DEVELOPMENT AND EVALUATION OF A TERRESTRIAL FOOD WEB BIOACCUMULATION MODEL

by

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ABSTRACT

Under the 1999 Canadian Environmental Protection Act (CEPA 1999), all chemicals listed on the Domestic Substances List (DSL) must be assessed in order to determine whether or not the substance is toxic, as defined in the Act. Chemicals are initially screened in terms of their persistence (P), bioaccumulative potential (B) and inherent toxicity (iT). The main purpose of this research project was to develop and evaluate a terrestrial food web bioaccumulation model to assess the validity of the CEPA bioaccumulation (B) screening criteria, which were derived solely from studies of aquatic organisms.

A steady-state bioaccumulation model was developed to predict chemical concentrations in soil-invertebrates and higher trophic level predators based on observed soil concentrations, site-specific soil properties, physical and physiological characteristics of modelled organisms and the physico-chemical properties of the modelled substances. The model was evaluated through comparisons of observed and predicted biota-soil accumulation factors (BSAFs) and biomagnification factors (BMFs) and through the use of Monte Carlo simulations to assess the sensitivity of model output to variation in key input parameters.

The model was then used to predict biomagnification factors (BMFs) as a function of the octanol-water partition coefficient (K_{OW}) and the octanol-air partition coefficient (K_{OA}). In contrast to the current bioaccumulation screening criteria, which

only classify substances with log K_{OW} values > 5 as bioaccumulative, all chemicals with a log K_{OW} > 2 and < 12 and log K_{OA} > 5 were found to have the potential to bioaccumulate in a terrestrial food web. These results indicate that the current bioaccumulation screening criteria are not appropriate for terrestrial organisms and should be re-evaluated as soon as possible.

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GLOSSARY

Bioaccumulation – the process of chemical uptake by all possible pathways (e.g. respiratory, dietary, dermal) which reflects the total exposure to chemicals in the surrounding environment

Bioaccumulation factor (BAF) – the ratio of the chemical concentration in the organism to the chemical concentration freely dissolved in water. BAFs can be expressed in terms of wet weight concentrations or lipid-normalized/lipid equivalent concentrations

Bioaccumulative (B) – any substance which exceeds the CEPA screening criterion for bioaccumulation (BAF, BCF or log K_{OW}) reflecting the tendency of a chemical to reach concentrations in organisms far in excess of concentrations in the ambient environment

Bioavailability – the fraction of the total chemical concentration in a particular environmental medium that is available for uptake into an organism across the respiratory surface or gastrointestinal tract

Bioconcentration – the process of chemical uptake across the respiratory surface (e.g. gills) which reflects the partitioning of chemicals between biota and water

Bioconcentration factor (BCF) – the ratio of the chemical concentration in the organism to the chemical concentration freely dissolved in water. BCFs can be expressed in terms of wet weight concentrations or lipid-normalized/lipid equivalent concentrations

Biomagnification – the process of chemical uptake from the gastrointestinal tract into an organism resulting from exposure to chemicals in the diet

Biomagnification factor (BMF) – the ration of the chemical concentration in the organism to the chemical concentration in the diet of the organism. BMFs can be expressed in terms of wet-weight concentrations but are much more informative if expressed in terms of lipid-normalized or lipid equivalent concentrations. A lipid-equivalent BMF greater than 1 indicates that the substance is bioaccumulative (B)

Biota-soil accumulation factor (BSAF) – the ratio of the chemical concentration in an organism to the chemical concentration in the soil. BSAFs can be expressed using the wet weight concentrations in the organism and dry weight concentrations in the soil or as a ratio of the lipid-normalized / lipid equivalent concentrations

Biotransformation – processes within an organism that result in changes to the molecular structure of a given compound. Typically, the compound is altered to become more polar which facilitates elimination

Distal consumer – an organism which feeds on proximate consumers

Equilibrium partitioning theory (EPT) – the theory which states that the lipid equivalent concentrations in any two environmental media (e.g. biota and soil) will be equal

Hazard Index (H) – a measure of the hazard (potential harm) faced by an organism due to exposure to chemicals in the environment. The Hazard Index is the ratio of the daily exposure ($mg_{chemical}\ kg^{-1}_{organism}\ day^{-1}$) to a daily exposure threshold related to some toxicological endpoint, typically the No Adverse Effects Level (NOAEL)

Inherent toxicity (iT) – any substance which exceeds the CEPA screening criterion for human or non-human toxicity

Lipid-equivalent concentration (Lipid EQ) – the wet weight concentration (ug / kg wet weight) divided by the lipid equivalent content of the organism (lipid, NLOM) resulting in concencentrations expressed in terms of μg / kg lipid equivalent. This measure is a surrogate for fugacity

Lipid-normalized concentration – the wet weight concentration (ug / kg wet weight) divided by the lipid content of the organism resulting in concencentrations expressed in terms of μg / kg lipid

Persistent (P) – any substance which exceeds the CEPA screening criterion for the degradation half-life ($t_{1/2}$) in any one environmental medium (air, water, soil, sediment)

Steady-state (SS) – the situation when the total uptake or influx of chemicals into a system exactly equals the total elimination or outflux of chemicals from the system

LIST OF ABBREVIATIONS AND ACRONYMS

B - Bioaccumulative

BAF – Bioaccumulation factor

BCF – Bioconcentration factor

BMF – Biomagnification factor

BSAF – Biota-Soil Accumulation factor

CEPA – Canadian Environmental Protection Act

DEFRA – Department for Environment, Food and Rural Affairs

DSL – Domestic Substances List

EC50 – Effects Concentration (50^{th} percentile)

EPT – Equilibrium partitioning theory

IRIS – Integrated Risk Information System

iT – Inherent toxicity

K_{AS} – Air-soil partition coefficient

K_{BF} – Biota-feces partition coefficient

K_{BM} – Biota-milk partition coefficient

K_{BU} – Biota-urine partition coefficient

K_{OA} – Octanol-air partition coefficient

K_{OW} – Octanol-water partition coefficient

K_{SW} – Soil-water partition coefficient

LC50 – Lethal Concentration (50^{th} percentile)

