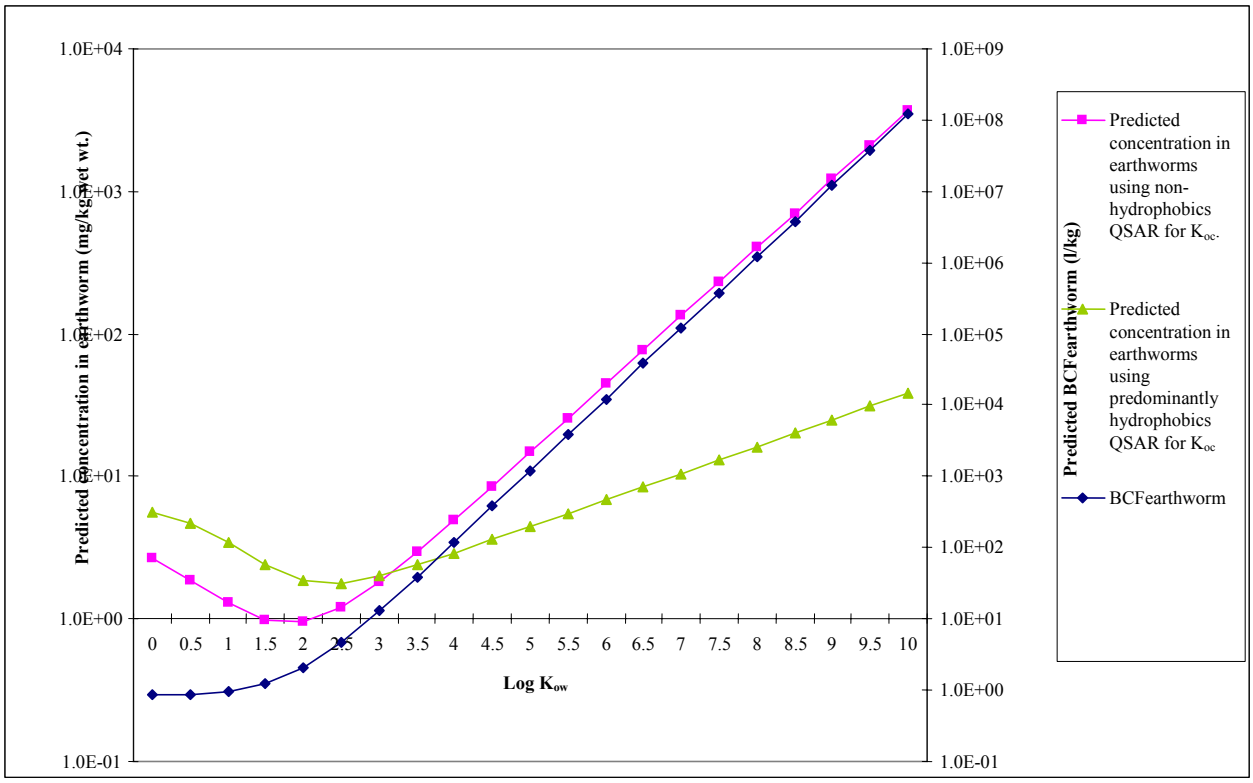

Figure 2.3 Estimated concentrations in earthworm exposed to a soil concentration of one mg/kg wet weight for a hypothetical chemical test set

As can be seen from these data, the predicted concentration in earthworms is a function of both the bioconcentration and the soil portioning properties of the substances. Indeed, it is clear that any uncertainties in the soil partitioning properties can have a very large influence on the resulting concentration in earthworms, as evidenced by the large differences in predicted concentrations for substances with log K_{ow} values above five when different methods for estimating K_{oc} are used.

The predicted concentration in earthworms shows a minimum value around a log K_{ow} of 1.5 to 2.5, and a generally linear increase with increasing log K_{ow} above this range. The minimum in the predicted concentration results from two competing effects: an increase in the earthworm BCF with increasing log K_{ow}, and an increase in the K_{oc} (and hence a reduction in the pore water concentration) with increasing log K_{ow}. At very low log K_{ow} values (up to log K_{ow} of around 1.5), the earthworm BCF is predicted to be relatively insensitive to the log K_{ow}, but K_{oc} increases with increasing log K_{ow} over the same range of zero to 1.5, resulting in lower concentrations of the substance in pore water.

At higher log K_{ow} values, the increase in K_{oc} with increasing log K_{ow} is offset by the increase in the earthworm BCF with increasing log K_{ow}. The net result is that the concentration predicted in earthworms increases with increasing log K_{ow} in this range, but the rate of increase is dependent on the K_{oc} value. A further factor which will affect the extent of accumulation is organism growth. This is not included in the TGD model. At high log K_{ow} values, even relatively low growth rates will tend to offset the increase in concentration.

2.4 Summary of findings

For predatory mammals, the Arctic Terrestrial Food-Chain model predicts that the BMF (relating the concentration in the mammal to the concentration in food) is dependent on both the log K_{ow} and the log K_{oa}. No significant accumulation (BMF of less than 0.1) is predicted for any chemical (regardless of the log K_{ow} value) when the log K_{oa} is below 3.5. The model also predicts that the maximum value for the BMF will be around 100 (or log BMF of around two). This occurs for substances with log K_{ow} values of around four, provided they also have a log K_{oa} value around seven or greater. The model also predicts that BMFs greater than one may be expected for substances of only moderate log K_{ow} value (between two and four), if they also have log K_{oa} values of five or more.

For the accumulation in earthworms, the TGD method predicts that the $BCF_{earthworm}$ (relating the concentration in earthworm to the concentration in soil pore water) will increase linearly with increasing log K_{ow} from a log K_{ow} of two upwards. For chemicals with a log K_{ow} below two, the predicted $BCF_{earthworm}$ is approximately constant. When the overall concentration predicted in earthworms is considered, this shows a minimum value around log K_{ow} of 2.5 to 3.5 (depending on the assumptions made over the partitioning of the chemical between soil and pore water), and then shows a linear increase with increasing log K_{ow} at higher log K_{ow} values. This minimum in the predicted concentrations results from two competing effects in the calculation methods.

It is also evident that the assumptions made over the soil-water partitioning properties of the chemical can have a large effect on the predicted concentration in earthworms, particularly for chemicals with log K_{ow} values above five.

3 Testing the Arctic Terrestrial Food-Chain model against field data

3.1 Comparison of predicted and experimental/field data

Testing of this model against experimental or field data proved problematic as there were few, if any, data directly relevant to the model other than those considered already by Kelly and Gobas (2003) in the development of the model. The analysis was further hampered by the lack of a working version of the model. Therefore, the model was only analysed here in very general terms.

One data set considered here was from a study by Leonards *et al.* (1998). This study investigated the accumulation of several polychlorinated biphenyls (PCBs) in mustelids – weasel (*Mustela nivalis*), stoat (*Mustela erminea*) and polecat (*Mustela putorius*) – from food in the wild. The animals used in the study were all from a restricted geographical area. The study determined BMFs based on a survey of the levels in the mustelids and their prey. The study also used data for otter[4] (*Lutra lutra*) taken from an earlier similar study by Leonards *et al.* (1997).

The prey surveyed included red vole (*Clethrionomys glareolus*), common vole (*Microtus arvalis*), wood mouse (*Apodemus sylvaticus*), common shrew (*Sorex araneous*), common hare (*Lepus europaeus*), frog (*Rana temporaria*), lake frog (*Rana esculenta*), common toad (*Bufo bufo*), natterjack toad (*Bufo calamita*) and various fish species.

The levels of PCBs in the mustelids were determined in the livers only. However, it was thought that levels in the liver were similar to those in other tissues when expressed on a lipid weight basis. Levels in the prey species were determined in whole animals (except for bones and skull). The prey species analysed accounted for 86%, 75%, 56% and 78% of the diets of weasel, stoat, polecat and otter respectively.

BMFs were calculated by determining the mean concentration of PCBs in each prey species, and then calculating the total concentration in the diet, based on the contribution each prey species made to the total diet of each predator. Similarly, the lipid content of the diet was estimated from the contribution of each prey species to the total diet. The final BMF was determined by dividing the concentration in the mustelid liver (on a mg kg^{-1} lipid basis) by the concentration in total diet (again on a mg kg^{-1} lipid basis); in other words, the BMFs were lipid-normalised. The BMFs derived by Leonards *et al.* (1998) are summarised in Table 2.2.

[4] Although the otter feeds mainly on aquatic organisms, it is relevant to consider the data here as they relate the concentration in the mammal to the concentration in feed.

Table 2.2 BMFs for mustelids from Leonards *et al.* (1998)

Chemical	BMF (lipid-normalised basis)[a]			
	Weasel	**Stoat**	**Polecat**	**Otter**
Group 1				
PCB 31	5	4	2	0.04 [0.2]
PCB 44	4	2	2	0.01 [0.06]
PCB 52	4	2	1	0.02 [0.1]
PCB 101	4	4	2	0.1 [0.6]
PCB 149	4	4	6	0.2 [1]
Group 2				
PCB 77	17	6	4	1 [6]
PCB 126	20	112	31	70 [395]
Group 3				
PCB 28	6	2	2	0.1 [0.6]
PCB 105	10	38	31	12 [67]
PCB 118	7	25	20	15 [85]
PCB 156	7	37	64	30 [169]
PCB 157	3	22	58	19 [107]
Group 4				
PCB 128	7	45	224	9 [51]
PCB 138	7	60	176	26 [145]
PCB 158	2	14	129	4 [23]
PCB 170	8	44	126	15 [85]
Group 5				
PCB 153	5	26	180	15 [85]
PCB 167	8	26	12	6 [34]
PCB 169	-	-	-	348 [1,960]
PCB 180	10	39	243	23 [130]

a) The BMFs given in the paper were based on the concentration in liver and prey on a lipid-normalised basis. The actual lipid contents of the livers were given (mean lipid contents were 3.2% for weasel, 4.1% for stoat, 5.4% for polecat and 4.4% for otter). The mean lipid contents for the diet were not available for weasel, stoat and polecat (although the lipid contents for the diet species were in the range 1-5%) but the mean lipid content of the diet of otter was 0.78%. The figures in [ ] for otter represent the BMF on a wet weight liver/wet weight prey basis. It is not possible to do a similar calculation for weasel, stoat and polecat, but for these species it can be assumed that the lipid content of the diet is similar to that of the liver, and so the wet weight BMF would be similar to the lipid-normalised BMF.

The pattern of uptake seen in mustelids was further analysed by Leonards *et al.* (1998). Firstly, the various PCBs were grouped according to their potential for metabolism based on the work of Boon *et al.* (1992). The key structural elements used to determine the metabolism potential included the position of vicinal H-atoms and the number of *ortho*-chlorine atoms. The groupings used (in order of decreasing potential for metabolism) are outlined below.

- Group 1 – PCB 31, PCB 44, PCB 49, PCB 52, PCB 101 and PCB 149.
- Group 2 – PCB 77 and PCB 126.
- Group 3 – PCB 28, PCB 105, PCB 114, PCB 118, PCB 156, PCB 157 and PCB 189.
- Group 4 – PCB 128, PCB 138, PCB 158, PCB 166 and PCB 170.
- Group 5 – PCB 153, PCB 167, PCB 169, PCB 180 and PCB 194.

Based on this grouping, and analysis of certain known metabolites, Leonards *et al.* (1998) rationalised the different patterns of accumulation seen amongst the different PCB congeners, and across the different species, in terms of differences in rates of metabolism. PCBs in groups 4 and 5 were thought to be relatively resistant to metabolism in all of the mustelids studied, whereas the chemicals in group 1 were thought to be metabolised by all species. Metabolic differences between species were thought to account for the differing patterns of accumulation seen with chemicals in groups 2 and 3 (where these congeners were thought to be metabolised in some species but not others).

To see how the magnitude of these BMFs compared with those estimated using the Arctic Terrestrial Food-Chain model, calculations according to the simplified (steady-state) wolf model given in Gobas *et al.* (2003) were carried out for each congener. Two sets of calculations were carried out. Firstly, it was assumed that no metabolism occurred in the organism. The second set of calculations assumed a nominal metabolism half-life for each of the five groupings as follows:

- Group 1 – assumed metabolism half-life 2 days.
- Group 2 – assumed metabolism half-life 10 days.
- Group 3 – assumed metabolism half-life 30 days.
- Group 4 – assumed metabolism half-life 100 days.
- Group 5 – assumed metabolism half-life 365 days.

These half-lives were purely for the purposes of illustrating the effect of metabolism rate on the predicted BMF, and were not necessarily related to the actual half lives in wolves (or mustelids). which are not known. The results of these calculations are summarised in Table 2.3

As can be seen from Table 2.3 etabolism is assumed in the model, BMFs of the order of 130-140 are estimated for all chemicals. These values are of a similar order to the lipid-normalised values found for group 4 and group 5 substances in mustelid livers that are thought to be resistant to metabolism; however, it should be remembered that the calculations are based on data for wolves. When a metabolism rate constant is introduced, the predicted BMF is reduced markedly, even if a relatively long metabolism half-life is assumed. This indicates that reliable data on the rate of metabolism would be needed in order to make accurate predictions using this method.

Table 2.3 BMFs calculated using the steady-state wolf model

Chemical	Physico-chemical properties			BMF (wet weight basis)	
	log K_{ow}	log K_{aw}	log K_{oa}	Assuming no metabolism	Assuming metabolism
			Group 1		
PCB 31	5.67	-2.09	7.76	134	0.07
PCB 44	6.00	-2.22	8.22	140	0.07
PCB 52	6.10	-2.07	8.17	139	0.07
PCB 101	6.40	-2.41	8.81	142	0.07
PCB 149	7.21	-1.23	8.44	141	0.07
			Group 2		
PCB 77	6.36	-2.33	8.69	142	0.34
PCB 126	6.95	-2.36	9.31	143	0.34
			Group 3		
PCB 28	5.80	-2.07	7.87	136	1.0
PCB 105	6.00	-1.92	7.92	137	1.0
PCB 118	6.40	-1.91	8.31	140	1.0
PCB 156	7.60	-2.21	9.81	143	1.0
PCB 157	7.44	-2.16	9.60	143	1.0
			Group 4		
PCB 128	6.74	-3.25	9.99	143	3.3
PCB 138	6.70	-3.05	9.75	143	3.3
PCB 158	7.37	-1.72	9.09	143	3.3
PCB 170	7.08	-3.41	10.49	143	3.3
			Group 5		
PCB 153	6.90	-3.01	9.91	143	11.4
PCB 167	7.68	-2.16	9.84	143	11.4
PCB 169	7.50	-2.33	9.83	143	11.4
PCB 180	7.20	-3.37	10.57	143	11.4

The above comparison was made using a model parameterised for arctic wolves. The organism-specific information required by the model is outlined below in Table 2.4. The equivalent values for mustelids are also given in Table 2.4. Using these species-specific parameters, the model was modified to given predictions for each of weasels, stoat, polecat and otter. The resulting predictions are summarised in Table 2.5.

Based on this analysis, the maximum BMF for non-metabolised substances for all species is roughly in the range 50 to 70, with a slight increase in the BMF from weasel to stoat to polecat to otter. These figures are again in reasonable agreement with the data obtained by Leonards et al. (1998) for the more persistent congeners (see Table 2). When metabolism is taken into account, the predicted BMFs decrease (as before) but this decrease is more marked for the larger organisms (such as otter) than for the smaller organism (such as weasel). The effect of this is that for substances that are expected to be metabolised relatively rapidly, there is a trend for the predicted BMF to increase from otter to polecat to stoat, with weasel generally showing the higher predicted BMF. This trend is also evident from the data reported in Table 2.2 for the group 1 substances (substances thought to be readily metabolised in all four organisms). Therefore, the model appears to perform reasonably well against this test set, and appears to predict species- (or size-) specific trends in accumulation. However, the model was tested using only a relatively small amount of data and, more importantly, was not tested using actual species-specific metabolism data, and so the tentative conclusions drawn on the predictive ability across species have yet to be properly tested.

Table 2.4 Species-specific parameters required for the Gobas *et al.* (2003) model

Model parameter	Wolves[a]	Weasel	Stoat	Polecat	Otter
Weight	80 kg	0.09 kg[d]	0.22 kg[d]	0.68 kg[d]	7 kg[h]
Lipid content (fraction)	0.12	0.032[e]	0.041[e]	0.054[e]	0.044[i]
Respiration rate	20,000 l day^{-1}	80 l day^{-1} [f]	160 l day^{-1} [f]	400 l day^{-1} [f]	2,500 l day^{-1} [f]
Feeding rate	2.1 kg day^{-1}	0.017 kg day^{-1} [f]	0.032 kg day^{-1} [f]	0.071 kg day^{-1} [f]	0.35 kg day^{-1} [f]
Urine excretion rate	1.0 l day^{-1}	0.010 l day^{-1} [f]	0.020 l day^{-1} [f]	0.046 l day^{-1} [f]	0.26 l day^{-1} [f]
Bile excretion rate	0.3 l day^{-1}	6.4×10^{-3} l day^{-1} [g]	0.011 l day^{-1} [g]	0.024 l day^{-1} [g]	0.1 l day^{-1} [g]
Faecal excretion rate	0.66 kg day^{-1}	0.014 kg day^{-1} [f]	0.025 kg day^{-1} [f]	0.052 kg day^{-1} [f]	0.22 kg day^{-1} [f]
Milk excretion rate (assumed male)	0 l day^{-1}	0 l day^{-1}	0 l day^{-1}	0 l day^{-1}	0 l day^{-1}
Growth rate constant (assumed adult)	0 kg kg^{-1} day^{-1}	0 kg kg^{-1} day^{-1}	0 kg kg^{-1} day^{-1}	0 kg kg^{-1} day^{-1}	0 kg kg^{-1} day^{-1}
Air uptake efficiency	30%	30%[c]	30%[c]	30%[c]	30%[c]
Dietary uptake efficiency	90%	90%[c]	90%[c]	90%[c]	90%[c]
Organism to faeces partition coefficient	50	50[c]	50[c]	50[c]	50[c]
β[b]	10	10[c]	10[c]	10[c]	10[c]

a) Values taken from Gobas *et al.* (2003).
b) Factor representing the degree to which bile fluids exceed the solubility of contaminants over that in water.
c) The same value as for wolves is assumed.
d) The weights of organisms are given in Leonards *et al.* (1998) without pelt and/or head. The weights given are based on the mean weights reported in Leonards *et al.* (1998), but have been increased by 20% to account for this.
e) Mean value for liver from Leonards *et al.* (1998).
f) Estimated from the organism weight using the allometric equations in Hendriks (1999).
g) Estimated based on the ratio of the bile excretion rate to the faecal excretion rate for wolves.
h) Based on the typical weight of otters being in the range 5-12 kg.
i) Based on the lipid contents of liver reported in Leonards *et al.* (1997).