LOAEL – Lowest observed adverse effects level

LTS – List of Toxic Substances

NOAEL - No observed adverse effects level

P - Persistent

RfD – Reference Dose

SS – Steady-state

TSCA – Toxic Substances Control Act

TSMP – Toxic Substance Management Plan

US EPA – United States Environmental Protection Agency

X_{NLOM} – Non-lipid organic matter-octanol proportionality constant

X_{OC} – Organic carbon-octanol proportionality constant

1.0 INTRODUCTION

Modern societies are highly dependent on the production and use of chemical compounds. For example, there are over 75,000 chemicals on the US EPA Toxic Substances Control Act (TSCA) Inventory of Substances (www.epa.gov, 2004) and 24,000 on the Domestic Substances List (DSL) in Canada (www.ec.gc.ca/ CEPARegistry, 2004). Legislators have recognized the need to identify substances with the greatest potential to cause harm in order to enact appropriate regulations regarding the use and disposal of these substances. In Canada, the government has declared that by 2006, all substances on the DSL must be evaluated in order to determine the risk they present to human health and the environment. The details of this process are discussed below.

1.1 Categorization Process for Substances on the DSL

Under the 1999 Canadian Environmental Protection Act (CEPA 1999), the Minister of the Environment and the Minister of Health are required to categorize (Section 73) and if necessary, conduct screening assessments (Section 74) of all chemicals listed on the Domestic Substances List (DSL) to determine whether these substances are "toxic" or capable of becoming "toxic" as defined in the Act. According to CEPA 1999, a substance is toxic if it is entering or may enter the environment in a quantity or concentration or under conditions that; (a) have or may have an immediate or long-term harmful effect on the environment or its biological diversity; (b) constitute or may constitute a danger to the environment on which life depends; or (c) constitute or

may constitute a danger in Canada to human life or health. Substances which are definitively assessed to be "CEPA toxic" are added to the CEPA Schedule 1 List of Toxic Substances (LTS) and become subject to some form of regulation.

Chemicals are initially categorized in terms of their persistence (P), bioaccumulative potential (B), and inherent toxicity (iT). The criteria for defining persistence and bioaccumulative potential under CEPA 1999 are the same as those developed under the 1995 Toxic Substances Management Policy (TSMP 1995). These criteria were developed by the *ad hoc* Science Group based on available empirical data, computer modelling, expert opinion and group consensus (Environment Canada, 1995). The adopted critical values for persistence and bioaccumulation are presented below. iT criteria for non-human organisms were formalized only recently by Environment Canada (Environment Canada, 2003).

1.1.1 Persistence

The critical values for persistence are based on transformation rates and are expressed in terms of half-life ($t_{1/2}$), which refers to the amount of time required for 50% of the chemical to be degraded in one of four environmental media (see Table 1.1). The data used to derive the critical values did not consider movement between media (advective transport) or dilution. A chemical is considered persistent if the critical value in any medium is exceeded.

Table 1-1 Critical values for Persistence in the Environment

Medium	Critical value for half-life
Air	>= 2 days*
Water	>= 6 months
Soil	>= 6 months
Sediment	>= 1 year
* or evidence of atmospheric transport to remote regions such as the Arctic	

1.1.2 Bioaccumulative Potential

Bioaccumulation refers to the uptake of contaminants by organisms resulting in chemical concentrations in biota being greater than those found in the surrounding environment. The potential for a substance to bioaccumulate is related to the relative rates of uptake (e.g. dietary, passive diffusion across respiratory surfaces) and depuration (e.g. biotransformation, fecal elimination). The *ad hoc* Science Group chose to express bioaccumulative potential in terms of bioaccumulation factor (BAF), bioconcentration factor (BCF) and the octanol-water partition coefficient (K_{OW}), and derived the critical values primarily from studies on freshwater fish (Environment Canada, 1995). The BAF, a field measurement that incorporates both dietary and diffusive uptake as well as bioavailability, is the preferred value for screening purposes but unfortunately has not been measured for the majority of substances on the DSL. As a result, critical values for BCF and K_{OW} were also developed since these measurements, particularly K_{OW}, are far more readily available. It is stressed that BAFs and BCFs as defined under the CEPA categorization scheme refer to aquatic systems only.

Table 1-2 Critical Values for Bioaccumulative Potential

Measurement	Critical Value
BAF (L / kg) or BCF (L / kg) and/or log K_{OW}	>= 5000* >= 5000* >= 5
* wet weight, whole body basis	

1.1.3 Inherent Toxicity

Criteria for inherent toxicity for humans are still being developed by Health Canada. Proposed iT critical values for non-humans are an external median lethal concentration$_{50}$ (LC_{50}) or effects concentration$_{50}$ (EC_{50}) of 1 mg / L or less for acute toxicity and a no-effects concentration of < 0.1 mg / L for chronic toxicity (Environment Canada, 2003). The chronic toxicity critical value will be applied preferentially for chemicals where reliable data exists. It should again be noted that the iT critical values apply only to biota in aquatic systems.

Under the DSL categorization scheme, if a substance is classified as inherently toxic (to humans or non-humans) and persistent or bioaccumulative, a more thorough screening level risk assessment must be conducted. According to Environment Canada, screening level risk assessments, "involve a more in-depth analysis of a substance to determine whether the substance is toxic or capable of becoming toxic as defined in CEPA 1999. This determination of toxic consists of integrating the assessment of known or potential exposure of a substance with known or potential adverse effects on the environment" (Environment Canada). The possible outcomes of the screening level risk

assessment include taking no action (for substances not deemed CEPA Toxic), adding the substance to the Priority Substances List (PSL) for further review or adding the substance to the LTS. A summary of the overall categorization strategy for substances on the DSL is presented below.

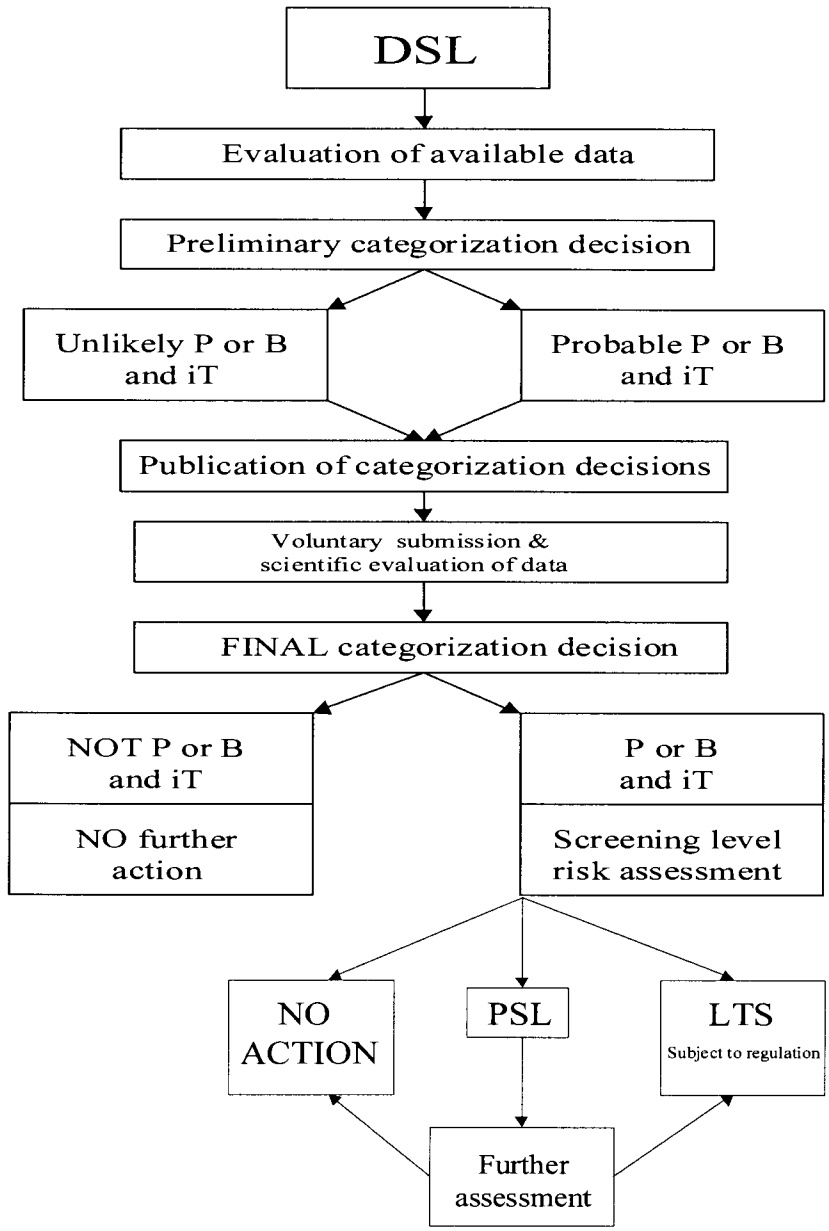


Figure 1-1 Overall DSL Categorization Scheme

The ability of the overall DSL categorization scheme to correctly assess substances on the DSL is of great concern due to the potential environmental, economic and social implications of mismanagement. The fundamental question is whether or not the established criteria for P and B (and iT when determined) as well as the procedures for the screening level risk assessments will lead to appropriate decisions. Given the current categorization scheme, undesirable outcomes could result from the following situations:

1) Insufficiently stringent or incorrect screening criteria and screening level assessment procedures

2) Overly stringent screening criteria and screening level assessment procedures (triggering unnecessary regulation and compliance costs)

3) Inappropriate physico-chemical properties used to describe the behaviour of chemicals in the environment

4) Incorrect data for the physico-chemical properties or degradation rates used to describe the behaviour of chemicals in the environment

Situation 1 could conceivably lead to undesirable biological impacts (human, non-human) and associated economic and social consequences while situation 2 could lead to negative economic and social impacts related to reduced competitiveness in the global marketplace. In the case of situation 3 and 4, both outcomes are possible. Accordingly, appropriate initial screening criteria are critical to the entire categorization and assessment process.

1.2 Rationale of the Research Project

The purpose of this research project is to investigate the appropriateness of one component of screening criteria, namely the critical values for assessing bioaccumulative potential (B). The most striking fact about the development of the screening criteria for

bioaccumulation is the preponderant reliance on data from aquatic organisms. Since the TSMP was intended to, "ensure the protection of the environment and human health" (Environment Canada, 1995), the reliance on data from studies of aquatic species should be of concern. Although the TSMP acknowledges that evidence of bioaccumulation in terrestrial organisms is relevant to the policy, no measures are in place to address the overwhelming number of chemicals for which empirical data in terrestrial species is completely absent.

The appropriateness of the bioaccumulation criteria for aquatic species is not at issue. Critical values were based on analyses of a significant amount of empirical data, the vast majority of which provide solid information on the potential for bioaccumulation to occur in these systems. The real question is whether or not bioaccumulation criteria derived from analyses of data from aquatic systems can be extrapolated to terrestrial organisms. If there are reasons why critical values derived from freshwater fish studies should be considered protective of all other organisms for all chemicals, they are not discussed in text of the TSMP, the TSMP Persistence and Bioaccumulation Criteria document (Environment Canada, 1995) or CEPA 1999. Theoretically, the only reasons why critical values derived from aquatic species would be protective of all other organisms are if;

1) Key pathways and relative rates of uptake and depuration in other organisms mimic those in aquatic species

2) Uptake pathways in other organisms are sufficiently limited compared to aquatic species while depuration is relatively similar

3) Depuration processes are sufficiently enhanced in other organisms compared to aquatic species while uptake is relatively similar

Unless at least one of these conditions is met, there is no defensible rationale for assuming that the adopted bioaccumulation critical values are appropriate for all other species.