Table 2.5 Predicted BMF for weasel, stoat, polecat and otter

Chemical	Predicted BMF (wet weight basis)							
	Weasel		Stoat		Polecat		Otter	
	I	II	I	II	I	II	I	II
				Group 1				
PCB 31	52	0.5	55	0.4	59	0.3	66	0.1
PCB 44	54	0.5	56	0.4	60	0.3	70	0.1
PCB 52	54	0.5	56	0.4	60	0.3	69	0.1
PCB 101	54	0.5	57	0.4	61	0.3	71	0.1
PCB 149	54	0.5	57	0.4	61	0.3	71	0.1
				Group 2				
PCB 77	54	2	57	2	61	1	71	1
PCB 126	55	2	57	2	61	1	71	1
				Group 3				
PCB 28	53	6	55	5	59	4	67	2
PCB 105	53	6	56	5	60	4	68	2
PCB 118	54	6	57	5	61	4	70	2
PCB 156	55	7	58	5	61	4	72	2
PCB 157	55	7	58	5	61	4	72	2
				Group 4				
PCB 128	55	17	58	14	61	11	71	6
PCB 138	55	17	58	14	61	11	71	6
PCB 158	55	17	57	14	61	11	71	6
PCB 170	55	17	58	14	61	11	72	6
				Group 5				
PCB 153	55	34	58	31	61	27	71	18
PCB 167	55	34	58	31	61	27	72	18
PCB 169	55	34	58	31	61	27	72	18
PCB 180	55	34	58	31	61	27	72	18

I) Calculation assuming no metabolism.
II) Calculation assuming a nominal metabolism rate as discussed above.

Trends in the BMF across the various species for group 2 and group 3 substances are related to the ability of each species to metabolise the specific isomers; Leonards *et al.* (1998) concluded that these isomers are metabolised in some species but not in others. This implies that species-specific metabolism data are needed in order to correctly predict the BMFs for these types of chemicals.

Throughout the above analysis, the BMFs calculated using the Gobas *et al.* (2003) method are probably on a whole animal wet weight basis (see Section 2.1), whereas the measured BMFs are for livers on a lipid-normalised basis. However, the difference between lipid-normalised and wet weight basis for weasels, stoat and polecat is thought to be relatively minor (the lipid content of livers and prey appear to be similar). For the otter data, the difference is more marked and the lipid-normalised BMFs are thought to be higher than the equivalent BMFs on a wet weight basis by a factor of around 5.6. Also, only the lipid contents of the livers were available for the mustelids, and this may not be the same as for the whole body.

3.2 Summary of findings

It was not possible to test fully the Arctic Terrestrial Food-Chain model owing to a lack of suitable test sets and the unavailability of the model in a computerised form. However, it was possible to test a simplified, steady-state version of the model. This model was parameterised for arctic wolves and the predicted BMFs obtained were in broad agreement with available data on non-metabolised PCBs in four species of mustelids. The importance of reliable metabolism data for the reliable prediction of BMFs for substances that undergo metabolism in terrestrial mammals was demonstrated.

The simplified model used only a relatively small amount of species-specific data and the model was parameterised with the relevant properties for weasel, stoat, polecat and otter. The model was found to give reasonably good predictions of the actual BMFs for these species for non-metabolised PCBs and further, it appeared to predict the relative order of the BMF across the various species for both non-metabolised and metabolised PCBs (although it was only possible to test this in a semi-quantitative way owing to the lack of suitable data). However, the available data set indicates that metabolism of some PCBs is species-specific and this implies that species-specific metabolism data would be needed in order to reliably predict the BMF for this type of substance.

The relatively small data requirements for this simplified model (and the ease with which most of these data can be estimated) means that this model could potentially be easily adapted to any terrestrial mammalian species. The calculations are relatively straight forward to carry out using a simple spreadsheet. The full version of the Arctic Terrestrial Food-Chain model needs a similar, but slightly larger, set of species-specific parameters. Therefore, it should also be possible to adapt this model for other terrestrial species. This would, however, need to be programmed into a spreadsheet or similar computerised version to make it routinely useable.

There are a number of similarities between this model and the cattle/milk model included in ACC-HUMAN that has been reviewed in Part C of this report series. The findings for ACC-HUMAN, in particular the crucial importance of data on the rate of metabolism in mammals, are also highly relevant here, given the findings above from the Leonards *et al.* (1998) data set.

4 Testing the TGD method against laboratory and field earthworm accumulation data

4.1 Comparison of predicted and experimental data

A number of experimental and field data was available on the uptake of organic chemicals from soil by earthworms. Data were available for laboratory experiments for the uptake into earthworms from solution and also laboratory and field data on the accumulation in earthworms from soil. Water-exposure experiments were used to test estimates of the $BCF_{earthworm}$ part of the TGD method and soil experiments/field data were used to test the overall TGD method. Water-exposure only data are summarised in Table 4.1.

Table 4.1 Comparison of experimental and predicted $BCF_{earthworm}$ for water-only exposure

Substance	log K_{ow}	Species	log $BCF_{earthworm}$ (l kg^{-1} wet weight)		Reference
			Experimental	Predicted	
Oxamyl	-0.47	*Eisenia fetida*	-1.06	-0.07	Sternsen and Øien, 1980, as reported in Jager, 1998
Aldicarb	1.15	*Lumbricus terrestris*	-0.16	0.00	Briggs and Lord, 1983, as quoted in Jager, 1998
Carbofuran	2.32	*Eisenia fetida*	0.22	0.52	Sternsen and Øien, 1980, as reported in Jager, 1998
Isoproturon	2.87	*Lumbricus terrestris*	0.05	0.99	Branquart *et al*., 1985, as reported in Jager, 1998
Linuron	3.20	*Lumbricus terrestris*	1.24	1.30	Branquart *et al*., 1985, as reported in Jager, 1998
Lindane	3.70	*Lumbricus terrestris*	1.85	1.79	Branquart *et al*., 1985, as reported in Jager, 1998
1,2,3-Trichlorobenzene	4.10	*Eisenia andrei*	2.12	2.18	Belfroid *et al*., 1993
1,3,5-Trichlorobenzene	4.20	*Eisenia andrei*	1.86	2.28	Belfroid *et al*., 1993
1,2,3,4-Tetrachlorobenzene	4.64	*Eisenia andrei*	2.75	2.72	Belfroid *et al*., 1993
Pentachlorobenzene	5.18	*Eisenia andrei*	3.24	3.26	Belfroid *et al*., 1993
Hexachlorobenzene	5.50	*Eisenia andrei*	3.61	3.58	Belfroid *et al*., 1993

A comparison of predicted and experimental BCFearthworm is shown in Figure 4.1. This shows very good agreement between predicted and experimental BCF, particularly at log K_{ow} values above 2.5. Based on these data, the method used in the TGD to estimate the BCFearthworm appears to be reasonably reliable. However, the reliability of the method has not been established for substances with relatively high log K_{ow} values (of six and above). This aspect is discussed later in this section.

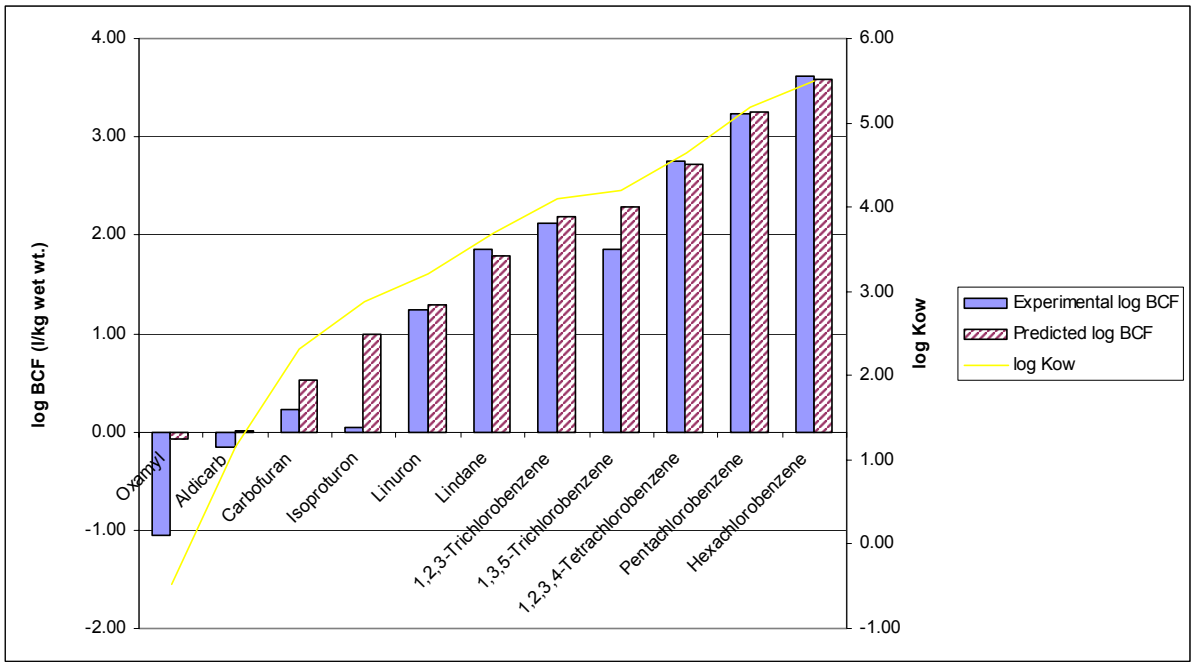

Figure 4.1 Comparison of predicted and experimental $BCF_{earthworm}$

These data were also considered by Jager *et al.* (1998) in the development of the method for estimating the $BCF_{earthworm}$; the authors came to similar conclusions based on the same data.

Many more data are available on the accumulation of organic chemicals in earthworms from soil. The data used for verification of the TGD method are summarised in Appendix A.

For this analysis, the data were converted where necessary for a $BAF_{earthworm}$ (based on the concentration in earthworms (mg kg^{-1} wet weight)/concentration in soil (mg kg^{-1} wet weight)) to be derived. This then allowed a direct comparison with predictions from the TGD. In order to carry out this conversion, information was often needed on the soil water contents, soil organic carbon contents and earthworm lipid contents. These values were taken from the original publications where available; however, in some cases the default values from the TGD were used. These default values are as follows:

- Soil water content = 12% by weight of the bulk soil.
- Soil organic carbon content = 2% of the bulk soil (or 0.02 if expressed as a fraction).
- Lipid content of earthworm = 1% by weight (or 0.01 if expressed as a fraction).

As discussed in Section 2.2, the TGD method requires a value of $K_{soil\text{-}water}$. This was estimated using either the TGD method with specific properties of the soil (water content and organic carbon content)[5] or, in the absence of one or more of these data, the recommended default values from the TGD for a standard soil, using K_{oc} and Kp_{soil} values estimated from log K_{ow}. As the TGD prediction depends crucially on the K_{oc} value, two methods for predicting log K_{ow} (the default QSAR for non-hydrophobic chemicals[2] and the specific QSAR for predominantly hydrophobic chemicals[3]) were used in this analysis. However, for some chemicals (such as certain halogenated phenols), Kp_{soil} values were also generated in the study for the specific soil used, and in this case measured Kp_{soil} values were used in the calculations. For all chemicals, it was assumed that the contribution of the K_{aw} to the $K_{soil\text{-}water}$ was small and could be neglected.

Plots of predicted against experimental log $BAF_{earthworm}$ (on a mg kg^{-1} wet weight worm/mg kg^{-1} wet weight soil basis) are shown in Figure 4.2 (for the TGD default QSAR for K_{oc}) and Figure 4.3 (for the QSAR for predominantly hydrophobics for K_{oc}). Both figures show that the TGD method overestimates the actual log $BAF_{earthworm}$ for the vast majority of the data set (where most datapoints lie above the 1:1 correspondence line in the plots).

Plots of the residual in the prediction (defined here as the actual log $BAF_{earthworm}$ – predicted log $BAF_{earthworm}$) are shown in Figure 4.4 (for the TGD default QSAR for K_{oc}) and Figure 4.5 (for the QSAR for predominantly hydrophobics for K_{oc}). In these plots, a positive residual indicates that the TGD method is underestimating the actual log $BAF_{earthworm}$, and a negative residual indicates that the TGD method is overestimating the actual log $BAF_{earthworm}$. Both plots show a similar trend, with a strong correlation of the residual with log K_{ow}. At lower log K_{ow} values (up to around three to four), there is a tendency for the TGD method to underestimate the actual $BAF_{earthworm}$, although this underestimation is small (generally within one log unit of the log $BAF_{earthworm}$ or within factor of 10 of the actual BAF). Above a log K_{ow} of around three to four, the TGD method tends to overestimate the actual $BAF_{earthworm}$, with this overestimation becoming progressively worse with increasing log K_{ow}. The overestimation is worse when the TGD default QSAR is used to estimate K_{oc}: the log $BAF_{earthworm}$ is overestimated by up to four log units at log K_{ow} of eight (meaning that the actual $BAF_{earthworm}$ is overestimated by a factor of 10,000) compared with when the QSAR for predominantly hydrophobics is used to estimate the K_{oc}, where the log $BAF_{earthworm}$ is overestimated by up to 2.5 log units at a log K_{ow} of eight (meaning that the actual log $BAF_{earthworm}$ is overestimated by a factor of around 320).

Figure 4.4 and Figure 4.5 also reveal a series of possible outliers whose experimental BAFs appear to lie around two to three log units below those of the bulk of the data set (these are also evident in Figure 4.2 and Figure 4.3 as the line of datapoints to the left hand side of the plots). On further inspection, it was revealed that these data were all from the study by Matscheko *et al.* (2002a). As discussed in Appendix A, there are some uncertainties over the actual units for $BAF_{earthworm}$ given in this paper (particularly whether the soil concentrations are on a mass or molar basis) and so these values are excluded from the further analysis of this data set.

The complete data set used for Figure 4.2 to Figure 4.5 also contains the data of Allard *et al.* (2005). As discussed in Appendix A, this study used an unusual exposure medium of a mixture of contaminated soil, agar medium and ground oatmeal. This unusual medium makes it difficult to relate the results from this study to field situations, and so this data set is also not considered further in the analysis of the data sets.

[5] Many studies report the soil organic matter content rather than the soil organic carbon content. In these cases, the organic carbon content was assumed to be 58 per cent of the quoted organic matter content.

A similar analysis of the residuals, with the data sets of Matschenko *et al.* (2002a) and Allard *et al.* (2005) removed, is shown in Figure 4.6 (for the TGD default QSAR for K_{oc}) and Figure 4.6 Plot of residual in log BAFearthworm against log Kow for the test set minus outliers (TGD default QSAR for Koc)

4.7 (for the QSAR for predominantly hydrophobics for K_{oc}). As can be seen, a good correlation of residual with log K_{ow} is obtained, particularly for the plot using the TGD default QSAR for K_{oc}. Regression equations from these plots are as follows:

TGD default QSAR for K_{oc}:

$$\text{Residual} = -0.69 \times \log K_{ow} + 2.72 \qquad R^2 = 0.70$$

QSAR for predominantly hydrophobics for K_{oc}:

$$\text{Residual} = -0.39 \times \log K_{ow} + 1.72 \qquad R^2 = 0.43$$

Given these correlations, it would therefore be possible to adjust the $BAF_{earthworm}$ obtained using the TGD method to correct for over/underpredictions as follows.

For the TGD default QSAR for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.69 \times \log K_{ow}) + 2.72$$

For the QSAR for predominantly hydrophobics for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.39 \times \log K_{ow}) + 1.72$$

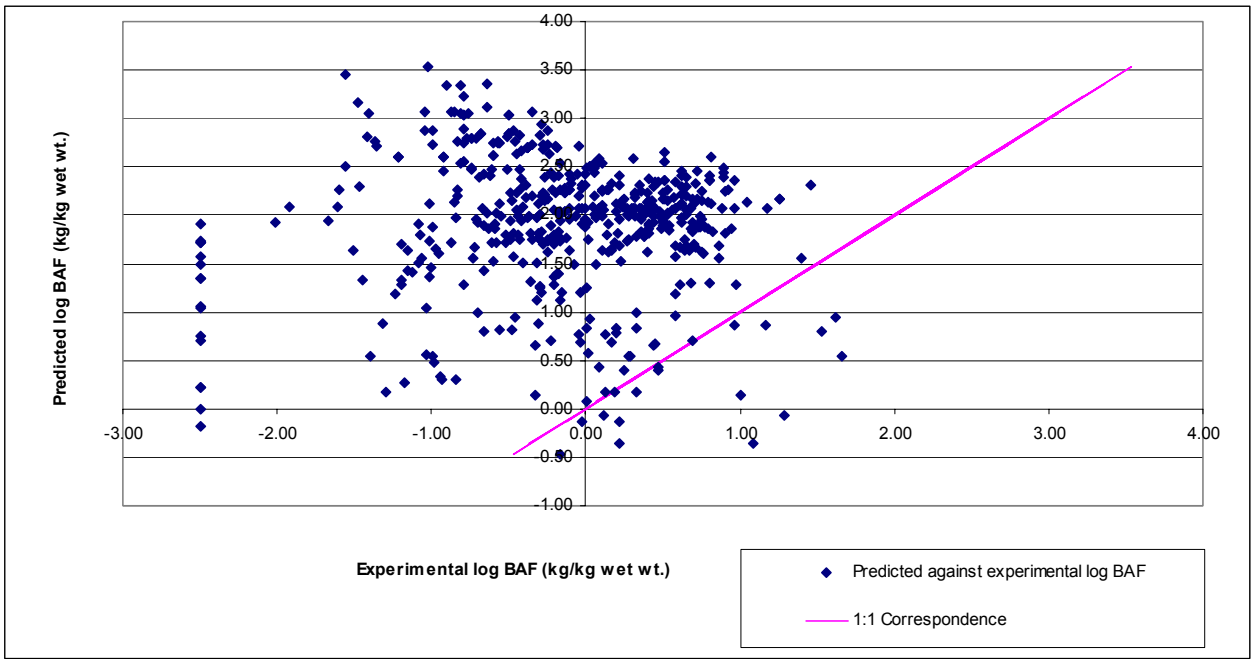

Figure 4.2 Plot of predicted against experimental log $BAF_{earthworm}$ for the complete test set (TGD default QSAR for K_{oc})

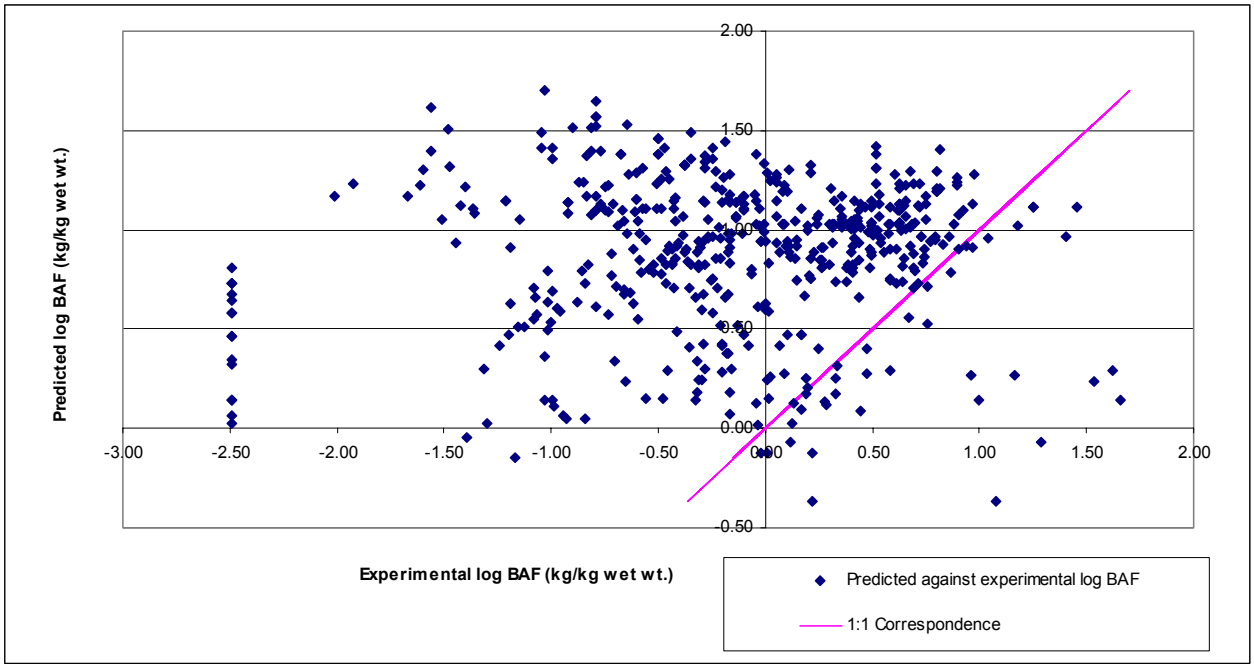

Figure 4.3 Plot of predicted against experimental log $BAF_{earthworm}$ for the complete test set (TGD QSAR for predominantly hydrophobic chemicals for K_{oc})