There are several reasons to suspect that in fact, none of these conditions will be met. First, terrestrial organisms typically have greater digestive efficiencies than aquatic species. Given that digestive efficiency is an important determinant of the rate of chemical uptake from the diet, it is likely that terrestrial organisms have relatively greater dietary uptake rates than aquatic species. Another key physiological difference between aquatic and terrestrial organisms is that respiratory exchange in terrestrial organisms does not occur in a purely aqueous environment. Respiratory exchange in an aqueous environment can be modelled solely as a function of the octanol-water partition coefficient (K_{OW}). For terrestrial organisms, respiratory exchange may be accurately represented and modelled as a function of the octanol-air partition coefficient (K_{OA}). Thus, elimination of chemical across the respiratory surface in aquatic species can not automatically be assumed to characterize the same process in terrestrial organisms. The implications of this fundamental difference are not accounted for by the current bioaccumulation criteria. Finally, many aquatic species have indeterminant growth whereas most terrestrial organisms do not. Given that growth often has an important influence on chemical concentrations in organisms, this difference could also be important.

The goal of this project is to develop a model of the bioaccumulation of organic chemicals in terrestrial food-webs which relates contaminant levels in soils to concentrations in representative soil invertebrates and higher trophic level predators. The

model is similar to mechanistic models of bioaccumulation successfully developed for aquatic organisms (Gobas FAPC, 1993, Morrison HA et al., 1996, Mackay D & Fraser A, 2000) but is modified to characterize uptake and elimination processes in terrestrial organisms. The model will be used to investigate biomagnification factors (BMFs) in a terrestrial food-chain in relation to physico-chemical properties such as K_{OW} and K_{OA}. The results of the model will then be used to suggest appropriate screening criteria to assess the inherent bioaccumulative potential of chemicals on the DSL, with respect to terrestrial organisms. The model will also be applied to investigate the effect of metabolism on bioaccumulative potential. Metabolism of parent compounds can potentially reduce BMFs to a significant degree. The model will be used to investigate the relative rate of metabolism required to counteract the inherent bioaccumulative potential of a substance based on it physico-chemical properties.

Mechanistic models of bioaccumulation can also be used for the purpose of conducting hazard assessments and establishing soil remediation targets. In combination with toxicological endpoints based on exposure (dose) or internal body burdens, the threshold concentration of chemical in the soil of a contaminated site which has the potential to cause harm can be estimated. To demonstrate the utility of the model in this respect, an illustrative hazard assessment is conducted.

2.0 THEORY

2.1 General

The objective of this study is to develop a terrestrial food-web bioaccumulation model which relates (i) chemical concentrations in soil to soil-dwelling organisms by estimating a biota-soil accumulation factor (BSAF) and (ii) concentrations in soil-invertebrate (SI) prey items to those in proximate consumers by estimating biomagnification factors (BMF). The bioaccumulation model can also be used to estimate concentrations in distal consumers using both BSAFs and BMFs. Biota-soil accumulation factors are defined as:

$$BSAF = C_{SI} / C_{SOIL} \quad \text{(dry kg / wet kg)} \quad [1]$$

where C_{SI} is the concentration in soil-dwelling organisms (ug / kg wet weight) and C_{SOIL} is the concentration in the soil (ug / kg dry soil). Biomagnification factors are defined as:

$$BMF = C_{BIOTA} / C_{DIET} \quad [2]$$

where C_{BIOTA} is the concentration in the organism of interest (ug / kg wet weight) and C_{DIET} is the concentration in the diet of that organism's diet (ug / kg wet weight). Concentrations in soil invertebrates (C_{SI} in ug / kg wet weight) are estimated as:

$$C_{SI} = C_{SOIL} * BSAF_{SI} \quad [3]$$

Concentrations in proximate consumers (C_{PC} in ug / kg wet weight) are estimated as:

$$C_{PC} = C_{SI} * BMF_{PC} \quad [4]$$
$$= C_{SOIL} * BSAF_{SI} * BMF_{PC}$$

Concentrations in distal consumers (C_{DC} in ug / kg wet weight) are estimated as:

$$C_{DC} = C_{PC} * BMF_{DC} \quad [5]$$
$$= C_{SOIL} * BSAF_{SI} * BMF_{PC} * BMF_{DC}$$

For a proximate consumer with multiple prey items, concentrations can be estimated as

$$C_{PC} = [\Sigma (P_{SI(i)} * C_{SI(i)})] * BMF_{PC} \quad [6]$$
$$= [\underset{\text{For } i=1 \text{ to } n}{\Sigma} (P_{SI(i)} * BSAF_{SI(i)} * C_{SOIL})] * BMF_{PC}$$

where n is the number of prey items and $P_{SI(i)}$ is the proportion of the diet (%) that each prey item(i) represents. Similarly, concentrations in distal consumers feeding on multiple prey items can be estimated as

$$C_{DC} = [\underset{\text{For } i=1 \text{ to } n}{\Sigma} P_{PC(i)} * C_{PC(i)}] * BMF_{DC} \quad [7]$$

where n is the number of prey items and $P_{PC(i)}$ is the proportion of the diet (%) that each prey item(i) represents. The overall food-chain model is represented conceptually in Figure 2.1

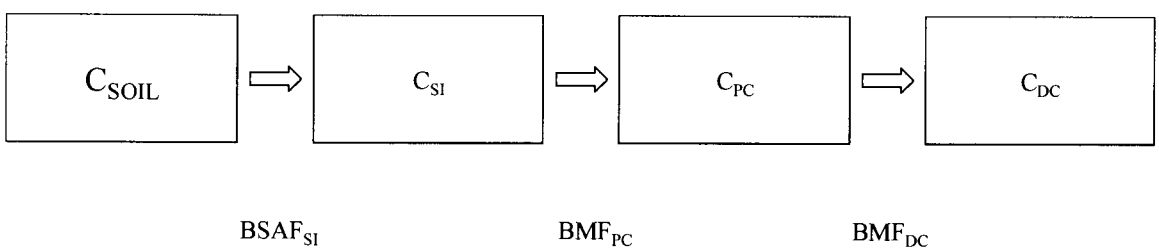


Figure 2-1 – Conceptual Representation of a Terrestrial Food-chain Model

Each component of the model requires input parameters that can be obtained from either measured values (e.g. soil organic matter content) or values estimated from literature sources or submodels (e.g. feeding rate). The performance of the model is then evaluated

by comparing model-predictions to observations from an appropriate field study. The process of parameterizing and evaluating the model are discussed in Chapter 3.0.

2.2 Soil-to-Soil Invertebrate Bioaccumulation Model

Two different soil-to-soil invertebrate bioaccumulation models were developed and compared for this study. The first model is based on an application of equilibrium partitioning theory (EPT). This approach was selected because of its simplicity and the small number of required inputs. Equilibrium partitioning theory assumes that the octanol-equivalent chemical concentrations of phases in contact will be equal, given an appropriate amount of equilibration time. The process of partitioning between soil and biota is dependent on an intermediary partitioning process from soil into interstitial water which is then followed by uptake into biota (Connell DW & Markwell RD, 1990, Belfroid AC et al., 1996). A soil-biota system is represented conceptually in Figure 2.2.

Figure 2-2 – Conceptual Representation of a Soil-Biota System

Partitioning of chemicals between water and biota can be estimated by the bioconcentration factor (BCF) which is defined as:

$$\begin{aligned} BCF &= C_{SI} / C_W \text{ (L / kg wet weight)} \\ &= (F_L + F_{NLOM} * X_{NLOM}) * K_{OW} \end{aligned} \qquad [8]$$

where C_W is the freely dissolved concentration of chemical in water (ug / m^3), F_L is the lipid content of the organism (%), F_{NLOM} is the non-lipid organic matter (NLOM) content of the organism (%,) X_{NLOM} is the proportionality constant relating the sorptive capacity of NLOM to that of octanol and K_{OW} is the octanol-water partition coefficient. Partitioning of chemical between soil and water can be estimated by the soil-water partition coefficient (K_{SW}) defined as:

$$K_{SW} = C_{SOIL} / C_W \text{ (L / kg dry soil)} = (F_{OC} * X_{OC}) * K_{OW} \quad [9]$$

where F_{OC} is the organic carbon (OC) content of the soil (%) and X_{OC} is the proportionality constant relating the sorptive capacity of OC to that of octanol. Based on these equations, BSAFs can be estimated as follows:

$$BSAF = \frac{C_{SI}}{C_{SOIL}} \text{ (kg dry / kg wet)} \quad [10]$$

$$= \frac{C_{SI} / C_W}{C_{SOIL}/C_W}$$

$$= \frac{BCF}{K_{SW}}$$

$$= \frac{(F_L + F_{NLOM}*X_{NLOM})}{F_{OC} * X_{OC}}$$

The EPT soil-to-soil invertebrate bioaccumulation model implicitly includes the following assumptions;

1) Contaminants are 100% bioavailable to soil invertebrates

2) Other pathways of elimination (e.g. growth, metabolism) are insignificant

Model performance may be affected negatively if any (or all) of these assumptions are violated.

Although the EPT approach is attractive due to its simplicity and broad applicability, bioaccumulation studies of benthic invertebrates have demonstrated that EPT can be unreliable, particularly in field studies (Lake JL et al.,1990, Landrum PF et al., 1992, Parkerton TF, 1993). Therefore, a more detailed steady-state (SS) model incorporating dietary uptake and other elimination pathways was developed. The equations used to characterize uptake and elimination pathways were based on bioaccumulation models for aquatic organisms presented in Gobas FAPC (1993) and Morrison HA et al (1996). The overall model is represented conceptually in Figure 2.3.

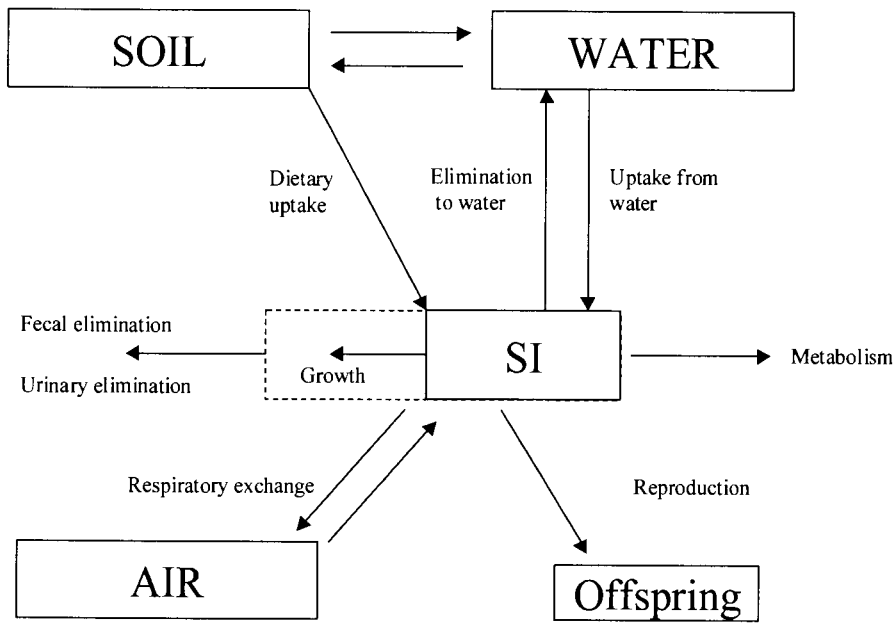


Figure 2-3 – Steady-state Bioaccumulation Model for Soil Invertebrates

Soil invertebrates can accumulate chemicals via uptake from the air, interstitial water and ingested soil and eliminate chemical directly back to the air and interstitial

water and also via fecal elimination, urinary elimination, reproduction (transfer of chemical to offspring) and metabolism. Growth, which results in the dilution of chemical concentrations, is also included as a pseudo-elimination pathway. Uptake of chemicals from air, water and ingested soil is represented by first-order rate constants multiplied by the concentration in air, water and soil respectively (ug / m^3) while elimination pathways are represented by the sum of first-order elimination rate constants and the concentration in the soil invertebrate (ug / m^3). Thus, the change in the chemical concentration in a soil invertebrate over time can be represented as:

$$dC_{SI} / dt = k_{UA}*C_{AIR} + k_{UW}*C_W + k_{UD}*C_{DIET} - (k_{EA} + k_{EW} + k_{FE} + k_{UE} + k_{GD} + k_{MT} + k_{RD}) * C_{SI} \quad [11]$$