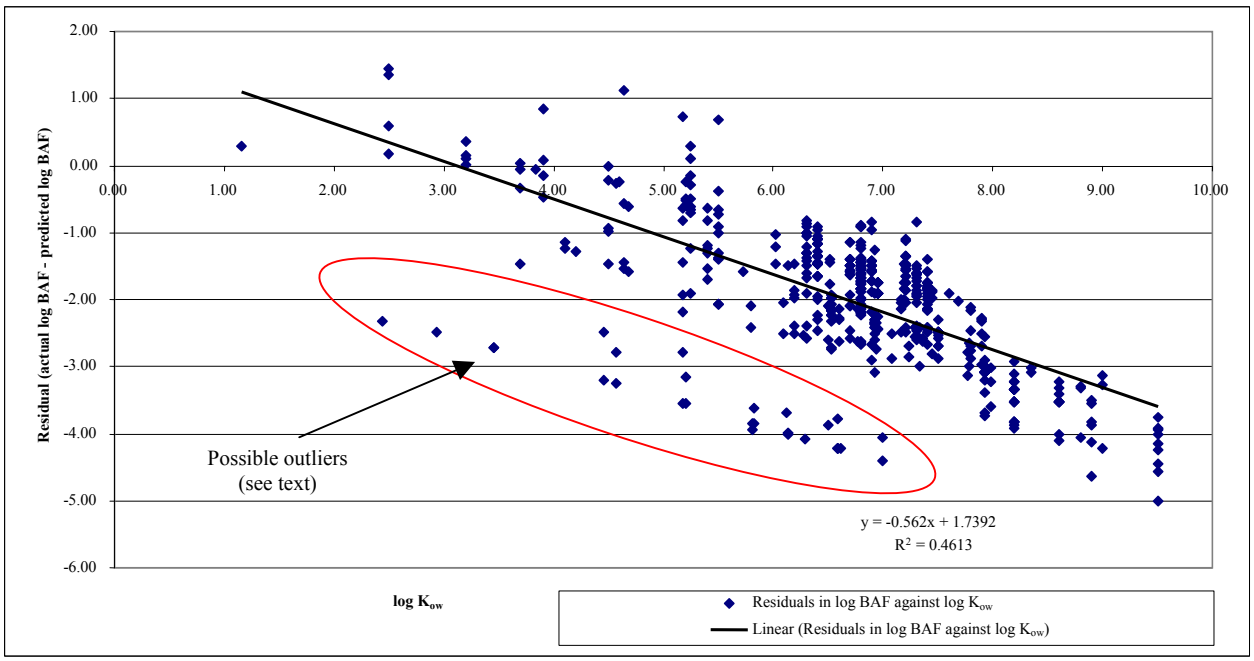

Figure 4.4 Plot of residual in log $BAF_{earthworm}$ against log K_{ow} for the complete test set (TGD default QSAR for K_{oc})

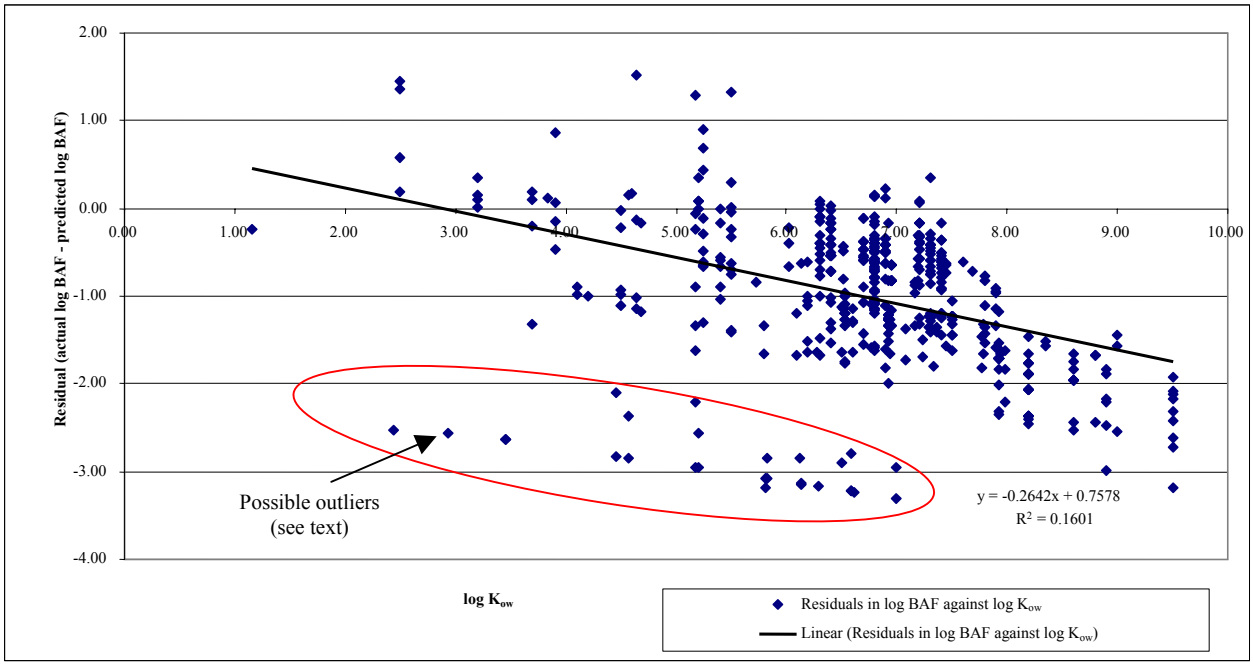

Figure 4.5 Plot of residual in log $BAF_{earthworm}$ against log K_{ow} for the complete test set (TGD QSAR for predominantly hydrophobic chemicals for K_{oc})

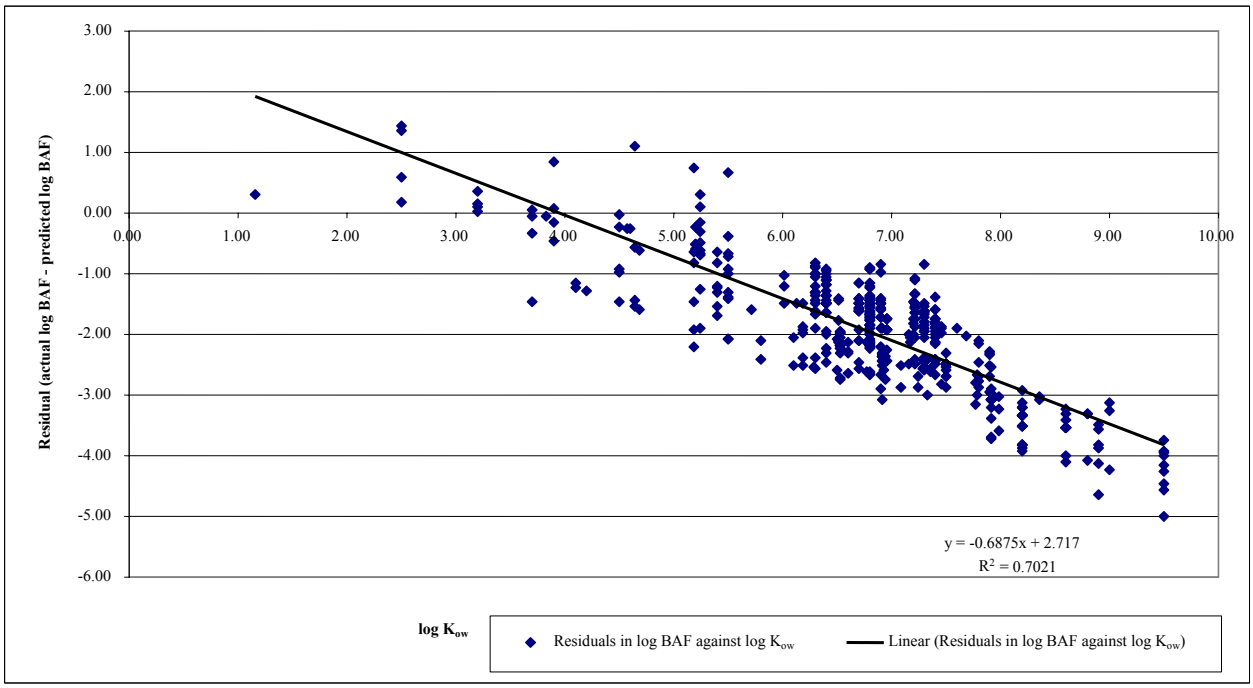

Figure 4.6 Plot of residual in log $BAF_{earthworm}$ against log K_{ow} for the test set minus outliers (TGD default QSAR for K_{oc})

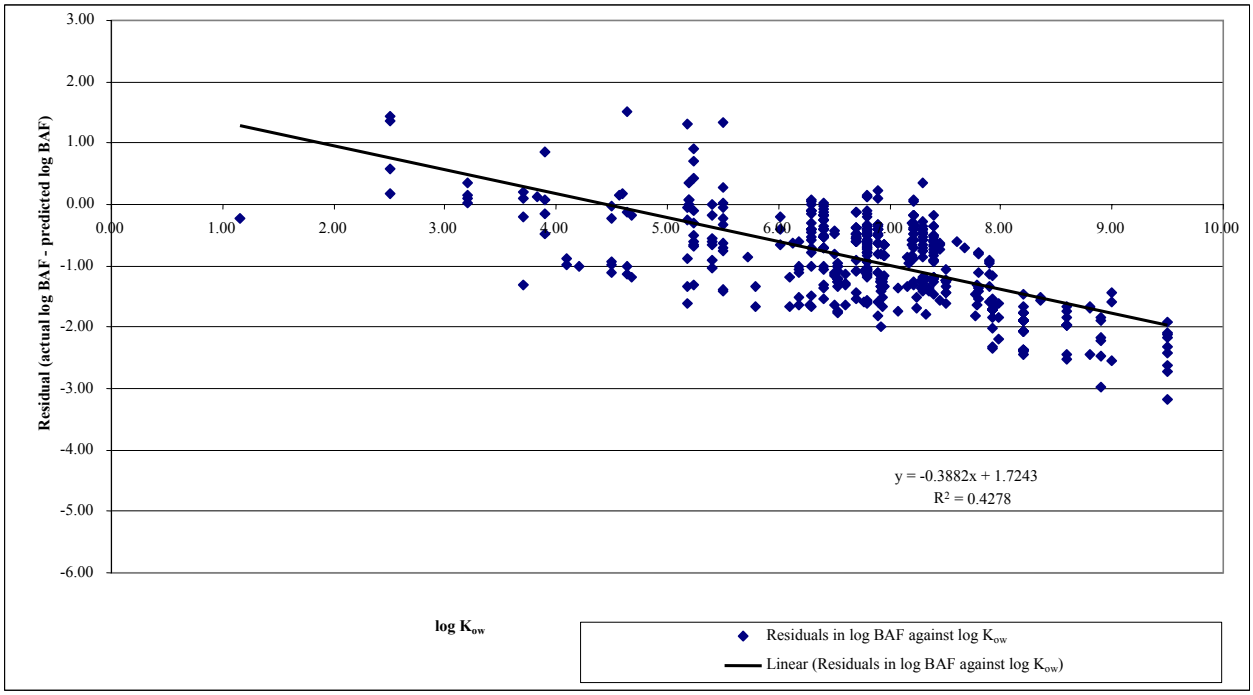

Figure 4.7 Plot of residual in log $BAF_{earthworm}$ against log K_{ow} for the test set minus outliers (TGD QSAR for predominantly hydrophobic chemicals for K_{oc})

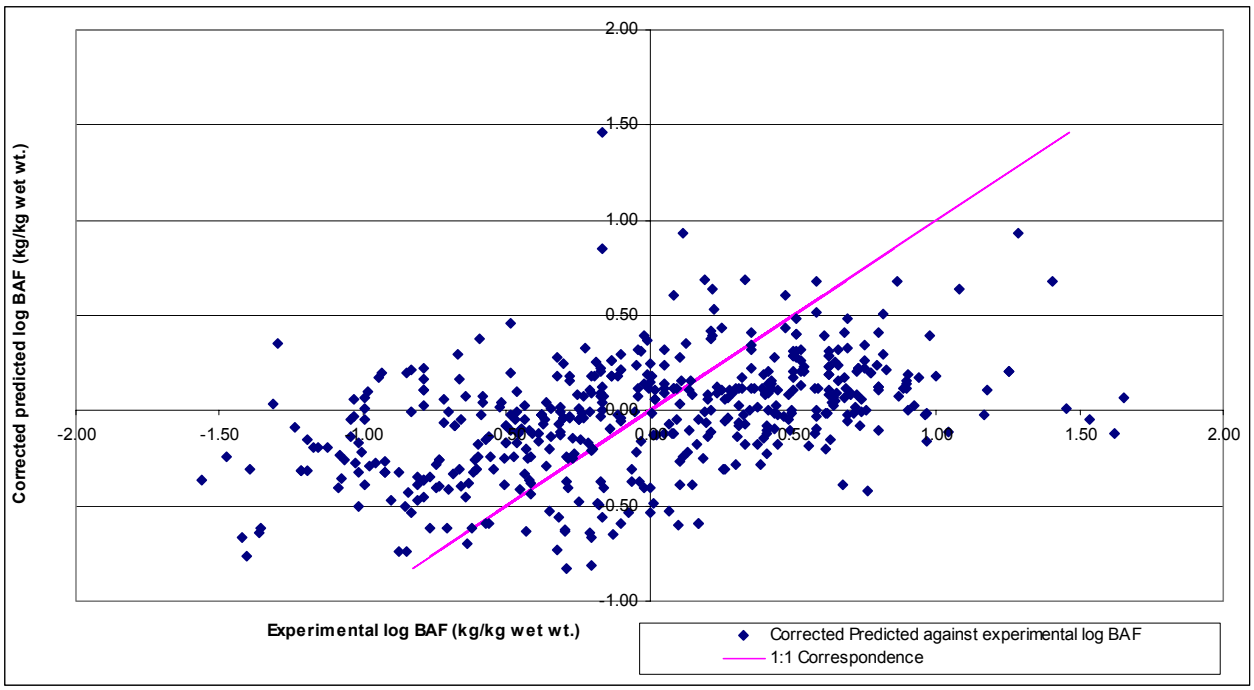

Figure 4.8 Comparison of predicted log $BAF_{earthworm}$ and experimental log $BAF_{earthworm}$ for the corrected TGD method (TGD default QSAR for K_{oc})

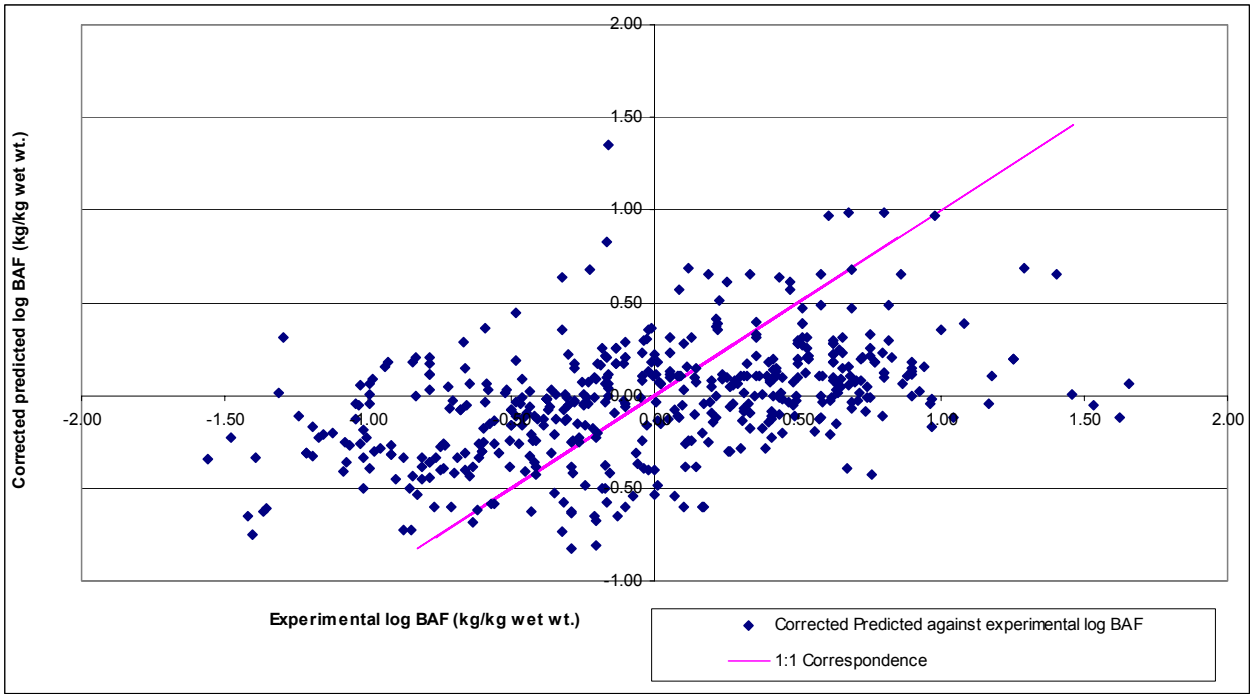

Figure 4.9 Comparison of predicted log $BAF_{earthworm}$ and experimental log $BAF_{earthworm}$ for the corrected TGD method (TGD QSAR for predominantly hydrophobic chemicals for K_{oc})

Using these equations, it was possible to calculate the $BAF_{earthworm\_corrected}$ for the chemicals used in this analysis. Plots of corrected BAF against experimental BAF for the data set (without the outliers) are shown in Figure 4.8 (the TGD default QSAR for K_{oc}) and Figure 4.8 Comparison of predicted log BAFearthworm and experimental log BAFearthworm for the corrected TGD method (TGD default QSAR for Koc)4.9 (the QSAR for predominantly hydrophobics for K_{oc}). Comparing these plots with Figure 4.2 and Figure 4.3, it is evident that there is much closer agreement between the corrected predicted $BAF_{earthwom}$ and the experimental data. A more detailed statistical analysis of the performance of the corrected method compared with the uncorrected TGD method without the outliers is summarised in Table 4.2.

Table 4.2 Basic statistical analysis of the residuals in the prediction for the TGD method and the corrected method

	TGD method		Corrected method	
	Default QSAR for K_{oc}	**QSAR for predominantly hydrophobics for K_{oc}**	**Default QSAR for K_{oc}**	**QSAR for predominantly hydrophobics for K_{oc}**
Mean residual[a]	-1.97	-0.92	0.00	0.00
Mean absolute residual[b]	2.00	0.98	0.44	0.44
Maximum absolute residual	5.01	3.18	1.74	1.74
95th percentile absolute residual	3.68	2.09	1.04	1.04
Number of data points	488	488	488	488

a) Residual = actual log $BAF_{earthworm}$ – predicted log $BAF_{earthworm}$.

b) Absolute residual is the difference between the actual log $BAF_{earthworm}$ and predicted log $BAF_{earthworm}$ disregarding the sign.