where k_{UA} is the rate constant characterizing uptake from air (day^{-1}), k_{UW} is the rate constant characterizing uptake from interstitial water (day^{-1}), k_{UD} is the rate constant characterizing uptake from ingested soil (day^{-1}) and k_{EA}, k_{EW}, k_{FE}, k_{UE}, k_{GD}, k_{MT}, and k_{RD} are the rate constants (day^{-1}) characterizing elimination to air, interstitial water, fecal elimination, urinary elimination, growth dilution, metabolism and reproduction respectively. Observed C_{SOIL} was converted from ug / kg dry soil to ug / m^3 dry soil and C_{AIR} (ug / m^3) was then estimated from C_{SOIL} assuming equilibrium partitioning as:

$$C_{AIR} = K_{AS} * C_{SOIL} \quad [12]$$

where K_{AS} is the partition coefficient describing the distribution of chemical into air and soil. K_{AS} is estimated as:

$$K_{AS} = C_{AIR} / C_{SOIL} \quad [13]$$

$$= 1 / (F_{OC}*X_{OC}*K_{OA})$$

where K_{OA} is the octanol-air partition coefficient.

C_W, which is the freely dissolved concentration in interstitial water (ug / m^3), is also estimated from C_{SOIL} assuming equilibrium partitioning as:

$$C_W = C_{SOIL} / K_{SW} \quad [14]$$

Assuming that the organism has reached steady state (i.e. $dC_{SI} / dt = 0$), equation 11 can be used to estimated C_{SI} (ug / m^3) as:

$$C_{SI} = \frac{[k_{UA}*C_{AIR} + k_{UW}*C_W + k_{UD}*C_{DIET}]}{[k_{EA} + k_{EW} + k_{FE} + k_{UE} + k_{GD} + k_{MT} + k_{RD}]} \quad [15]$$

BSAFs can then be estimated by dividing the predicted C_{SI} by the observed soil concentration C_{SOIL}.

Uptake

Uptake from air results from passive diffusion across the respiratory surface. The rate constant for uptake from air (k_{UA}, day^{-1}) can be defined as:

$$k_{UA} = (E_A * G_A) / V_{SI} \quad [16]$$

where E_A is the efficiency of chemical uptake from air (%), G_A is the volume of air respired (m^3 / day) and V_{SI} is the volume of the organism (m^3).

Uptake from water also results from passive diffusion across the respiratory surface. The rate constant for uptake from interstitial water (k_{UW}, day^{-1}) can be defined as:

$$k_{UW} = (E_W * G_W) / V_{SI} \quad [17]$$

where E_W is the efficiency of chemical uptake from water (%), G_W is the amount of water turned over by the organisms (m^3 / day) and V_{SI} is the volume of the organism (m^3).

Dietary uptake results from chemical solubilizing in the gastrointestinal tract and then moving across the gut wall. The rate constant for chemical uptake from ingested food (k_{UD}, day^{-1}) can be defined as:

$$k_{UD} = (E_D * G_D) / V_{SI} \quad [18]$$

where E_D is the efficiency of chemical uptake from the diet (%) and G_D is the amount of food ingested by the organism (m^3 / day).

Elimination

The rate constant for elimination to air (k_{EA}) is defined as:

$$k_{EA} = (E_A * G_A) / (V_{SI} * K_{BA}) \quad [19]$$

where K_{BA} is the partition coefficient describing the distribution of chemical between the organism and the air. K_{BA} is estimated as:

$$K_{BA} = (F_L + F_{NLOM}*X_{NLOM})* K_{OA} + F_W/K_{AW} \quad [20]$$

where K_{AW} is the dimensionless Henry's Law constant, otherwise known as the air-water partition coefficient.

The rate constant for elimination to interstitial water (k_{EW}, day^{-1}) is defined as:

$$k_{EW} = k_{UW} / BCF \quad [21]$$

This process reflects the process of chemical diffusing back across in the respiratory surface.

The rate constant for fecal elimination (k_{FE}, day^{-1}) can be defined as:

$$k_{FE} = (G_F * E_D)/ (V_{SI} * K_{BF}) \quad [22]$$

where G_F is the amount of fecal matter excreted (m^3 / day) and K_{BF} is the partition coefficient describing the distribution of chemical between the organism (C_{SI}) and its fecal matter (C_F). K_{BF} can be interpreted as the ratio of sorptive capacities of the organism and its fecal matter. Digestion of lipids and organic matter in the gut tends to reduce the sorptive capacity of the ingested material and contributes to the uptake of chemical into the organism. For soil-invertebrates, K_{BF} can be defined as:

$$K_{BF} = C_{SI} / C_F \quad [23]$$

$$= \frac{(F_L + F_{NLOM}*X_{NLOM}) + F_W/K_{OW}}{F_{OC\text{-}F}*X_{OC}}$$

where F_L, F_{NLOM} and F_W represent the reported lipid, non-lipid organic matter and water content of the organism (%) respectively and $F_{OC\text{-}F}$ represents the organic carbon of the fecal matter (%). The fraction of organic carbon in fecal matter is calculated as a function of the pre-digestion organic matter fraction and the organic matter assimilation efficiency (A_{OM}) as follows:

$$F_{OC\text{-}F} = \frac{0.58 * [G_D * F_{OM} * (1 - A_{OM})]}{G_F} \quad [24]$$

where F_{OM} is the reported fraction of organic matter in the ingested soil and 0.58 represents the proportion of the organic matter composed of organic carbon (MACKAY Fugacity textbook). G_F is calculated as:

$$G_F = G_D - G_D * F_{OM} * A_{OM} \quad [25]$$

The rate constant for urinary elimination (k_{UE}, day^{-1}) can be defined as:

$$k_{UE} = G_U / (V_{SI} * K_{BU}) \quad [26]$$

where G_U is the amount of urine excreted (m^3 / day) and K_{BU} is the partition coefficient describing the partitioning of chemical between the organism (C_{SI}) and its urine (C_U).

K_{BU} is defined as:

$$K_{BU} = C_{SI} / C_U = (F_L + F_{NLOM} * X_{NLOM}) * K_{OW} + F_W \quad [27]$$

The rate constant for growth dilution (k_{GD}, day^{-1}) is estimated using the growth rate of the organism. This rate constant accounts for the change in volume and associated decrease in concentration even though the volume of the organism (V_{SI}) remains constant in the model.