From the data given in Table 4.2, for the TGD method the mean residual is -1.97 using the default QSAR for K_{oc} and -0.92 for the QSAR for predominantly hydrophics for K_{oc}. This indicates (as is also evident from the plots) that the TGD method systematically overpredicts the $BAF_{earthworm}$ for the majority of chemicals; the mean residuals are equivalent to an overprediction of around 100 times using the default QSAR for K_{oc} and around 10 times using the QSAR for predominantly hydrophobics for K_{oc}. For the corrected method, the mean residual is zero for both methods for estimating the K_{oc}, indicating that there is no systematic under- or overprediction of the test data.

Absolute residuals indicate the level of agreement between actual and predicted BAF regardless of whether the prediction is an underestimate or overestimate. Here, the mean absolute residual for the TGD method is 2.00 for the default QSAR for K_{oc} and 0.98 for the predominantly hydrophobics method, indicating that the mean difference between experimental and predicted BAF is a factor of 100 for the former or a factor of 10 for the latter. The 95th percentile value for the residual is 3.68 for the first and 2.09 for the second. This means that 95 per cent of the test data are predicted to within a factor of around 4,800 using the default QSAR for K_{oc} or around 120 using the QSAR for predominantly hydrophobics.

For the corrected method, the mean and 95th percentiles of the absolute residuals are 0.44 and 1.74 respectively for both methods for calculating the K_{oc}. A mean residual of 0.44 means that the mean under/overprediction is a factor of 2.8 on the actual BAF, and 95 per cent of BAFs are estimated to within a factor of 55.

This analysis shows that applying the empirical correction to the $BAF_{earthworm}$ predicted by the TGD method results in significant improvements in the accuracy and reliability of the prediction. The test set used here contains some chemicals of extreme hydrophobicity, such as decabromodiphenyl ether (PBDE 209) that has a log K_{ow} of 9.5, along with several other chemicals with log K_{ow} greater than eight; the observed $BAF_{earthworm}$ is also well predicted for these chemicals using the corrected method.

However, there are still areas of uncertainty when using the corrected method. Figures 4.8 and 4.9 show that the method tends to underpredict higher BAF values (values on the right of the plots tend to fall below the 1:1 line) and overpredict lower values (those to the left of the plots tend to fall above the 1:1 line). This suggests that there are other aspects which could be considered in a more mechanistically complete model, relating to soil bioavailability and possible non-linearity at high log K_{ow} values (possible reasons being low solubility or availability and growth).

A number of other studies have also investigated the reliability of an equilibrium partitioning-type approach for estimating concentrations in earthworms, generally based on similar assumptions as those used by TGD in estimating $BCF_{earthworm}$. These studies generally found that the concentration in earthworms was overpredicted using an equilibrium partitioning approach when compared with data from field studies. Jager (2003) suggested this related to the difficulties in estimating (or measuring) the bioavailable fraction of a chemical in soil pore water, and this would be in line with the analysis here, as the predicted $BAF_{earthworm}$ is dependent on the method used to estimate the K_{oc}. Factors such as sequestration or ageing in natural soils may be important here.

However, another possible explanation emerges from this analysis. It is clear that the overprediction of the concentration in earthworms is related to the log K_{ow}, and becomes particularly apparent at high log K_{ow} values. Thus, it is possible that the assumption that $BCF_{earthworm}$ increases with increasing log K_{ow} could fall down at very high log K_{ow} values (as seen with fish bioconcentration, for example). The relationship of $BCF_{earthworm}$ with log K_{ow} has been tested here only up to a log K_{ow} of around 5.5.

Thus, for chemicals with very high log K_{ow} values, uptake could be more related to accumulation from soil ingestion rather than bioconcentration through the skin from soil pore water.

This was considered by Jager (2003), who concluded that a linear increase in log $BCF_{earthworm}$ with log K_{ow} held even for very hydrophobic chemicals (based mainly on modelling studies). Further, Jager (2003) and Jager *et al.* (2003) concluded that, although gut uptake becomes increasingly important with increasing log K_{ow} (and may become dominant for very hydrophobic chemicals), uptake through the gut is a passive diffusion process that can also be explained by equilibrium partitioning. It is thought that processes in the gut can act to increase the fugacity of substances, through extraction of the carrier material (lipids, possibly proteins) and compaction of the gut content (see Kelly and Gobas, 2003). In worms, food taken into the gut is soil and it is not greatly changed in the gut due to their limited digestive capacities. Hence, the partition within the worm is likely to be similar to that between the worm and the external soil.

Although models have been developed to look at the role of soil and food ingestion, these also assume that $BCF_{earthworm}$ increases with increasing log K_{ow} at higher log K_{ow} values, and so still tend to overpredict the concentration in worms when compared to field data.

Despite these limitations, it has been argued that the equilibrium-partitioning approach to predicting concentrations in earthworms is fail-safe, as it consistently overpredicts the concentrations observed in reality. This is not itself a problem when using the method for conservative risk assessment applications, but if used for setting environmental standards, could lead to overly conservative standards being applied. Although the precise reasons for the consistent overpredictions of the method are not clear, it is still possible to use the method in a pragmatic way if an empirical correction for overprediction is applied as suggested above.

4.2 Summary of findings

The TGD method was extensively tested against a large data set of experimental and field earthworm accumulation data. The analysis showed that the TGD method consistently overpredicts $BAF_{earthworm}$ (and hence concentration in earthworm) at log K_{ow} values above four to five. This overprediction appears to be linearly related to the log K_{ow} value, and the following corrections can be applied to the predicted $BAF_{earthworm}$.

For the TGD default QSAR for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.69 \times \log K_{ow}) + 2.72$$

For the QSAR for predominantly hydrophobics for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.39 \times \log K_{ow}) + 1.72$$

Using these corrections, very good agreement with the experimental data was obtained for chemicals across a large range of log K_{ow} values (up to around 9.5) and for a variety of soil types.

The actual cause of the overprediction at high log K_{ow} values for the uncorrected TGD method is unclear, but may be related to difficulties in estimating the bioavailable fraction of these chemicals in soil pore water and/or assumptions in the model that $BCF_{earthworm}$ increases with log K_{ow} at high log K_{ow} values. Although it would be useful to investigate the causes of overprediction of $BAF_{earthworm}$ further and so refine the model,

from a practical point of view the above corrections appear to work very well, and so at this stage further development of the model is probably not warranted.

5 Conclusions and recommendations

5.1 Arctic Terrestrial Food-Chain model

In this study, it was not possible to fully test the Arctic Terrestrial Food-Chain model, owing to a lack of suitable test data and the unavailability of a computerised version of the model. A simplified, steady-state version of the model developed for wolves was used in this analysis, and this appeared to provide reasonable predictions of the accumulation from food of substances that are not readily metabolised in a predator. However, for substances that are metabolised, information on the rate of metabolism in the species being modelled would be necessary in order to provide reliable predictions.

There were some similarities between these models and the ACC-HUMAN model reviewed in Part C of this report series. Again, it was found that ACC-HUMAN only provided reliable predictions for the concentrations in cattle and milk for chemicals that were resistant to metabolism. For other substances, actual information on the rate of metabolism in cattle would be needed. This was particularly evident for substances with log K_{ow} values below six.

This report raises the problem of the availability of suitable metabolism rate constant data for terrestrial mammal modelling. Ideally, this should be generated with experiments on the species being modelled. However, such experiments are costly and difficult to carry out, and the available data would be generated as part of feeding studies in any case. Thus, for chemicals where metabolism data are available, it is likely that a BAF would also be available from the same study, so an actual prediction would not be needed. The second potential problem here is that most studies looking at metabolism measure the total depuration rate (the total loss of chemical from the organism) rather than metabolism specifically (experimentally, it is very difficult to separate out the different rates of the various loss processes). As other loss processes (such as faecal egestion) are already built into terrestrial mammal models, rate constants derived from total depuration half-lives in a mammal may overestimate the rate of metabolism. This then raises the question of whether a predictive method that relies on the availability of metabolism data is useful in practice. One approach would be to investigate if it is possible to extrapolate or predict rates of metabolism in terrestrial species of interest from species that are more commonly studied (for example, laboratory rodents).

In terms of setting standards for terrestrial species, a model that predicts concentrations in top predators such as wolves and otters is not necessarily useful, as it is the concentration in the food (prey) of predators that is most relevant. In this respect, both the models given in Kelly and Gobas (2003) and Gobas *et al.* (2003) could easily be modified to predict the concentration in, for example, a worm- or plant-eating small mammal such as rabbit, vole or shrew that then constitutes the diet for a top predator (such as foxes, polecats and so on). If such a model was developed to predict the accumulation in the plant-eater or worm-eater from diet (as is currently the case with the Arctic Terrestrial Food-Chain model), this could be combined with either a plant model (see Part C review of plant models) or the earthworm model (see Section 5.2) in order to relate the concentration in the small mammal to the concentration in soil (or in the case of plants, air if necessary). This would provide a link through the food chain from soil to the prey of top predators and would allow an overall bioaccumulation factor from soil to the prey species to be defined. The model could then be used to

back-calculate from a 'safe' concentration in the diet of the top predator to an equivalent concentration in soil when setting standards as outlined by the Environment Agency (2007).

In conclusion, the Arctic Terrestrial Food-Chain model, and in particular the simplified steady-state wolf model, appears to show promise in being able to predict accumulation from food in terrestrial mammals. It is recommended that the steady-state model described in Gobas *et al.* (2003) is parameterised for small plant-eating and worm-eating mammals, and is combined with the plant models described in Part C of this report series, and the earthworm model. However, at present such a terrestrial mammal model will only provide reliable predictions for substances that do not undergo metabolism in the mammal. For other substances, species-specific metabolism data would be needed. As these data are not widely available for chemicals in terrestrial mammals, this will undoubtedly limit the general applicability of the model. Further work would be needed to determine if it is possible to reliably estimate the rates of metabolism of chemicals in terrestrial species from laboratory animal data or other methods.

5.2 Accumulation in earthworms

The TGD method was extensively tested against a large data set of experimental and field earthworm accumulation data. The analysis showed that the TGD method consistently overpredicts $BAF_{earthworm}$ (and hence concentration in earthworm) at log K_{ow} values above four to five. This overprediction appears to be linearly related to the log K_{ow} value, and the following corrections could be applied to the predicted $BAF_{earthworm}$.

For the TGD default QSAR for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.69 \times \log K_{ow}) + 2.72$$

For the QSAR for predominantly hydrophobics for K_{oc}:

$$\log BAF_{earthworm\_corrected} = \log BAF_{earthworm\_predicted} - (0.39 \times \log K_{ow}) + 1.72$$

Using these corrections, very good agreement with the experimental data was obtained across chemicals with a large range of log K_{ow} values (up to around 9.5) and for a variety of soil types.

The actual cause of the overprediction at high log K_{ow} values for the uncorrected TGD method is unclear, but may be related to difficulties in estimating the bioavailable fraction of these chemicals in soil pore water and/or assumptions in the model that $BCF_{earthworm}$ increases with log K_{ow} at high log K_{ow} values. Although it would be useful to investigate the causes of overprediction of $BAF_{earthworm}$ further and so refine the model, from a practical point of view the above corrections appear to work very well, and so at this stage further development of the model is probably not warranted.

Other parts of the TGD method have been tested in Part A (accumulation in fish) and Part C (accumulation in plants and cattle).

In terms of setting standards, the corrected TGD method could be applied relatively easily for the protection of a worm-eating predator. In this case, the 'safe' level of chemical in the diet of the predator (a concentration in worms) could be used to back-calculate, using the $BAF_{earthworm}$ to the equivalent concentration in soil. It would be possible to do this calculation on either a wet weight soil or dry weight soil basis. It would also be possible to take account of different soil organic carbon contents if desired. Taking the $PNEC_{oral}$ as the 'safe' level, the relevant concentration in soil is

$$C_{soil} = \frac{PNEC_{oral}}{BAF_{earthworm}}$$

If measured values of $BAF_{earthworm}$ are not available, Section 2.2 provides equations to calculate $BAF_{earthworm}$ from the log K_{ow} of the substance which incorporate the organic carbon content of the soil. The section also includes the conversion from wet weight to dry weight soil concentration basis. These equations give the uncorrected BAF value, which can be adjusted using the equations above.

It would also be possible to incorporate the corrected earthworm method into a more sophisticated model, whereby a top predator consumes a worm-eating mammal. Here, it would be necessary to construct an accumulation model for the worm-eating mammal that calculated the concentration in the mammal resulting from consuming contaminated food. The framework outlined in Section 5.1 could provide a useful starting point for this.

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Glossary of terms

Adapted from USEPA (2000).

Allometric	Relative growth of a part of an organism in relation to the growth of the whole.
Bioaccumulation	The net accumulation of a substance by an organism as a result of uptake from all environmental sources.
Bioaccumulation factor	The ratio of the concentration of a substance in tissue to its concentration in ambient water (or other media). The concentration in the organism can be expressed on a wet or fresh weight basis (BAF = concentration in organism (mg/kg wet wt.)/concentration in water (mg/l)) or on a lipid weight basis (BAF = concentration in organism mg/kg lipid/concentration in water (mg/l)). The concentration in water would normally refer to the dissolved concentration, but it is also possible to define the BAF on the basis of the total concentration, depending on the system being considered.
Bioconcentration	The net accumulation of a substance by an aquatic organism as a result of uptake directly from the ambient water, through gill membranes or other external body surfaces.
Bioconcentration factor	The ratio of the concentration of a substance in tissue of an aquatic organism to its concentration in the ambient water. It can be expressed in terms of a wet or fresh weight concentration in fish (BCF = concentration in fish (mg/kg wet weight)/concentration in water (mg/l)), or a lipid weight concentration in fish (BCF_{lipid} = concentration in fish (mg/kg lipid)/concentration in water (mg/l)). The concentration in water usually refers to the dissolved concentration.
Biomagnification	The increase in tissue concentration of a chemical in organisms at successive trophic levels through a series of predator-prey associations.
Biomagnification factor	The ratio of the tissue concentration of a chemical in a predator at a particular trophic level to the tissue concentration in its prey at the next lower trophic level for a given water body and chemical exposure. The BMF can be expressed in terms of concentrations on a wet or fresh weight basis (BMF = concentration in organism at trophic level x (mg/kg wet wt.)/concentration in organism at trophic level y (mg/kg wet wt.); where x>y) or on a lipid weight basis (BMF_{lipid} = concentration in organism at trophic level x (mg/kg lipid)/concentration in organism at trophic level y (mg/kg lipid)).
Depuration	The loss of a substance from an organism as a result of any active or passive process.
Hydrophilic	A term that refers to the extent to which a chemical is attracted to partitioning into the water phase. Hydrophilic chemicals have a greater tendency to partition into polar phases (such as

	water) compared to hydrophobic chemicals.
Hydrophobic	A term that refers to the extent to which a chemical avoids partitioning into the water phase. Highly hydrophobic chemicals have a greater tendency to partition into nonpolar phases (such as lipid, organic carbon) compared with chemicals of lower hydrophobicity.
Lipid-normalized concentration	The total concentration of a contaminant in tissue or whole organism, divided by the lipid fraction in that tissue, organism or media.
Octanol-water partition coefficient (P)	The ratio of the concentration of a substance in the n-octanol phase to its concentration in the aqueous phase in an equilibrated two-phase octanol-water system. The value is often expressed as a base 10 logarithm value (log K_{ow}).
Organic-carbon normalized concentration	For sediments, the total concentration of a contaminant in sediment divided by the fraction of organic carbon in the sediment.
Uptake	The acquisition by an organism of a substance from the environment as a result of any active or passive process.

List of abbreviations

BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BFAF	Biota-food accumulation factor
BMF	Biomagnification factor
BSAF	Biota-sediment accumulation factor
BTF	Biotransfer factor
bw	Bodyweight
CLEA	Contaminated Land Exposure Assessment
DDD	Dichlorodiphenyldichloroethane
DDE	Dichlorodiphenyldichloroethylene
DDT	Dichlorodiphenyltrichloroethane
DDT - Total	Total DDT compounds. Includes all isomers of DDT, DDD (Dichlorodiphenyldichloroethane)and DDE (Dichlorodiphenyldichloroethylene)
Defra	Department for Environment, Food and Rural Affairs
ERA	Ecological risk assessment framework
EU	European Union
EUSES	European Uniform System for Evaluation of Substances
HCH	Hexachlorocyclohexane. Also known as lindane.
K_{aw}	Air-water partition coefficient (also known as dimensionless Henry's Law constant; log K_{aw} = logarithmic value).
K_{oc}	Organic carbon-water partition coefficient (log K_{oc} = logarithmic value)
K_{oa}	Octanol-air partition coefficient (log K_{oa} = logarithmic value)
K_{ow}	Octanol-water partition coefficient (log K_{ow} = logarithmic value)
Kp_{soil}	Solids-water partition coefficient for soil (units of l kg^{-1})
$K_{soil\text{-}water}$	Bulk soil-water partition coefficient for wet soil (units of m^3 m^{-3})
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
PCB	Polychlorinated biphenyl
ΣPCB	Total PCBs as defined by the International Council for the Exploration of the Sea. These are the congeners PCB 28, PCB 52, PCB 101, PCB 118, PCB 138, PCB 153 and PCB 180.
PEC	Predicted environmental concentration
QSAR	Quantitative structure-activity relationship

R^2	Correlation coefficient
wet wt.	Wet weight basis

Appendix A Equations for the Arctic Terrestrial Food-Chain model

The model is presented in two parts in Kelly and Gobas (2003). The first part is an air-to-vegetation distribution model. The overall model is described by the following equation.

$$\frac{dC_{VT}}{dt} = \left(\frac{A_V}{V_V}\right) \times \left\{ \delta_G \times \left(C_{AG} - \frac{C_{VD}}{K_{VG}}\right) + \delta_W \times \left(C_{WD} - \frac{C_{VD}}{K_{VW}}\right) + \left(\delta_P \times C_{AP} - k_E \times V_V \times C_{VP}\right) \right\}$$

where C_{VT} = total concentration in vegetation (mol m^{-3}).

A_V = projected leaf surface area (m^2).

V_V = volume of vegetation (m^3).

δ_G = mass transfer coefficient for air-to-vegetation diffusion (m $hour^{-1}$).

C_{AG} = gas-phase concentration of the chemical in air (mol m^{-3}).

C_{VD} = adsorbed concentration in vegetation (mol m^{-3}).

K_{VG} = vegetation gas-phase partition coefficient (dimensionless).

δ_W = mass transfer coefficient for meltwater-to-vegetation diffusion (m $hour^{-1}$).

C_{WD} = freely dissolved concentration in meltwater (mol m^{-3}).

K_{VW} = vegetation-water partition coefficient (dimensionless).

δ_P = deposition velocity of particle-bound chemical to the leaf surface (a combined value for both wet and dry deposition is used) (m $hour^{-1}$).

C_{AP} = particulate-bound concentration of the chemical in air (mol m^{-3}).

k_E = first-order rate constant for erosion of particulate-bound chemical once associated with the vegetation surface ($hour^{-1}$).

C_{VP} = adsorbed vegetation concentration resulting from particulate decomposition.

This equation can be solved to give either time-dependent or steady-state concentrations. The plant model is designed for arctic plants such as lichens. As can be seen from the above, the processes considered in the model are air-to-vegetation partitioning, direct deposition of particulate-bound substance, and accumulation from the overlying snow packs. This part of the model is therefore of limited relevance to the United Kingdom. However, it should be noted that a model covering similar uptake processes (without the accumulation from overlying snow packs) is included in the ACC-HUMAN model that is reviewed in Part C of this report series. This, and the lack of suitable data for verification, means that the plant model within the Actic Terrestrial Food-chain model has not been considered further here.

The second part of the model concerns the uptake into terrestrial herbivores (caribou) and carnivores (arctic wolves) from food. The following equation describes the model for both terrestrial herbivores and carnivores.

$$\frac{dV_B C_B}{dt} = (G_A \times E_A \times C_{AG}) + (G_D \times E_D \times C_D) - \left(\frac{G_A \times E_A}{K_{BA}} + \frac{E_D \times G_F}{K_{BG}} + \frac{G_U}{K_{BU}} + \frac{G_M}{K_{BM}} + (k_M \times V_B) \right) \times C_B$$

where V_B = volume of organism (m^3).

C_B = concentration of chemical in organism (mol m^{-3}).

G_A = inhalation rate (m^3 $hour^{-1}$).

E_A = inhalation efficiency (dimensionless).

C_{AG} = gas-phase concentration in air (mol m^{-3}).

G_D = ingestion rate of food (m^3 $hour^{-1}$).

E_D = gross chemical dietary uptake efficiency (dimensionless).

C_D = concentration in diet (mol m^{-3}).

K_{BA} = volume-normalised partition coefficient between the organism and air (dimensionless).

G_F = faecal egestion rate (m^3 $hour^{-1}$).

K_{BG} = mass transfer coefficient for diffusion from the organism into the gastrointestinal tract (m $hour^{-1}$).

G_U = urinary excretion rate (m^3 $hour^{-1}$).

K_{BU} = volume-normalised partition coefficient between the organism and urine.

G_M = milk excretion rate (m^3 $hour^{-1}$).

K_{BM} = volume-normalised partition coefficient between the organism and milk (dimensionless).

k_M = metabolic transformation rate constant ($hour^{-1}$).

The term dV_BC_B/dt represents the net chemical flux of the chemical into the organism in mol/h and is also termed N_B in the paper.

At steady-state $dV_BC_B/dt = 0$, and the concentration in the organism can be estimated from the following equation.

$$C_B = \frac{(G_A \times E_A \times C_{AG}) + (G_D \times E_D \times C_D)}{\left(\frac{G_A \times E_A}{K_{BA}} + \frac{E_D \times G_F}{K_{BG}} + \frac{G_U}{K_{BU}} + \frac{G_M}{K_{BM}} + (k_M \times V_B) \right)}$$

From this equation it is relatively straight forward to estimate the accumulation factor for uptake from food alone (C_B/C_D assuming $C_{AG} = 0$) and air alone (C_B/C_{AG} assuming $C_D = 0$).

Within the model, the various partition coefficients needed are estimated as follows:

$$K_{BA} = \nu_{LB} \times K_{OA} + 0.035 \times \nu_{NB} \times K_{OA} + \frac{\nu_{WB}}{K_{AW}}$$

$$K_{BG} = \frac{\left(\nu_{LB} + 0.035 \times \nu_{NB} + \frac{\nu_{WB}}{Kow} \right)}{\left(\nu_{LG} + 0.035 \times \nu_{NG} + \frac{\nu_{WG}}{Kow} \right)}$$

$$K_{BU} = \left(\nu_{LB} + 0.035 \times \nu_{NB} \right) \times Kow + \nu_{WB}$$

$$K_{BM} = \frac{\left(\left(\nu_{LB} + 0.035 \times \nu_{NB} \right) \times Kow + \nu_{WB} \right)}{\left(\left(\nu_{LM} + 0.035 \times \nu_{NM} \right) \times Kow + \nu_{WM} \right)}$$

where ν_{LB} = lipid content of the organism (kg lipid kg^{-1} wet weight organism).

ν_{NB} = non-lipid organic matter content of the organism (kg non-lipid organic matter kg^{-1} wet weight organism).

ν_{WB} = water content of the organism (kg water kg^{-1} wet weight organism).

ν_{LG} = lipid content of intestinal content (kg lipid kg^{-1} wet weight digesta).

ν_{NG} = non-lipid organic matter content of intestinal content (kg non-lipid organic matter kg^{-1} wet weight digesta).

ν_{WG} = water content of intestinal content (kg water kg^{-1} wet weight digesta).

ν_{LM} = lipid content of milk (kg lipid kg^{-1} milk).

ν_{NM} = non-lipid organic matter content of milk (kg non-lipid organic matter kg^{-1} milk).

ν_{WM} = water content of milk (kg water kg^{-1} milk).

K_{oa} = octanol-air partition coefficient, corrected for internal body concentration (~37°C).

K_{aw} = air-water partition coefficient, corrected for internal body concentration (~37°C).

K_{ow} = octanol-water partition coefficient.

The lipid, non-lipid and water contents of intestinal contents depend on the digestibility of the ingested diet and can be estimated using the following equations.

$$\nu_{LG} = \frac{(1-\varepsilon_L)\times \nu_{LD}}{\{(1-\varepsilon_L)\times \nu_{LD} + (1-\varepsilon_N)\times \nu_{ND} + (1-\varepsilon_W)\times \nu_{WD}\}}$$

$$\nu_{NG} = \frac{(1-\varepsilon_N)\times \nu_{ND}}{\{(1-\varepsilon_L)\times \nu_{LD} + (1-\varepsilon_N)\times \nu_{ND} + (1-\varepsilon_W)\times \nu_{WD}\}}$$

$$\nu_{WG} = \frac{(1-\varepsilon_W)\times \nu_{WD}}{\{(1-\varepsilon_L)\times \nu_{LD} + (1-\varepsilon_N)\times \nu_{ND} + (1-\varepsilon_W)\times \nu_{WD}\}}$$

where ε_L = absorption efficiency of lipid.

ε_N = absorption efficiency of non-lipid.

ε_W = absorption efficiency of water.

Kelly and Gobas (2003) tested the model using time trend data for the levels of PCB 153 in both male and female wolves and caribou from Bathhurst Inlet. In general, the model predictions were comparable to the observed concentrations. In particular, the model was able to reasonably predict a) the seven times increase in male caribou tissue concentrations that occurred between September and July and b) the lower concentrations in female animals compared to male animals.

Appendix B – Data sets used to verify the TGD method for earthworms

The data used to verify the TGD method for predicting the accumulation in earthworms are summarised in Table B1. The data used were taken from the following studies.

Belfroid et al. (1994)

The study was a laboratory study using artificial soil spiked with the test substance. Exposure was for over 49 days but steady state was reached within two days. The organic carbon content of the soil was not given and so the organic matter content of 10% for artificial soil taken from Belfroid *et al*. (1995) was assumed, and it was assumed that organic carbon accounted for 58% of the organic matter content. The water content of the wet soil was 35%. The gut contents of the worms were voided prior to analysis.

Belfroid et al. (1995)

The study was a laboratory soil using field soils that were already contaminated with the test substance. Exposure was for up to 60 days and steady state was obtained within this time period. The soil organic matter content of the soil was 20%, and the soil organic carbon content was taken to be 58% of this value. The water content of the wet soil was 45%. The gut contents of the worms were voided prior to analysis.

Van Gestel and Ma (1988)

The study was a laboratory study using two agricultural field soils that were spiked with the test substance. Exposure was for up to 14 days. The soil organic matter content of the soils were 3.7% (Kooyenburg soil) and 6.1% (Holten soil), and the soil organic carbon content was taken to be 58% of these values. BAFs in the paper were reported on a dry weight soil basis, but the underlying soil concentrations were not reported. For the analysis here, a soil concentration of one mg/kg dry weight was assumed and the resulting concentration in the earthworm was estimated using the given BAF. This was then corrected to give a BAF on a wet weight soil basis (the water content of the wet soil was 16%). The gut contents of the worms were voided prior to analysis.

Hendriks et al. (1995)

This study was a field study that reported levels of worms collected from polluted soils in the Rhine delta. The concentrations in soil were also reported. Both the dry matter contents of soil (Ochten 81% and Gelderse Poort 73%) and organic matter contents (Ochten 5% and Gelderse Poort 9%) were given. The organic carbon contents were estimated assuming the assuming that the organic carbon content of the soil was 58% of the organic matter content). The gut contents of the worms were voided prior to analysis.

Jager et al. (2003)

This study was a laboratory study using artificial soil spiked with the chemicals of interest. Exposure was for up to 21 days. The organic matter content of the soil was 10.5% and the organic carbon content was assumed to be 58% of this value. The water content of the wet soil was 40%. The gut contents of the worms were voided prior to analysis.

Lord et al. (1980)

This study was a laboratory study using pesticide-free natural soil spiked with the chemicals of interest, and exposure was for up to 55 days. The organic matter content was 26 mg/g and the organic carbon content was taken to be 58% of the organic matter content. The water content of the wet soil was 21%. The gut contents of the worms were voided prior to analysis. Both the concentration in soil and the ratio of the concentration in worm to soil are shown graphically only in the paper and so the data used were read from the graph.

Sample et al. (1998)

This study was a compilation of field results of concentrations in worms and soil from a literature review. The gut contents were voided prior to analysis in some cases. Both the soil and earthworm concentrations were given on a dry weight basis. To convert the concentration in worms to a wet earthworm basis, a water content of 84% was assumed. The organic matter contents of the soils were reported and these were converted to organic carbon contents assuming organic matter is 58% organic carbon. The water contents of the soils were not given and so a default wet soil water content of 12% was assumed in the calculations.

Jager et al. (2000)

This study was a laboratory study using artificial soil spiked with the test substance. Exposure was for up to seven days. BAF was found to decline with increasing exposure time in many cases and the maximum BAF found was used in the analysis here. The concentrations in the earthworms were not given in the paper but were estimated for this analysis using the maxiumum BAF and the soil concentrations reported. The organic matter content of the soil was 10.5% and the organic carbon content was taken to be 58% of this value. The water content of the wet soil was 35%. The gut contents were voided prior to analysis.

Jager (2003) and van der Wal et al. (2004a)

This study was a laboratory study using soils that were already contaminated with the test substances in the field. Exposure was for up to 28 days. The water contents of the soils are not given in the paper. The tests appear to have been carried out at the maximum water holding capacities. The water holding capacities of similar soils (as g water/g dry weight soil) are given in Jager *et al*. (2005) as 0.50 for ESCH 3 and 0.53 for ESCH 4. Therefore, the water contents (as a percentage of the total wet weight) are 33% for ESCH 3 and 35% for ESCH 4. These were used here. The organic carbon contents of the soil were estimated to be 6.6% (ESCH 3) and 8.5% (ESCH 4). The concentrations in worms were the estimated steady-state concentrations. The lipid

contents of the worms were as reported at 2.3%. The guts were allowed to empty for 24 hours prior to analysis.

Beyer (1996)

This study was a laboratory study using an artificial soil contaminated with the test substance. Exposure was for up to eight weeks. The water content of soil was adjusted to 30% of dry weight ingredients; therefore, the water content of the wet soil = 30/(100+30) = 23%. The peat content of soil was given as 10% and the organic carbon content of the soil was estimated here to be 58% of this value. The total worm, including the gut contents were analysed and the soil content of the whole worm was determined to be around 10% of the wet weight.

Matscheko et al. (2002a)

This study was a laboratory study using a contaminated soil from an old gas works site in Stockholm. Exposure was for up to 19 days. The water content of the wet soil was 10%. The organic matter content of the soil was 6.2% and the organic carbon content was assumed here to be 58% of this value, that is, 3.6%. The gut contents of the worms were voided prior to analysis. $BAF_{earthworm}$ was reported to be around 0.02 for all chemicals studied on a worm lipids/soil organic matter basis. As the organic carbon content is assumed to be 58% of the organic matter content, the equivalent factor is 0.034 on a worm lipid/soil organic carbon basis or ~0.00122 on a lipid/wet soil basis. A worm lipid content of one per cent was assumed in these conversions. However, the units for soil concentrations used in this study were not clear (they may be µmol/g as these units were used elsewhere in this paper) and so it was not clear if these derived BAFs were in the same form as the other BAFs used in this analysis. This is discussed further in the main report.

Mosleh et al. (2003)

This study was a laboratory study using uncontaminated natural soil that was spiked with the test substance. The exposure was for 15 days. The organic carbon content of the soil was 7.7%. In the study, 500 g of dry soil was mixed with 100 ml (~100 g) water and so the water content of the soil =100/(500+100) = 16.7%. The gut contents of the earthworms were voided prior to analysis. Toxic effects were seen in this study and BAF was found to decrease with increasing concentration. The highest BAF found was used in this analysis.

Allard et al. (2005)

This study was a laboratory study using soil from a creosote-contaminated site mixed with sand. The test soil had a water content of 7% and an ignition loss of 1.6% dry weight. For this analysis, the ignition loss was assumed to be equal to the organic matter content, and the organic carbon content was taken to be 58% of this value, that is 0.93%. The gut contents were voided prior to analysis. The exposures to the contaminated soil were carried out in a mixture of agar medium (15 ml), ground oatmeal (1.5 g/l) and soil (15 g) for up to 42 days. The unusual exposure medium used makes these results difficult to relate to field situations. This is discussed further in the main report.

Hu et al. (2005)

This study was a laboratory study using two soils from Beijing, one an agricultural soil and one a forest soil, spiked with the test substance. Exposure was for up to 30 days. The organic matter contents were determined as 1.35% (agricultural soil) and 4.53% (forest soil) and the corresponding organic carbon contents of 0.78% and 2.63% were estimated assuming the organic matter = 58% organic carbon. The water content of the soils was 40% of the water holding capacities. The water holding capacities of the two soils were not given and so a water content of 12% of the wet weight was assumed as a default. The guts contents were voided prior to analysis.

Haque and Ebing (1988)

This study was a laboratory study using an OECD artificial soil spiked with ^{14}C-labelled test substance. The organic carbon content was not given and so an organic matter content of 10% (as is typical for the OECD artificial soil) was assumed, and it was further assumed that the organic carbon content was 58% of this value. The soil moisture was 40% of the water holding capacity. The water holding capacity was not given and so a water content of 12% was assumed by default. Gut contents were voided prior to analysis. The test chemical was added to soil 14 days prior to the worms and the uptake was determined based on ^{14}C-measurements.

Van der Wal et al. (2004b)

This study was a laboratory study using OECD artificial soil. The organic carbon content was not given and so an organic matter content of 10% (as is typical for the OECD artificial soil) was assumed, and it was further assumed that the organic carbon content was 55% of this value. The soil was moistened to 55% of maximum water holding capacity, which is equivalent to 70% moisture content on a dry weight. The water content on a wet weight basis is therefore 70/(100=70) = 41%. Steady state was reached after two to four days exposure ,but the concentrations in worms then fell until a new lower (by a factor of two to three) steady state was reached after 8-12 days. The values used in this analysis were read from a graph after around four days for the nominal 25 mg/kg dry soil experiments (these results showed the lowest subsequent decrease with time). The gut contents were not voided prior to analysis

Sellström et al., 2005

This study was a field study reporting the levels in worms and soil from several soils from Sweden. The organic matter contents and worm lipid contents were given in the paper, and for this analysis the organic carbon content of soil assumed to be 58% of the organic matter content. The water contents of the soils were not given and so a default value of 12% was assumed here. It is not clear if worm gut contents were voided prior to analysis and so for the calculations here it was assumed that they were not voided prior to analysis.

Harris et al. (2000)

This study was a field study reporting the concentrations of chemicals in earthworms and soils from historically contaminated orchard soils. It was not clear if gut contents were purged prior to analysis. All earthworm concentrations were given on a dry

weight basis and so a water content of 75% was assumed in this analysis by default for the earthworm. The soil water contents were not given and so a water content of 12% was assumed as a default in this analysis. The soil organic matter content was 2.3% (Niagara soil), 3.3% (Simcoe soil) and 3.8% (Okanagan soil) and it was assumed that organic carbon content was 58% of organic matter content. It was not clear if worm gut contents were voided prior to analysis and so for the calculations here, it was assumed that they were not voided prior to analysis.

Matscheko et al. (2002b)

This study was a field study reporting the concentrations of chemicals in earthworms and soils from a number of soils from Sweden, including soils that had received sewage sludge. The organic matter contents were given as 4.7% (IR soil)[6], 4.8% (I1 soil), 5.4% (I2 soil), 2.6% (PR soil), 2.8% (P1 soil), 2.8% (P2 soil), 3.4% (LR spring soil), 3.7% LS spring soil), 3.3% (LR autumn soil), 3.5% (LS autumn soil), 5.7% (BR soil), 4.9% (BS), 1.8% (HR) and 2.6% (Hsed). It was assumed here that the organic carbon content was 58% of the organic matter content. Soil water contents were not given and so a water content of 12% was assumed as a default in this analysis. The gut contents of the worms were voided prior to analysis. Soil concentrations were given but only the resulting lipid BAF (on a lipid worm/soil organic matter) basis was reported, rather than the concentrations in worms. The BAF on a wet worm/whole soil basis was calculated here using the known soil organic matter contents and assuming the worm had a lipid content of 1.5% of the fresh weight (mean value found in the study).

[6] The soil names relate to the abbreviations used in the original paper and are used here for identification purposes only. For original paper should be consulted for further details of the soil types and locations.