The rate constant for metabolism (k_{MT}, day^{-1}) is estimated as the fraction of chemical in biota that is biotransformed to a metabolite. Accumulation of metabolites is not considered in this model because metabolites are not typically reported.

The rate constant for reproduction (k_{RD}, day^{-1}) is estimated as the fraction of chemical in the biota that is eliminated during the production of offspring.

The steady-state bioaccumulation model includes the following major assumptions;

1) Steady-state conditions have been reached (i.e. $dC_{SI}/dt = 0$)

2) Concentrations in interstitial water are at a chemical equilibrium with the soil and with the organism

3) The fraction of lipid, NLOM and water remains constant over time

2.3 Terrestrial Organism Bioaccumulation Model

Uptake and elimination pathways for terrestrial organisms are represented conceptually in Figure 2.4.

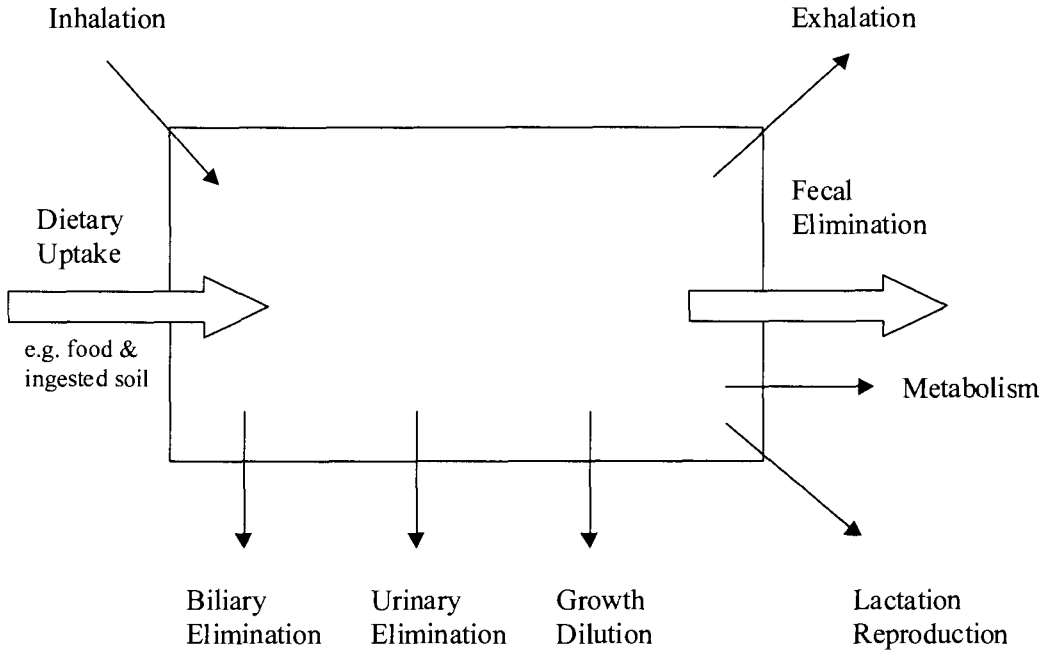


Figure 2-4 – Steady-state Terrestrial Bioaccumulation Model

For terrestrial organisms the two major routes of uptake are inhalation and dietary uptake. When developing models for aquatic organisms, uptake via respiration can be modelled as a function of K_{OW} since exchange occurs in a purely aqueous environment. This approach is obviously not valid for pulmonates (air-breathing organisms) so instead,

respiratory exchange is modelled as a function of the octanol-air partition coefficient (K_{OA}).

Dietary uptake is viewed as being mainly controlled by the degree to which net chemical exchange in the gastrointestinal tract favours movement of chemical into the organism over movement into the gut. Since partitioning of chemical between biota and feces (K_{BF}) is largely dependent on the digestive capability of the organism (i.e. the degree to which dietary lipids and NLOM [including organic carbon] are assimilated), the efficiency of digestion is expected to be an important determinant of the steady-state chemical concentration in the animal. The relative efficiency of the various elimination pathways in terrestrial organisms is also an extremely important determinant of bioaccumulation.

The change in concentration in biota (C_B, ug / m^3) over time can be expressed as a product of a 1st-order uptake rate constant for each uptake and elimination pathway and the concentrations in the relevant phase. Since many terrestrial consumers ingest soil incidentally while feeding, uptake of chemicals from ingested soil was included in the model such that:

$$dC_B / dt = k_{UA}*C_{AIR} + k_{UD} * C_{DIET} + k_{US}*C_{SOIL} - (k_{EA} + k_{UE} + k_{FE} + k_{BE} + k_{LA} + k_{MT} + k_{GD} + k_{RD}) * C_B \quad [28]$$

where C_{AIR} is the concentration in ambient air (ug / m^3), C_{DIET} is the concentration in the diet (ug / m^3), C_{SOIL} is the concentration in soil (ug / m^3), k_{UA}, k_{UD} and k_{US} are the rate constants (day^{-1}) characterizing uptake from air, diet and ingested soil respectively, and k_{EA}, k_{UE}, k_{FE}, k_{BE}, k_{LA}, k_{MT}, k_{GD} and k_{RD} are the rate constants (day^{-1}) characterizing elimination via respiratory exchange, urination, defecation, biliary elimination, lactation,

metabolism of parent compound and pseudo-elimination via growth dilution and parturition/egg-laying respectively. C_{DIET} can be based on observations or output from the soil-to-soil invertebrate model.

Assuming steady state conditions ($dC_B / dt = 0$), equation 6 can then be rearranged to arrive at an estimate of C_B as:

$$C_B = \frac{k_{UA}*C_{AIR} + k_{UD} * C_{DIET} + k_{US}*C_{SOIL}}{(k_{EA} + k_{UE} + k_{FE} + k_{BE} + k_{LA} + k_{MT} + k_{GDR} + k_{RD})} \quad [29]$$

BMFs can then be calculated by dividing the predicted biota concentrations by observed or predicted concentrations in the diet.