Table B1 Data sets used for verification of the TGD method for earthworms

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
Aldicarb	1.15	4.15E+01	1.08E+01	*Lumbricus terrestris*	Uncontaminated natural soil	7.7%	-0.16	-0.46	0.08	1.46	1.29	Mosleh *et al*., 2003
9,10-Anthraquinone	2.44	1.94E+02	1.19E+02	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	-0.18	0.03	0.86	0.75	Matscheko *et al*., 2002a
Anthracene	4.46	2.18×10^3	5.16×10^3	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.19	1.28	0.91	0.93	0.89	Allard *et al*., 2005
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	0.70	0.33	0.35	0.30	Matscheko *et al*., 2002a
Benzo[a]anthracene	5.82	1.11×10^4	6.52×10^4	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.67	1.94	1.17	0.65	0.64	Allard *et al*., 2005
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	1.35	0.58	0.07	0.05	Matscheko *et al*., 2002a
1,2-Benzo anthraquinone	3.45	6.52E+02	7.84E+02	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	0.22	0.14	0.57	0.49	Matscheko *et al*., 2002a
Benzo[b]fluoranthene	6.29	1.95×10^4	1.57×10^5	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	1.58	0.67	-0.03	-0.04	Matscheko *et al*., 2002a
Benzo[b+k]fluoranthene	6.12	1.59×10^4	1.14×10^5	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.61	2.08	1.23	0.59	0.58	Allard *et al*., 2005
Benzo[k]fluoranthene	6.59	2.80×10^4	2.74×10^5	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	1.72	0.73	-0.09	-0.09	Matscheko *et al*., 2002a
Benzo[ghi]perylene	7.00	4.57×10^4	5.89×10^5	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.56	2.50	1.40	0.41	0.42	Allard *et al*., 2005
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	1.92	0.81	-0.18	-0.17	Matscheko *et al*., 2002a
Benzo[a]pyrene	6.13	1.61×10^4	1.16×10^5	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	1.50	0.64	0.00	-0.01	Matscheko *et al*., 2002a
				Enchytraeus crypticus	Creosote-contaminated soil mixed with sand	0.9%	-1.92	2.09	1.23	0.59	0.58	Allard *et al*., 2005
				Eisenia andrei	Artificial soil	5.9%	-0.20	1.29	0.43	-0.21	-0.22	Jager *et al*., 2000
Carbazole	2.94	354	303	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	0.00	0.06	0.69	0.61	Matscheko *et al*., 2002a
3-Chlorophenol	2.50	12[b]	12[b]	*Eisenia fetida andrei*	Agricultural field soil - Holten soil	3.5%	0.22	-0.36	-0.36	0.63	0.34	van Gestel and Ma, 1988

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Lubricus rubellus	Agricultural field soil - Holten soil	3.5%	1.08	-0.36	-0.36	0.63	0.34	
		6[b]	6[b]	*Eisenia fetida andrei*	Agricultural field soil - Kooyenburg soil	2.1%	0.12	-0.07	-0.07	0.93	0.64	
				Lubricus rubellus	Agricultural field soil - Kooyenburg soil	2.1%	1.29	-0.07	-0.07	0.93	0.64	
Chrysene	5.81	1.10×10^4	6.40×10^4	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-2.01	1.93	1.17	0.66	0.64	Allard *et al*., 2005
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	1.35	0.58	0.07	0.05	Matscheko *et al*., 2002a
DDD (sum o,p' and p,p'-isomers)	6.02	1.4×10^4	9.47×10^4	Several species	Canadian orchard soil - Niagara	1.3%	0.36	1.83	1.01	0.41	0.40	Harris *et al*., 2000
					Canadian orchard soil - Simcoe	1.9%	0.65	1.68	0.86	0.26	0.25	
					Canadian orchard soil - Okanagan	2.2%	0.40	1.62	0.80	0.19	0.19	
DDE (sum o,p' and p,p'-isomers)	6.51	2.54×10^4	2.36×10^5	Several species	Canadian orchard soil - Niagara	1.3%	-0.03	2.07	1.10	0.31	0.31	Harris *et al*., 2000
					Canadian orchard soil - Simcoe	1.9%	0.15	1.91	0.95	0.15	0.16	
					Canadian orchard soil - Okanagan	2.2%	0.40	1.85	0.89	0.09	0.10	
DDE (*p,p'*-isomer)	6.51	2.54×10^4	2.36×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	0.38	1.78	0.81	0.02	0.02	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.60	1.52	0.55	-0.24	-0.24	
DDT (sum o,p'- and pp'-isomers)	6.19	1.73×10^4	1.30×10^5	Several species	Canadian orchard soil - Niagara	1.3%	-0.59	1.91	1.04	0.38	0.37	Harris *et al*., 2000
					Canadian orchard soil - Simcoe	1.9%	-0.17	1.76	0.89	0.22	0.22	
					Canadian orchard soil - Okanagan	2.2%	-0.28	1.70	0.83	0.16	0.16	
DDT (o,p'-isomer)	6.19	1.73×10^4	1.30×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	0.15	1.62	0.75	0.08	0.08	Hendriks *et al*., 1995
DDT (*p,p'*-isomer)	6.19	1.73×10^4	1.30×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.25	1.62	0.75	0.08	0.08	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.02	1.37	0.49	-0.17	-0.18	
Dibenzo[a]anthracene	6.61	2.87×10^4	2.85×10^5	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	1.73	0.73	-0.10	-0.09	Matscheko *et al*., 2002a

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
Dibenzo[a,h]anthracene	6.50	2.51×10^4	2.32×10^5	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.60	2.26	1.30	0.51	0.51	Allard *et al*., 2005
Dibenzotiophene	3.46	659	799	*Eisenia fetida*	Contaminated soil from gas works site	3.6%	-2.49	0.23	0.14	0.56	0.49	Matscheko *et al*., 2002a
3,4-Dichlorophenol	3.20	30[b]	30[b]	*Eisenia fetida andrei*	Agricultural field soil - Holten soil	3.5%	-0.02	-0.13	-0.13	0.39	0.32	van Gestel and Ma, 1988
				Lubricus rubellus	Agricultural field soil - Holten soil	3.5%	0.22	-0.13	-0.13	0.39	0.32	
		15[b]	15[b]	*Eisenia fetida andrei*	Agricultural field soil - Kooyenburg soil	2.1%	0.33	0.17	0.17	0.69	0.62	
				Lubricus rubellus	Agricultural field soil - Kooyenburg soil	2.1%	0.19	0.17	0.17	0.69	0.62	
Dieldrin	5.40	6.73×10^3	2.98×10^4	*Lubricus rubellus*	Ochten field soils	2.9%	-0.30	1.24	0.60	0.25	0.22	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.70	0.99	0.34	-0.01	-0.03	
				Eisenia andrei	Field-contaminated soil - Esch 4[a]	8.5%	0.13	0.77	0.13	-0.22	-0.25	Jager, 2003; van der Wal *et al*., 2004
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4[a]	8.5%	-0.04	0.78	0.13	-0.22	-0.25	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3	6.6%	-0.31	0.89	0.24	-0.11	-0.13	
				Lubricus terrestris	Natural soil	1.5%	0.23	1.53	0.88	0.53	0.51	Lord *et al*., 1980
Endosulfan	3.83	1.03×10^3	1.59×10^3	*Lumbricus terrestris*	Uncontaminated natural soil	7.7%	0.01	0.07	-0.12	0.15	0.09	Mosleh *et al*., 2003
Fluoranthene	5.20	5.30×10^3	2.05×10^4	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.51	1.64	1.05	0.78	0.75	Allard *et al*., 2005
				Eisenia andrei	Artificial soil	5.9%	0.33	0.84	0.25	-0.02	-0.05	Jager *et al*., 2000
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	1.05	0.47	0.20	0.16	Matscheko *et al*., 2002a
1,2,3,4, 6,7,8-Heptachlorodibenzo-*p*-dioxin	8.20	1.92×10^5	5.52×10^6	Several species	Field soils - Sweden – IR[a]	2.7%	-0.60	2.61	1.16	-0.31	-0.30	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	-1.21	2.60	1.15	-0.32	-0.31	
					Field soils - Sweden - I2[a]	3.1%	-0.79	2.55	1.10	-0.37	-0.36	
					Field soils - Sweden – PR[a]	1.5%	-0.47	2.87	1.41	-0.05	-0.05	
					Field soils - Sweden - PR1[a]	1.6%	-0.68	2.84	1.38	-0.08	-0.08	
					Field soils - Sweden - PR2[a]	1.6%	-0.50	2.84	1.38	-0.08	-0.08	
					Field soils - Sweden – BS[a]	2.8%	-0.92	2.60	1.14	-0.32	-0.32	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
					Field soils - Sweden – HR[a]	1.0%	-0.79	3.03	1.57	0.11	0.11	
					Field soils - Sweden - Hsed	1.5%	-1.04	2.87	1.41	-0.05	-0.05	
1,2,3,4, 6,7,8-Heptachlordibezofuran	7.92	1.38×10^{5}	3.27×10^{6}	Several species	Field soils - Sweden – IR[a]	2.7%	-0.43	2.48	1.10	-0.25	-0.21	Matscheko *et al.*, 2002b
					Field soils - Sweden - I1[a]	2.8%	-0.61	2.47	1.09	-0.26	-0.22	
					Field soils - Sweden - I2[a]	3.1%	-0.66	2.42	1.04	-0.31	-0.27	
					Field soils - Sweden – PR[a]	1.5%	-0.25	2.74	1.36	0.01	0.04	
					Field soils - Sweden - PR1[a]	1.6%	-0.38	2.70	1.33	-0.02	0.01	
					Field soils - Sweden - PR2[a]	1.6%	-0.38	2.70	1.33	-0.02	0.01	
					Field soils - Sweden – LR[a] - Autumn	1.9%	-0.45	2.63	1.26	-0.09	-0.06	
					Field soils - Sweden – BR[a]	3.3%	-0.69	2.40	1.02	-0.33	-0.30	
					Field soils - Sweden – HR[a]	1.0%	-0.79	2.90	1.52	0.17	0.20	
					Field soils - Sweden - Hsed	1.5%	-0.99	2.74	1.36	0.01	0.04	
Heptachlorepoxide	5.40	6.73×10^{3}	2.98×10^{4}	*Lubricus rubellus*	Ochten field soils	2.9%	0.00	1.24	0.60	0.25	0.22	Hendriks *et al*., 1995
Hexachlorobenzene	5.50	7.59×10^{3}	3.59×10^{4}	*Eisenia andrei*	Artificial soil	5.8%	0.33	0.99	0.32	-0.07	-0.10	Belfroid *et al*., 1994
				Eisenia andrei	Field-contaminated soil	11.6%	-0.04	0.69	0.01	-0.38	-0.40	Belfroid *et al*., 1995
				Lumbricus terrestris	OECD standard soil	5.8%	-0.46	0.95	0.29	-0.12	-0.12	Beyer, 1996
				Lubricus rubellus	Ochten field soils	2.9%	-0.79	1.29	0.62	0.23	0.20	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.03	1.04	0.36	-0.03	-0.05	
				Eisenia andrei	Artificial soil	6.1%	0.58	0.97	0.29	-0.10	-0.12	Jager *et al*., 2003

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Eisenia andrei	Field-contaminated soil - Esch 4[a]	8.5%	-0.47	0.82	0.15	-0.24	-0.27	Jager, 2003; van der Wal *et al*., 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4[a]	8.5%	-0.56	0.82	0.15	-0.24	-0.26	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3[a]	6.6%	0.02	0.94	0.26	-0.13	-0.15	
				Lubricus terrestris	Natural soil	1.5%	0.58	1.58	0.90	0.51	0.49	Lord *et al*., 1980
				Enchytraeus crypticus	OECD standard soil	5.8%	1.62	0.95	0.29	-0.12	-0.12	van der Wal *et al*., 2004b
Hexachlorocyclohexane (beta- isomer)	3.70	879	1.25×10^3	*Lubricus rubellus*	Ochten field soils	2.9%	0.47	0.43	0.28	0.60	0.54	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.30	0.18	0.02	0.35	0.28	
Hexachlorocyclohexane (gamma- isomer or lindane)	3.70	879	1.25×10^3	*Lubricus rubellus*	Ochten field soils	2.9%	0.09	0.43	0.28	0.60	0.54	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	0.13	0.18	0.02	0.35	0.28	
1,2,3,6,7,8-Hexachloro dibenzo-*p*-dioxin	7.98	$1.48X10^5$	3.66×10^6	Several species	Field soils - Sweden - PR2[a]	1.6%	-0.28	2.73	1.34	-0.04	0.00	Matscheko *et al*., 2002b
					Field soils - Sweden – BS[a]	2.8%	-0.74	2.49	1.10	-0.28	-0.24	
					Field soils - Sweden – Hsed[a]	1.5%	-0.83	2.77	1.37	0.00	0.03	
1,2,3,4,7,8-Hexachloro dibenzofuran	7.92	1.38×10^5	3.27×10^6	Several species	Field soils - Sweden – IR[a]	2.7%	-0.50	2.48	1.10	-0.25	-0.21	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	-0.74	2.47	1.09	-0.26	-0.22	
					Field soils - Sweden – PR[a]	1.5%	-0.34	2.74	1.36	0.01	0.04	
					Field soils - Sweden - PR1[a]	1.6%	-0.38	2.70	1.33	-0.02	0.01	
					Field soils - Sweden - PR2[a]	1.6%	-0.38	2.70	1.33	-0.02	0.01	
					Field soils - Sweden – BS[a]	2.8%	-0.92	2.46	1.08	-0.27	-0.23	
1,2,3,6,7,8-Hexachloro dibenzofuran	7.92	1.38×10^5	3.27×10^6	Several species	Field soils - Sweden - PR1	1.6%	-0.38	2.70	1.33	-0.02	0.01	Matscheko *et al*., 2002b
					Field soils - Sweden - PR2	1.6%	-0.38	2.70	1.33	-0.02	0.01	
Indeno[1,2,3-cd]pyrene	6.58	2.76×10^4	2.69×10^5	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.47	2.30	1.32	0.50	0.50	Allard *et al*., 2005

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	1.72	0.73	-0.09	-0.09	Matscheko *et al.*, 2002a
Octachlorodibenzo-*p*-dioxin	8.20	1.92×10^{5}	5.52×10^{6}	Several species	Field soils - Sweden – IR[a]	2.7%	-0.60	2.61	1.16	-0.31	-0.26	Matscheko *et al.*, 2002b
					Field soils - Sweden - I1[a]	2.8%	-1.21	2.60	1.15	-0.32	-0.27	
					Field soils - Sweden - I2[a]	3.1%	-0.79	2.55	1.10	-0.37	-0.33	
					Field soils - Sweden – PR[a]	1.5%	-0.25	2.87	1.41	-0.05	-0.01	
					Field soils - Sweden - PR1[a]	1.6%	-0.68	2.84	1.38	-0.08	-0.04	
					Field soils - Sweden - PR2[a]	1.6%	-0.50	2.84	1.38	-0.08	-0.04	
					Field soils - Sweden – LR[a] - Spring	2.0%	-0.46	2.75	1.30	-0.17	-0.12	
					Field soils - Sweden – LS[a] - Spring	2.1%	-0.20	2.72	1.26	-0.20	-0.16	
					Field soils - Sweden – LR[a] - Autumn	1.9%	-0.57	2.77	1.31	-0.15	-0.11	
					Field soils - Sweden – LS[a] - Autumn	2.0%	-0.60	2.74	1.28	-0.18	-0.14	
					Field soils - Sweden – BR[a]	3.3%	-0.81	2.53	1.07	-0.39	-0.35	
					Field soils - Sweden – BS[a]	2.8%	-0.92	2.60	1.14	-0.32	-0.28	
					Field soils - Sweden – HR[a]	1.0%	-0.79	3.03	1.57	0.11	0.15	
					Field soils - Sweden – Hsed[a]	1.5%	-0.99	2.87	1.41	-0.05	-0.01	
Octachlorodibenzofuran	8.60	3.10×10^{5}	1.16×10^{7}	Several species	Field soils - Sweden – IR[a]	2.7%	-0.50	2.81	1.23	-0.39	-0.34	Matscheko *et al.*, 2002b
					Field soils - Sweden - I1[a]	2.8%	-0.74	2.80	1.22	-0.40	-0.35	
					Field soils - Sweden - I2[a]	3.1%	-0.79	2.75	1.17	-0.45	-0.40	
					Field soils - Sweden – PR[a]	1.5%	-0.34	3.06	1.49	-0.13	-0.08	
					Field soils - Sweden - PR1[a]	1.6%	-0.50	3.03	1.46	-0.16	-0.11	
					Field soils - Sweden - PR2[a]	1.6%	-0.50	3.03	1.46	-0.16	-0.11	
					Field soils - Sweden – LR[a] - Spring	2.0%	-0.29	2.95	1.37	-0.25	-0.20	
					Field soils - Sweden – BS[a]	2.8%	-0.74	2.79	1.21	-0.41	-0.36	
					Field soils - Sweden – HR[a]	1.0%	-0.79	3.22	1.65	0.03	0.08	
					Field soils - Sweden – Hsed[a]	1.5%	-1.04	3.06	1.49	-0.13	-0.08	
PBDE 47	6.80	3.60×10^{4}	4.06×10^{5}	Several species	Field soils - Sweden – IR[a]	2.7%	0.50	1.94	0.89	-0.02	-0.01	Matscheko *et al.*, 2002b
					Field soils - Sweden - I1[a]	2.8%	0.69	1.93	0.88	-0.03	-0.02	
					Field soils - Sweden - I2[a]	3.1%	0.74	1.88	0.83	-0.08	-0.07	
					Field soils - Sweden – PR[a]	1.5%	0.66	2.20	1.15	0.24	0.25	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
					Field soils - Sweden - PR1[a]	1.6%	0.50	2.17	1.11	0.21	0.22	
					Field soils - Sweden - PR2[a]	1.6%	0.72	2.17	1.11	0.21	0.22	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.24	2.08	1.03	0.12	0.13	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.20	2.05	0.99	0.09	0.10	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.43	2.10	1.04	0.14	0.15	
					Field soils - Sweden – LS[a] - Autumn	2.0%	1.18	2.07	1.02	0.11	0.12	
					Field soils - Sweden – BR[a]	3.3%	0.41	1.86	0.81	-0.10	-0.09	
					Field soils - Sweden – BS[a]	2.5%	0.31	1.98	0.93	0.02	0.03	
					Field soils - Sweden – HR[a]	1.0%	0.51	2.36	1.31	0.40	0.41	
					Field soils - Sweden – Hsed[a]	1.5%	-0.04	2.20	1.15	0.24	0.25	
PBDE 47 (continued	6.80	3.60×10^{4}	4.06×10^{5}	Unknown	Field soils from different locations	1.9%	0.45	2.06	1.02	0.11	0.12	Sellström *et al*., 2005
						1.9%	0.42	2.05	1.00	0.09	0.10	
						1.9%	0.65	2.05	1.00	0.09	0.10	
						3.3%	0.20	1.82	0.77	-0.14	-0.13	
						3.6%	0.33	1.78	0.73	-0.18	-0.16	
						3.6%	0.38	1.78	0.73	-0.18	-0.16	
						2.0%	0.48	2.04	0.99	0.08	0.09	
						2.2%	0.10	1.99	0.94	0.03	0.05	
						4.2%	0.19	1.71	0.67	-0.25	-0.23	
						3.8%	-0.43	1.75	0.71	-0.20	-0.19	
						1.2%	0.10	2.24	1.19	0.28	0.29	
						1.5%	-0.48	2.16	1.11	0.20	0.21	
PBDE 66	6.80	3.60×10^{4}	4.06×10^{5}	Several species	Field soils - Sweden - PR1[a]	1.6%	1.25	2.17	1.11	0.21	0.22	Matscheko *et al*., 2002b
					Field soils - Sweden - PR2[a]	1.6%	1.25	2.17	1.11	0.21	0.22	
					Field soils - Sweden – BR[a]	3.3%	0.49	1.86	0.81	-0.10	-0.09	
					Field soils - Sweden – BS[a]	2.5%	0.44	1.98	0.93	0.02	0.03	
					Field soils - Sweden – HR[a]	1.0%	0.51	2.36	1.31	0.40	0.41	
					Field soils - Sweden – Hsed[a]	1.5%	0.05	2.20	1.15	0.24	0.25	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Unknown	Field soils from different locations	3.8%	-0.35	1.75	0.71	-0.20	-0.19	Sellström *et al*., 2005
PBDE 85	7.30	6.55×10	$1.03x10^{6}$	Unknown	Field soils from different locations	3.8%	-0.55	1.99	0.80	-0.31	-0.28	Sellström *et al*., 2005
PBDE 99	7.40	7.38×10^{4}	1.24×10^{6}	Several species	Field soils - Sweden – IR[a]	2.7%	0.40	2.23	1.00	-0.14	-0.12	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	0.63	2.22	0.99	-0.15	-0.13	
					Field soils - Sweden – PR[a]	1.5%	0.90	2.49	1.26	0.12	0.14	
					Field soils - Sweden - PR1[a]	1.6%	0.62	2.45	1.23	0.08	0.11	
					Field soils - Sweden - PR2[a]	1.6%	0.72	2.45	1.23	0.08	0.11	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.41	2.37	1.14	0.00	0.02	
					Field soils - Sweden – LS[a] - Spring	2.1%	-0.10	2.33	1.11	-0.04	-0.01	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.97	2.36	1.13	-0.01	0.01	
					Field soils - Sweden – BR[a]	3.3%	0.41	2.15	0.92	-0.22	-0.20	
					Field soils - Sweden – BS[a]	2.5%	0.14	2.27	1.04	-0.10	-0.08	
					Field soils - Sweden – HR[a]	1.0%	0.51	2.65	1.42	0.28	0.30	
					Field soils - Sweden – Hsed[a]	1.5%	0.05	2.49	1.26	0.12	0.14	
				Unknown	Field soils from different locations	1.9%	0.45	2.35	1.13	-0.02	0.01	Sellström *et al*., 2005
						1.9%	0.47	2.34	1.12	-0.03	-0.01	
						1.9%	0.58	2.34	1.12	-0.03	-0.01	
						3.3%	0.11	2.11	0.89	-0.26	-0.24	
						3.6%	0.27	2.07	0.85	-0.30	-0.28	
						3.6%	0.26	2.07	0.85	-0.30	-0.28	
						2.0%	0.17	2.33	1.10	-0.04	-0.02	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
						2.2%	-0.14	2.28	1.06	-0.09	-0.07	
						4.2%	-0.06	2.00	0.78	-0.37	-0.34	
						3.8%	-0.43	2.04	0.82	-0.33	-0.30	
						1.2%	0.11	2.53	1.31	0.16	0.18	
						1.5%	-0.23	2.44	1.22	0.07	0.10	
PBDE 100	7.30	6.55×10^4	1.03×10^6	Several species	Field soils - Sweden – IR[a]	2.7%	0.57	2.18	0.99	-0.12	-0.10	Matscheko *et al*., 2002b
					Field soils - Sweden – PR[a]	1.5%	0.90	2.44	1.24	0.14	0.16	
					Field soils - Sweden - PR1[a]	1.6%	0.62	2.41	1.21	0.11	0.13	
					Field soils - Sweden - PR2[a]	1.6%	0.80	2.41	1.21	0.11	0.13	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.71	2.32	1.13	0.02	0.04	
					Field soils - Sweden – LS[a] - Autumn	2.0%	1.46	2.31	1.11	0.01	0.03	
					Field soils - Sweden – BR[a]	3.3%	0.62	2.10	0.90	-0.20	-0.18	
					Field soils - Sweden – BS[a]	2.5%	0.31	2.22	1.03	-0.08	-0.06	
					Field soils - Sweden - HR	1.0%	0.81	2.60	1.40	0.30	0.32	
					Field soils - Sweden - Hsed	1.5%	0.05	2.44	1.24	0.14	0.16	
				Unknown	Field soils from different locations	1.9%	0.35	2.30	1.11	0.00	0.03	Sellström *et al*., 2005
						1.9%	0.44	2.29	1.10	-0.01	0.01	
						1.9%	0.62	2.29	1.10	-0.01	0.01	
						3.3%	0.12	2.06	0.87	-0.24	-0.22	
						3.6%	0.30	2.02	0.83	-0.28	-0.26	
						3.6%	0.39	2.02	0.83	-0.28	-0.26	
						3.8%	-0.06	1.99	0.80	-0.31	-0.28	
						1.2%	0.01	2.48	1.29	0.18	0.20	
						1.5%	-0.20	2.39	1.20	0.09	0.12	
PBDE 153	7.90	1.34×10^5	3.16×10^6	Unknown	Field soils from different locations	1.9%	0.09	2.59	1.22	-0.12	-0.09	Sellström *et al*., 2005
						1.9%	0.30	2.58	1.21	-0.14	-0.10	
						3.6%	-0.02	2.31	0.94	-0.41	-0.37	
						3.6%	0.00	2.31	0.94	-0.41	-0.37	
						3.8%	-0.41	2.28	0.91	-0.43	-0.39	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
						1.5%	-0.28	2.68	1.31	-0.03	0.01	
PBDE 154	7.80	1.19×10^5	2.62×10^6	Unknown	Field soils from different locations	1.9%	0.08	2.53	1.19	-0.12	-0.08	Sellström *et al*., 2005
						3.6%	0.15	2.26	0.92	-0.39	-0.35	
						3.6%	0.11	2.26	0.92	-0.39	-0.35	
						3.8%	-0.45	2.23	0.90	-0.41	-0.38	
						1.2%	-0.04	2.72	1.38	0.08	0.11	
						1.5%	-0.23	2.63	1.30	-0.01	0.02	
PBDE 196	8.80	3.94×10^5	1.69×10^7	Unknown	Field soils from different locations	3.6%	-0.56	2.74	1.11	-0.59	-0.53	Sellström *et al*., 2005
						3.6%	-0.57	2.74	1.11	-0.59	-0.53	
						3.8%	-1.36	2.71	1.08	-0.62	-0.56	
PBDE 206	8.90	4.45×10^5	2.04×10^7	Unknown	Field soils from different locations	1.9%	-0.77	3.06	1.40	-0.34	-0.28	Sellström *et al*., 2005
						1.9%	-0.81	3.06	1.40	-0.34	-0.28	
						3.6%	-0.71	2.79	1.13	-0.62	-0.55	
						3.6%	-0.77	2.79	1.13	-0.62	-0.55	
						3.8%	-1.36	2.76	1.10	-0.64	-0.58	
						1.5%	-1.48	3.16	1.50	-0.24	-0.18	
PBDE 207	9.00	5.01×10^5	2.45×10^7	Unknown	Field soils from different locations	3.6%	-0.29	2.83	1.15	-0.64	-0.57	Sellström *et al*., 2005
						3.6%	-0.43	2.83	1.15	-0.64	-0.57	
						3.8%	-1.42	2.81	1.12	-0.66	-0.60	
PBDE 209	9.50	9.12×10^5	6.24×10^7	Unknown	Field soils from different locations	1.9%	-0.64	3.36	1.53	-0.45	-0.38	Sellström *et al*., 2005
						1.9%	-0.81	3.35	1.51	-0.47	-0.39	
						1.9%	-0.90	3.35	1.51	-0.47	-0.39	
						3.3%	-0.64	3.11	1.28	-0.70	-0.62	
						3.6%	-0.87	3.07	1.24	-0.74	-0.66	
						3.6%	-0.85	3.07	1.24	-0.74	-0.66	
						3.8%	-1.40	3.05	1.22	-0.77	-0.69	
						1.2%	-1.03	3.54	1.70	-0.28	-0.20	
						1.5%	-1.56	3.45	1.62	-0.36	-0.29	
PCB 22	5.72	9.87×10^3	5.41×10^4	*Lubricus rubellus*	Ochten field soils	2.9%	-0.19	1.40	0.66	0.18	0.16	Hendriks *et al*., 1995
PCB 52	6.10	1.56×10^4	1.10×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.46	1.58	0.73	0.10	0.09	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.19	1.32	0.47	-0.15	-0.16	
PCB 70/76	6.28	1.93×10^4	1.54×10^5	*Lubricus rubellus*	Gelderse Poort field soils	5.2%	-1.12	1.41	0.51	-0.19	-0.20	Hendriks *et al*., 1995
PCB 84/92	6.60	2.83×10^4	2.79×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.31	1.82	0.83	0.00	0.00	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.73	1.56	0.57	-0.26	-0.25	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
PCB 87	6.50	2.51×10^4	2.32×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.31	1.77	0.81	0.02	0.02	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.08	1.52	0.55	-0.24	-0.24	
PCB 95/66	5.80	1.09×10^4	6.28×10^4	*Lubricus rubellus*	Ochten field soils	2.9%	-0.66	1.44	0.67	0.16	0.15	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.24	1.18	0.42	-0.09	-0.11	
PCB 97	6.77	3.47×10^4	3.83×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.23	1.90	0.86	-0.04	-0.03	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.98	1.65	0.60	-0.29	-0.28	
PCB 99/113	6.60	2.83×10^4	2.79×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.46	1.82	0.83	0.00	0.00	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.07	1.56	0.57	-0.26	-0.25	
PCB 101	6.40	2.23×10^4	1.92×10^5	*Eisenia andrei*	Field-contaminated soil	11.6%	-0.32	1.12	0.19	-0.56	-0.56	Belfroid *et al*., 1995
				Several species	Field soils - Sweden – IR[a]	2.7%	0.64	1.75	0.81	0.07	0.07	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	0.74	1.99	0.90	-0.05	-0.04	
					Field soils - Sweden - I2[a]	3.1%	0.58	1.69	0.75	0.01	0.00	
					Field soils - Sweden – PR[a]	1.5%	0.66	2.01	1.07	0.32	0.32	
					Field soils - Sweden - PR1[a]	1.6%	0.62	1.97	1.04	0.29	0.29	
					Field soils - Sweden - PR2[a]	1.6%	0.62	1.97	1.04	0.29	0.29	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.54	1.89	0.95	0.21	0.21	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.94	1.85	0.92	0.17	0.17	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.73	1.90	0.97	0.22	0.22	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.77	1.88	0.94	0.19	0.19	
					Field soils - Sweden – BR[a]	3.3%	0.71	1.67	0.73	-0.02	-0.02	
					Field soils - Sweden – BS[a]	2.5%	0.14	1.79	0.85	0.11	0.11	
					Field soils - Sweden – HR[a]	1.0%	0.69	2.17	1.23	0.48	0.48	
					Field soils - Sweden – Hsed[a]	1.5%	0.35	2.01	1.07	0.32	0.32	
PCB 101/90	6.40	2.23×10^4	1.92×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.52	1.72	0.79	0.04	0.04	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.00	1.47	0.53	-0.22	-0.22	
PCB 107/108/144/135	6.94	4.25×10^4	5.27×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.37	1.98	0.89	-0.07	-0.06	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.02	1.73	0.63	-0.33	-0.32	
PCB 110	6.30	1.98×10^4	1.60×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.72	1.68	0.77	0.06	0.06	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.15	1.42	0.51	-0.19	-0.20	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Eisenia andrei	Field-contaminated soil - Esch 4[a]	8.5%	-0.16	1.21	0.30	-0.41	-0.41	Jager, 2003; van der Wal *et al*., 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4[a]	8.5%	-0.28	1.21	0.30	-0.41	-0.41	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3[a]	6.6%	-0.36	1.32	0.41	-0.29	-0.30	
				Several species	Field soils - Sweden – IR[a]	2.7%	0.70	1.70	0.80	0.09	0.08	Matscheko *et al.*, 2002b
					Field soils - Sweden - I1[a]	2.8%	0.87	1.69	0.79	0.08	0.07	
					Field soils - Sweden - I2[a]	3.1%	0.64	1.64	0.73	0.03	0.02	
					Field soils - Sweden – PR[a]	1.5%	0.75	1.96	1.05	0.34	0.34	
					Field soils - Sweden - PR1[a]	1.6%	0.62	1.93	1.02	0.31	0.31	
					Field soils - Sweden - PR2[a]	1.6%	0.50	1.93	1.02	0.31	0.31	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.54	1.84	0.94	0.23	0.22	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.90	1.81	0.90	0.19	0.19	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.79	1.86	0.95	0.24	0.24	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.83	1.83	0.92	0.22	0.21	
					Field soils - Sweden – BR[a]	3.3%	0.75	1.62	0.71	0.00	0.00	
					Field soils - Sweden – BS[a]	2.5%	-0.16	1.74	0.84	0.13	0.12	
					Field soils - Sweden – HR[a]	1.0%	0.81	2.12	1.21	0.50	0.50	
					Field soils - Sweden – Hsed[a]	1.5%	0.35	1.96	1.05	0.34	0.34	
PCB 111	6.92	4.15×10^4	5.07×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	0.07	1.97	0.89	-0.07	-0.06	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.61	1.72	0.63	-0.32	-0.31	
PCB 118	6.40	2.23×10^4	1.92×10^5	*Eisenia andrei*	Field-contaminated soil	11.6%	-0.17	1.12	0.19	-0.56	-0.56	Belfroid *et al*., 1995

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Lubricus rubellus	Ochten field soils	2.9%	-0.58	1.72	0.79	0.04	0.04	Hendriks *et al*., 1995
				Several species	Field soils - Sweden – IR[a]	2.7%	0.27	1.75	0.81	0.07	0.07	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	0.26	1.74	0.80	0.06	0.06	
					Field soils - Sweden - I2[a]	3.1%	0.21	1.69	0.75	0.01	0.00	
					Field soils - Sweden – PR[a]	1.5%	0.53	2.01	1.07	0.32	0.32	
					Field soils - Sweden - PR1[a]	1.6%	0.50	1.97	1.04	0.29	0.29	
					Field soils - Sweden - PR2[a]	1.6%	0.50	1.97	1.04	0.29	0.29	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.41	1.89	0.95	0.21	0.21	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.68	1.85	0.92	0.17	0.17	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.73	1.90	0.97	0.22	0.22	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.77	1.88	0.94	0.19	0.19	
					Field soils - Sweden – BR[a]	3.3%	0.62	1.67	0.73	-0.02	-0.02	
					Field soils - Sweden – BS[a]	2.5%	-0.21	1.79	0.85	0.11	0.11	
					Field soils - Sweden – HR[a]	1.0%	0.51	2.17	1.23	0.48	0.48	
					Field soils - Sweden – Hsed[a]	1.5%	0.05	2.01	1.07	0.32	0.32	
PCB 123/147	6.93	4.20×10^4	5.17×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.32	1.98	0.89	-0.07	-0.06	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.88	1.72	0.63	-0.33	-0.31	
PCB 126	6.95	4.31×10^4	5.36×10^5	Several species	Field soils - Sweden – IR[a]	2.7%	0.10	2.01	0.92	-0.05	-0.04	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	0.26	2.00	0.91	-0.06	-0.04	
					Field soils - Sweden - I2[a]	3.1%	0.21	1.95	0.86	-0.11	-0.10	
					Field soils - Sweden – PR[a]	1.5%	0.53	2.27	1.18	0.21	0.22	
					Field soils - Sweden - PR1[a]	1.6%	0.32	2.24	1.14	0.18	0.19	
					Field soils - Sweden - PR2[a]	1.6%	0.50	2.24	1.14	0.18	0.19	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.24	2.15	1.06	0.09	0.10	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.20	2.12	1.02	0.06	0.07	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.25	2.17	1.07	0.11	0.12	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.40	2.14	1.05	0.08	0.09	
					Field soils - Sweden – BR[a]	3.3%	0.01	1.93	0.83	-0.13	-0.12	
					Field soils - Sweden – BS[a]	2.5%	-0.21	2.05	0.96	-0.01	0.00	
					Field soils - Sweden – HR[a]	1.0%	-0.01	2.43	1.34	0.37	0.38	
					Field soils - Sweden – Hsed[a]	1.5%	-0.17	2.27	1.18	0.21	0.22	
PCB 132/105	7.24	6.09×10^4	9.21×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.56	2.13	0.95	-0.13	-0.12	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.00	1.87	0.69	-0.39	-0.37	
PCB 138	6.70	3.19×10^4	3.37×10^5	*Eisenia andrei*	Field-contaminated soil	11.6%	-0.29	1.27	0.24	-0.62	-0.62	Belfroid *et al*., 1995
				Eisenia andrei	Field-contaminated soil - Esch 4	8.5%	-0.17	1.40	0.38	-0.49	-0.49	Jager, 2003; van der Wal *et al*., 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4	8.5%	-0.18	1.40	0.38	-0.49	-0.48	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3	6.6%	-0.41	1.51	0.49	-0.38	-0.37	
				Several species	Field soils - Sweden – IR[a]	2.7%	0.50	1.89	0.87	0.00	0.01	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	0.74	1.88	0.86	0.00	0.00	
					Field soils - Sweden - I2[a]	3.1%	0.69	1.83	0.81	-0.06	-0.05	
					Field soils - Sweden – PR[a]	1.5%	0.75	2.15	1.13	0.26	0.27	
					Field soils - Sweden - PR1[a]	1.6%	0.62	2.12	1.10	0.23	0.24	
					Field soils - Sweden - PR2[a]	1.6%	0.62	2.12	1.10	0.23	0.24	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.41	2.03	1.01	0.15	0.15	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.50	2.00	0.97	0.11	0.11	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.43	2.05	1.02	0.16	0.16	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.53	2.02	1.00	0.13	0.14	
					Field soils - Sweden – BR[a]	3.3%	0.41	1.81	0.79	-0.08	-0.07	
					Field soils - Sweden – BS[a]	2.5%	-0.16	1.93	0.91	0.05	0.05	
					Field soils - Sweden – HR[a]	1.0%	0.21	2.31	1.29	0.42	0.43	
					Field soils - Sweden – Hsed[a]	1.5%	0.53	2.15	1.13	0.26	0.27	
PCB 138/163/164	6.70	3.19×10^4	3.37×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.59	1.87	0.84	-0.02	-0.02	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.95	1.61	0.59	-0.28	-0.27	
PCB 141	7.33	6.79×10^4	1.09×10^6	*Lubricus rubellus*	Ochten field soils	2.9%	-0.24	2.17	0.96	-0.15	-0.13	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.08	1.91	0.71	-0.41	-0.39	
PCB 146	7.36	7.03×10^4	1.15×10^6	*Lubricus rubellus*	Ochten field soils	2.9%	-0.39	2.18	0.97	-0.16	-0.14	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.70	1.93	0.71	-0.41	-0.39	
PCB 148	7.29	6.47×10^4	1.01×10^6	*Lubricus rubellus*	Ochten field soils	2.9%	-0.27	2.15	0.96	-0.14	-0.12	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.66	1.90	0.70	-0.40	-0.38	
PCB 149	7.21	5.88×10^4	8.71×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.31	2.11	0.94	-0.13	-0.11	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.63	1.86	0.69	-0.38	-0.37	
				Eisenia andrei	Field-contaminated soil - Esch 4[a]	8.5%	0.10	1.64	0.47	-0.60	-0.58	Jager, 2003; van der Wal *et al*., 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4[a]	8.5%	0.17	1.64	0.47	-0.59	-0.58	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3[a]	6.6%	0.01	1.76	0.59	-0.48	-0.47	
				Several species	Field soils - Sweden – IR[a]	2.7%	0.80	2.14	0.97	-0.10	-0.08	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	1.04	2.13	0.96	-0.11	-0.09	
					Field soils - Sweden - I2[a]	3.1%	0.97	2.08	0.91	-0.16	-0.14	
					Field soils - Sweden – PR[a]	1.5%	0.90	2.40	1.23	0.16	0.17	
					Field soils - Sweden - PR1[a]	1.6%	0.80	2.36	1.19	0.12	0.14	
					Field soils - Sweden - PR2[a]	1.6%	0.80	2.36	1.19	0.12	0.14	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.64	2.28	1.11	0.04	0.06	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.90	2.24	1.07	0.00	0.02	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.65	2.29	1.12	0.05	0.07	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.92	2.27	1.10	0.03	0.04	
					Field soils - Sweden – BR[a]	3.3%	0.56	2.06	0.88	-0.18	-0.17	
					Field soils - Sweden – BS[a]	2.5%	0.31	2.18	1.01	-0.06	-0.04	
					Field soils - Sweden – HR[a]	1.0%	0.51	2.56	1.38	0.32	0.33	
					Field soils - Sweden – Hsed[a]	1.5%	0.66	2.40	1.23	0.16	0.17	
PCB 151	7.16	5.54×10^4	7.94×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	-0.41	2.09	0.93	-0.12	-0.10	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.17	1.83	0.68	-0.37	-0.36	
PCB 153	6.90	4.06×10^4	4.89×10^5	*Eisenia andrei*	Field-contaminated soil	11.6%	-0.20	1.36	0.28	-0.67	-0.66	Belfroid *et al*., 1995
				Lubricus rubellus	Ochten field soils	2.9%	-0.71	1.96	0.88	-0.06	-0.05	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.19	1.71	0.63	-0.32	-0.31	
				Eisenia andrei	Artificial soil	6.1%	0.67	1.64	0.56	-0.39	-0.38	Jager *et al*., 2003
				Eisenia andrei	Field-contaminated soil - Esch 4[a]	8.5%	-0.08	1.49	0.41	-0.53	-0.52	Jager, 2003; van der Wal *et al*., 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4[a]	8.5%	0.07	1.50	0.42	-0.53	-0.52	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3[a]	6.6%	0.76	1.61	0.53	-0.42	-0.41	
				Several species	Field soils - Sweden – IR[a]	2.7%	0.27	1.99	0.91	-0.04	-0.03	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	0.49	1.98	0.90	-0.05	-0.04	
					Field soils - Sweden - I2[a]	3.1%	0.43	1.93	0.85	-0.10	-0.09	
					Field soils - Sweden – PR[a]	1.5%	0.75	2.25	1.17	0.22	0.23	
					Field soils - Sweden - PR1[a]	1.6%	0.62	2.21	1.13	0.19	0.20	
					Field soils - Sweden - PR2[a]	1.6%	0.62	2.21	1.13	0.19	0.20	
					Field soils - Sweden – LR[a] - Spring	2.0%	0.41	2.13	1.05	0.10	0.11	
					Field soils - Sweden – LS[a] - Spring	2.1%	0.68	2.09	1.01	0.07	0.08	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
					Field soils - Sweden – LR[a] - Autumn	1.9%	0.43	2.14	1.06	0.12	0.13	
					Field soils - Sweden – LS[a] - Autumn	2.0%	0.70	2.12	1.04	0.09	0.10	
					Field soils - Sweden – BR[a]	3.3%	0.41	1.91	0.83	-0.12	-0.11	
					Field soils - Sweden – BS[a]	2.5%	-0.16	2.03	0.95	0.00	0.01	
					Field soils - Sweden – HR[a]	1.0%	0.21	2.41	1.33	0.38	0.39	
					Field soils - Sweden – Hsed[a]	1.5%	0.35	2.25	1.17	0.22	0.23	
PCB 156	7.60	9.38×10^{4}	1.80×10^{6}	*Eisenia andrei*	Field-contaminated soil	11.6%	-0.20	1.70	0.41	-0.81	-0.78	Belfroid *et al*., 1995
PCB 167	7.68	1.03×10^{5}	2.09×10^{6}	*Eisenia andrei*	Field-contaminated soil	11.6%	-0.29	1.74	0.43	-0.83	-0.80	Belfroid *et al*., 1995
PCB 169	7.50	8.32×10^{4}	1.50×10^{6}	Several species	Field soils - Sweden – IR[a]	2.7%	-0.03	2.28	1.02	-0.16	-0.14	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	-0.21	2.27	1.01	-0.17	-0.15	
					Field soils - Sweden - I2[a]	3.1%	-0.26	2.22	0.96	-0.22	-0.20	
					Field soils - Sweden – PR[a]	1.5%	0.05	2.54	1.28	0.10	0.12	
					Field soils - Sweden - PR1[a]	1.6%	0.02	2.50	1.25	0.06	0.09	
					Field soils - Sweden - PR2[a]	1.6%	0.02	2.50	1.25	0.06	0.09	
					Field soils - Sweden – LR[a] - Spring	2.0%	-0.11	2.42	1.16	-0.02	0.00	
					Field soils - Sweden – LS[a] - Spring	2.1%	-0.10	2.38	1.13	-0.06	-0.03	
					Field soils - Sweden – LR[a] - Autumn	1.9%	-0.05	2.43	1.18	-0.01	0.02	
					Field soils - Sweden – LS[a] - Autumn	2.0%	-0.17	2.41	1.15	-0.03	-0.01	
					Field soils - Sweden – BR[a]	3.3%	-0.29	2.19	0.94	-0.25	-0.22	
					Field soils - Sweden – BS[a]	2.5%	-0.39	2.32	1.06	-0.12	-0.10	
					Field soils - Sweden – HR[a]	1.0%	-0.19	2.69	1.44	0.26	0.28	
					Field soils - Sweden – Hsed[a]	1.5%	-0.17	2.54	1.28	0.10	0.12	
PCB 170/190	7.08	5.03×10^{4}	6.84×10^{5}	*Lubricus rubellus*	Ochten field soils	2.9%	-0.45	2.05	0.92	-0.10	-0.09	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-1.07	1.79	0.66	-0.36	-0.34	
PCB 174	7.77	1.15×10^{5}	2.48×10^{6}	*Lubricus rubellus*	Ochten field soils	2.9%	-0.42	2.38	1.05	-0.24	-0.21	Hendriks *et al*., 1995

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
					Gelderse Poort field soils	5.2%	-1.02	2.13	0.79	-0.50	-0.47	
PCB 177	7.79	1.18×10^5	2.57×10^6	*Lubricus rubellus*	Ochten field soils	2.9%	-0.27	2.39	1.05	-0.25	-0.22	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.85	2.14	0.80	-0.50	-0.47	
PCB 179	7.45	7.83×10^4	1.36×10^6	*Lubricus rubellus*	Gelderse Poort field soils	5.2%	-0.84	1.97	0.73	-0.43	-0.41	Hendriks *et al*., 1995
				Eisenia andrei	Field-contaminated soil - Esch 4[a]	8.5%	-0.13	1.76	0.52	-0.65	-0.62	Jager, 2003; van der Wal *et al*., 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4	8.5%	-0.21	1.76	0.52	-0.64	-0.62	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3	6.6%	0.00	1.87	0.63	-0.53	-0.51	
PCB 180	7.20	5.81×10^4	8.55×10^5	*Eisenia andrei*	Field-contaminated soil	11.6%	-0.32	1.51	0.34	-0.73	-0.71	Belfroid *et al*., 1995
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4	8.5%	0.17	1.64	0.47	-0.59	-0.58	Jager, 2003; van der Wal *et al*., 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3	6.6%	-0.24	1.75	0.58	-0.48	-0.46	
				Eisenia andrei	Field-contaminated soil - Esch 4	8.5%	-0.10	1.64	0.47	-0.59	-0.58	
PCB 182/187	7.17	5.60×10^4	8.09×10^5	*Lubricus rubellus*	Ochten field soils	2.9%	0.05	2.09	0.93	-0.12	-0.10	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.29	1.84	0.68	-0.37	-0.36	
PCB 192/172	7.94	1.41×10^5	3.40×10^6	*Lubricus rubellus*	Gelderse Poort field soils	5.2%	-0.83	2.21	0.82	-0.53	-0.50	Hendriks *et al*., 1995
PCB 193	7.92	1.38×10^5	3.27×10^6	*Lubricus rubellus*	Gelderse Poort field soils	5.2%	-0.35	2.20	0.82	-0.53	-0.50	Hendriks *et al*., 1995
PCB201	8.35	2.30×10^5	7.30×10^6	*Lubricus rubellus*	Ochten field soils	2.9%	-0.42	2.66	1.16	-0.36	-0.32	Hendriks *et al*., 1995
					Gelderse Poort field soils	5.2%	-0.62	2.40	0.90	-0.62	-0.57	
Pentachlorobenzene	5.18	5.17×10^3	1.98×10^4	*Eisenia andrei*	Artificial soil	5.8%	0.19	0.84	0.25	-0.01	-0.04	Belfroid *et al*., 1994
				Eisenia andrei	Field-contaminated soil	11.6%	-1.39	0.54	-0.05	-0.31	-0.34	Belfroid *et al*., 1995

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Lumbricus terrestris	OECD standard soil	5.8%	-0.66	0.80	0.23	-0.05	-0.06	Beyer, 1996
				Lubricus rubellus	Gelderse Poort field soils	5.2%	-1.31	0.88	0.30	0.04	0.01	Hendriks *et al*., 1995
				Enchytraeus crypticus	OECD standard soil	5.8%	1.53	0.80	0.23	-0.05	-0.06	van der Wal *et al*., 2004b
1,2,3,7,8-Pentachloro dibenzofuran	6.92	4.15E+04	5.07E+05	Several species	Field soils - Sweden – IR[a]	2.7%	-0.30	2.00	0.91	-0.04	-0.03	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	-0.37	1.99	0.90	-0.05	-0.04	
					Field soils - Sweden - I2[a]	3.1%	-0.42	1.94	0.85	-0.10	-0.09	
					Field soils - Sweden – PR[a]	1.5%	-0.10	2.26	1.17	0.22	0.23	
					Field soils - Sweden - PR1[a]	1.6%	-0.13	2.22	1.14	0.18	0.19	
					Field soils - Sweden - PR2[a]	1.6%	-0.20	2.22	1.14	0.18	0.19	
2,3,4,7,8-Pentachloro dibenzofuran	6.92	4.15×10^{4}	5.07×10^{5}	Several species	Field soils - Sweden – IR[a]	2.7%	-0.30	2.00	0.91	-0.04	-0.03	Matscheko *et al*., 2002b
					Field soils - Sweden - I1[a]	2.8%	-0.43	1.99	0.90	-0.05	-0.04	
					Field soils - Sweden - I2[a]	3.1%	-0.49	1.94	0.85	-0.10	-0.09	
					Field soils - Sweden – PR[a]	1.5%	-0.10	2.26	1.17	0.22	0.23	
					Field soils - Sweden - PR1[a]	1.6%	-0.13	2.22	1.14	0.18	0.19	
					Field soils - Sweden - PR2[a]	1.6%	-0.28	2.22	1.14	0.18	0.19	
					Field soils - Sweden - Hsed	1.5%	-0.83	2.26	1.17	0.22	0.23	
Pentachlorophenol	5.24	5.56×10^{3}	2.21×10^{4}	*Eisenia fetida*	Uncontaminated natural soil - agricultural	0.8%	-0.16	1.74	1.14	0.85	0.82	Hu *et al*., 2005
					Uncontaminated natural soil - forest soil	2.6%	-0.04	1.21	0.61	0.32	0.29	
		125[b]	125[b]	*Eisenia fetida andrei*	Agricultural field soil - Holten soil	3.5%	0.61	1.28	1.28	0.39	0.96	van Gestel and Ma, 1988
				Lubricus rubellus	Agricultural field soil - Holten soil	3.5%	0.98	1.28	1.28	0.39	0.96	
		120[b]	120[b]	*Eisenia fetida andrei*	Agricultural field soil - Kooyenburg soil	2.1%	0.80	1.29	1.29	0.41	0.98	
				Lubricus rubellus	Agricultural field soil - Kooyenburg soil	2.1%	0.68	1.29	1.29	0.41	0.98	
Phenanthrene	4.57	2.49×10^{3}	6.33×10^{3}	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.44	1.34	0.93	0.91	0.87	Allard *et al*., 2005
				Eisenia andrei	Artificial soil	5.9%	0.28	0.54	0.13	0.11	0.07	Jager *et al*., 2000

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	0.75	0.35	0.33	0.28	Matscheko *et al.*, 2002a
Pyrene	5.18	5.17×10^{3}	1.98×10^{4}	*Enchytraeus crypticus*	Creosote-contaminated soil mixed with sand	0.9%	-1.15	1.63	1.05	0.79	0.76	Allard *et al.*, 2005
				Eisenia andrei	Artificial soil	5.9%	0.01	0.83	0.25	-0.02	-0.05	Jager *et al.*, 2000
				Eisenia fetida	Contaminated soil from gas works site	3.6%	-2.49	1.04	0.46	0.20	0.17	Matscheko *et al.*, 2002a
Sodium pentachlorophenate	5.24	5.56×10^{3}	2.21×10^{4}	*Allolobophora caliginosa*	OECD standard soil	5.8%	0.96	0.87	0.27	-0.02	-0.05	Haque and Ebing, 1988
				Allolobophora caliginosa	OECD standard soil	5.8%	1.16	0.87	0.27	-0.02	-0.05	
				Allolobophora caliginosa	Spiked natural soil	1.2%	0.86	1.56	0.96	0.68	0.65	
				Lumbricus terrestris	Spiked natural soil	1.2%	1.40	1.56	0.96	0.68	0.65	
Telodrin	5.20	5.30×10^{3}	2.05×10^{4}	*Eisenia andrei*	Field-contaminated soil - Esch 4[a]	8.5%	0.45	0.68	0.09	-0.18	-0.21	Jager, 2003; van der Wal *et al.*, 2004a
				Aporrectodea caliginosa	Field-contaminated soil - Esch 4[a]	8.5%	0.17	0.68	0.09	-0.18	-0.21	
				Aporrectodea caliginosa	Field-contaminated soil - Esch 3[a]	6.6%	0.20	0.79	0.20	-0.07	-0.10	
Tetrachlorobenzene	4.60	2.58×10	6.70×10^{3}	*Eisenia andrei*	Artificial soil	6.1%	0.29	0.54	0.12	0.09	0.05	Jager *et al.*, 2003
1,2,3,4-Tetrachloro benzene	4.64	2.71×10^{3}	7.22×10^{3}	*Eisenia andrei*	Artificial soil	5.8%	0.02	0.58	0.15	0.10	0.06	Belfroid *et al.*, 1994
				Eisenia andrei	Field-contaminated soil	11.6%	-1.17	0.28	-0.15	-0.20	-0.24	Belfroid *et al.*, 1995
				Lumbricus terrestris	OECD standard soil	5.8%	-0.99	0.54	0.14	0.07	0.05	Beyer, 1996
				Enchytraeus crypticus	OECD standard soil	5.8%	1.66	0.54	0.14	0.07	0.05	van der Wal *et al.*, 2004b
1,2,3,5-Tetrachloro benzene	4.68	2.84×10^{3}	7.78×10^{3}	*Lumbricus terrestris*	OECD standard soil	5.8%	-1.03	0.56	0.15	0.06	0.04	Beyer, 1996
				Lubricus terrestris	Natural soil	1.5%	0.58	1.18	0.75	0.68	0.64	Lord *et al.*, 1980
1,2,4,5-Tetrachloro	4.50	2.29E+03	5.56E+03	*Lumbricus*	OECD standard soil	5.8%	-0.98	0.48	0.11	0.10	0.07	Beyer, 1996

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
benzene				*terrestris*								
2,3,7,8-Tetrachloro dibenzo-*p*-dioxin	6.80	3.60×10^{4}	4.06×10^{5}	Unknown		2.0%[d]	-0.16	2.03	0.98	0.07	0.08	Sample *et al*., 1998
				Unknown		2.0%[d]	-0.64	2.03	0.98	0.07	0.08	
				Unknown		2.0%[d]	-0.58	2.03	0.98	0.07	0.08	
				Unknown		2.0%[d]	-0.17	2.03	0.98	0.07	0.08	
				Aporrectodea caliginosa[e]		2.0%[d]	0.08	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.36	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.58	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.68	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.09	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.08	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.39	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.00	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	-0.04	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.30	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.59	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.31	2.08	1.02	0.12	0.13	
				Aporrectodea rosea[e]		2.0%[d]	0.32	2.08	1.02	0.12	0.13	
				Aporrectodea caliginosa[e]		2.0%[d]	0.35	2.08	1.02	0.12	0.13	
				Aporrectodea rosea[e]		2.0%[d]	0.88	2.08	1.02	0.12	0.13	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
2,3,7,8-Tetrachloro dibenzofuran	6.53	2.60×10^{4}	2.45×10^{5}	Several species	Field soils - Sweden – IR[a]	2.7%	-0.36	1.81	0.84	0.04	0.04	Matscheko *et al.*, 2002b
					Field soils - Sweden - I1[a]	2.8%	-0.43	1.80	0.83	0.03	0.03	
					Field soils - Sweden - I2[a]	3.1%	-0.49	1.75	0.78	-0.02	-0.02	
					Field soils - Sweden – PR[a]	1.5%	-0.10	2.07	1.10	0.30	0.30	
					Field soils - Sweden - PR1[a]	1.6%	-0.13	2.04	1.06	0.26	0.27	
					Field soils - Sweden - PR2[a]	1.6%	-0.13	2.04	1.06	0.26	0.27	
					Field soils - Sweden – LR[a] Spring	2.0%	-0.11	1.95	0.98	0.18	0.18	
					Field soils - Sweden – LS[a] - Spring	2.1%	-0.02	1.92	0.94	0.14	0.15	
					Field soils - Sweden – LR[a] - Autumn	1.9%	-0.01	1.97	0.99	0.19	0.19	
					Field soils - Sweden – BR[a]	3.3%	-0.25	1.73	0.75	-0.04	-0.04	
					Field soils - Sweden – BS[a]	2.8%	-0.52	1.79	0.82	0.02	0.02	
					Field soils - Sweden – HR[a]	1.0%	-0.49	2.23	1.26	0.46	0.46	
					Field soils - Sweden – Hsed[a]	1.5%	-0.67	2.07	1.10	0.30	0.30	
2,3,4,5-Tetrachloro phenol	4.50	95[b]	95[b]	*Eisenia fetida andrei*	Agricultural field soil - Holten soil	3.5%	-0.32	0.66	0.66	0.28	0.62	van Gestel and Ma, 1988
				Lubricus rubellus	Agricultural field soil - Holten soil	3.5%	0.44	0.66	0.66	0.28	0.62	
		85[b]	85[b]	*Eisenia fetida andrei*	Agricultural field soil - Kooyenburg soil	2.1%	-0.23	0.70	0.70	0.33	0.66	
				Lubricus rubellus	Agricultural field soil - Kooyenburg soil	2.1%	0.69	0.70	0.70	0.33	0.66	
1,2,3-Trichlorobenzene	4.10	1.42E+03	2.64E+03	*Lumbricus terrestris*	OECD standard soil	5.8%	-0.85	0.30	0.05	0.19	0.16	Beyer, 1996
1,2,4-Trichloro benzene	4.10	1.42E+03	2.64E+03	*Lumbricus terrestris*	OECD standard soil	5.8%	-0.93	0.30	0.05	0.19	0.16	Beyer, 1996
1,3,5-Trichlorobenzene	4.20	1.60E+03	3.18E+03	*Lumbricus terrestris*	OECD standard soil	5.8%	-0.94	0.34	0.06	0.17	0.14	Beyer, 1996
2,4,5-Trichlorophenol	3.90	78[b]	78[b]	*Eisenia fetida andrei*	Agricultural field soil - Holten oils	3.5%	-0.32	0.14	0.14	0.18	0.33	van Gestel and Ma, 1988
				Lubricus rubellus	Agricultural field soil - Holten oils	3.5%	1.00	0.14	0.14	0.18	0.33	
		43[b]	43[b]	*Eisenia fetida andrei*	Agricultural field soil - Kooyenburg soil	2.1%	0.25	0.40	0.40	0.44	0.59	

Substance[c]	Log K_{ow}	Predicted K_{oc} (l/kg)		Species	Field or laboratory data	Soil organic carbon content	Exprmntl/ field log BAF (kg/kg wet wt.)	Predicted log BAF				Reference
								TGD method		Corrected TGD method		
		I	II					I	II	I	II	
				Lubricus rubellus	Agricultural field soil - Kooyenburg soil	2.1%	0.47	0.40	0.40	0.44	0.59	

I – Calculation using the TGD default QSAR for K_{oc}.

II – Calculation using the TGD QSAR for predominantly hydrophobic chemicals.

a) The abbreviations used relate to the different soil types in the original paper. The same designations have been used here for ease of reference.

b) These values are soil-water partition coefficients (Kp values in units of l/kg) measured in the soils tested. Strictly speaking. the TGD default QSAR and the QSAR for predominantly hydrophobic chemicals are not applicable to the estimation of the K_{oc} value for phenols and so the Kp values measured by van Gestel and Ma (1988) for the soils tested have been used in this analysis.

c) Polychlorinated biphenyls (PCBs) and polybrominated diphenyl ethers (PBDEs) are identified here by the IUPAC congener numbering system. Other names are as they appear in the original papers. No attempt has been made to verify the identities of the chemicals studied.

d) No data available. The TGD default organic carbon content of two per cent was assumed.

e) The exact species is unclear. The paper gives the species only as *A. caliginosa* and *A. rosea.*

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