Uptake

For pulmonates, exchange of chemical occurs across the respiratory surfaces in the lungs. The inhalation uptake rate constant (k_{UA}, day^{-1}) can be defined as:

$$k_{UA} = (E_A*G_A) / V_B \quad [30]$$

where E_A is the efficiency of chemical uptake from air (%), G_A is the amount of air respired (m^3 / day) and V_B is the volume of the organism (m^3).

The dietary uptake rate constant (k_{UD}, day^{-1}) is defined the same as for the soil invertebrate model such that:

$$k_{UD} = (E_D * G_D) / V_B \quad [31]$$

where E_D is the efficiency of chemical uptake from the diet (%) and G_D is the feeding rate (m^3 / day).

The ingested soil uptake rate constant (k_{US}, day^{-1}) can be defined as:

$$k_{US} = (E_S * G_S) / V_B \quad [32]$$

where E_S is the efficiency of chemical uptake from ingested soil (%) and G_S is the amount of soil ingested by the animal (m^3 / day).

Elimination

The respiratory elimination rate constant (k_{EA}, day^{-1}) can be defined as:

$$k_{EA} = (E_A * G_A) / (V_B * K_{BA}) \quad [33]$$

The urinary excretion rate constant (k_{UE}, day^{-1}) can be defined as:

$$k_{UE} = G_U / (V_B * K_{BU}) \quad [34]$$

where G_U is the urinary excretion rate (m^3 / day) and K_{BU} is the partition coefficient describing the partitioning of chemical between the organism and its urine. K_{BU} is defined as:

$$K_{BU} = (F_L + F_{NLOM} * X_{NLOM}) * K_{OW} + F_W \quad [35]$$

The fecal excretion rate constant (k_{FE}, day^{-1}) can be defined as:

$$k_{FE} = (G_F * E_D) / (V_B * K_{BF}) \quad [36]$$

where G_F is the fecal excretion rate (m^3 / day) and K_{BF} is the organism-to-feces partition coefficient. K_{BF} is defined as:

$$K_{BF} = \frac{[(F_L + F_{NLOM} * X_{NLOM}) + F_W/K_{OW}]}{[(F_{L\text{-}F} + F_{NLOM\text{-}F} * X_{NLOM} + F_{OC\text{-}F} * X_{OC}) + F_{W\text{-}F}/K_{OW}]} \quad [37]$$

where F_L, F_{NLOM}, F_W are the lipid content (%), NLOM content (%) and water content (%) of the biota respectively. $F_{L\text{-}F}$, $F_{NLOM\text{-}F}$ and $F_{W\text{-}F}$ are the lipid content, NLOM content and water content of the fecal matter and are based on the F_L, F_{NLOM} and F_W of the ingested diet and the ability of the animal to assimilate ingested material. The composition of the feces can be calculated as the post-digestion volume of substance (lipid, NLOM, OC or water) divided by the total post-digestion volume of material (G_F) such that:

$$F_{L\text{-}F} = [(1 - A_L) * F_{L\text{-}D}] / G_F \quad [38]$$

$$F_{NLOM\text{-}F} = [(1 - A_{NLOM}) * F_{NLOM\text{-}D}] / G_F \quad [39]$$

$$F_{OC\text{-}F} = [0.58 * (1 - A_{OM}) * F_{OM}] / G_F \quad [40]$$

$$F_{W\text{-}F} = [(1 - A_W) * F_{W\text{-}D}] / G_F \quad [41]$$

where $F_{L\text{-}D}$, $F_{NLOM\text{-}D}$, F_{OM} and $F_{W\text{-}D}$ are the lipid, NLOM, OM and water content (%) respectively of the diet and A_L, A_{NLOM}, A_{OM} and A_W are the absorption efficiencies (%) of lipid, NLOM, OC and water respectively. G_F can be calculated as:

$$G_F = G_D + G_S - (G_D*F_{L\text{-}D}*A_L + G_D*F_{NLOM\text{-}D}*A_{NLOM} + G_D*F_{W\text{-}D}*A_W) - (G_S*F_{OM}*A_{OM} + G_S*(1-F_{OM})*A_S) \quad [42]$$

where A_S is the absorption efficiency of inorganic soil.

The biliary elimination rate constant (k_{BE}, day^{-1}) can be defined as:

$$k_{BE} = G_B / (V_B*F_L*K_{OB}) \quad [43]$$

where G_B is the bile excretion rate (m^3 / day) and K_{OB} is the octanol-bile partition coefficient. K_{OB} is defined as:

$$K_{OB} = K_{OW}/\beta \quad [44]$$

where β represents the increase in solubility of chemicals in bile fluids compared to water.

The lactation rate constant (k_{LA}) can be defined as:

$$k_{LA} = G_M / (V_B * F_L * K_{BM}) \quad (day^{-1}) \quad [45]$$

where G_M is the lactation rate (m^3 / day) in female animals and K_{BM} is the octanol-milk partition coefficient. K_{BM} is defined as:

$$K_{BM} = \frac{(F_L + F_{NLOM} * X_{NLOM}) + F_W / K_{OW}}{(F_{L\text{-}M} + F_{NLOM\text{-}M} * X_{NLOM}) + F_{W\text{-}M}/K_{OW}} \quad [46]$$

where $F_{L\text{-}M}$, $F_{NLOM\text{-}M}$, and $F_{W\text{-}M}$ are the lipid, NLOM and water content (%) of the milk respectively. This elimination pathway is only relevant for nursing mammalian females.

The metabolic transformation rate constant k_{MT} (day^{-1}) represents the fraction of chemical that is biotransformed per day. Accumulation of metabolites is not considered in this model.

The growth dilution rate constant, k_{GD}, which represents the diluting effect of any increase in body mass over time, can be estimated as the proportional increase in mass per day. For adult animals, this rate constant is usually considered insignificant (Gobas FAPC et al., 2003).

Loss of chemical via maternal transfer to eggs or offspring *in utero* (k_{RD}) can also be considered a form of growth dilution and represents the proportion of maternal mass directed towards the development of embryonic tissues.

The proposed terrestrial organism bioaccumulation model implicitly includes the following major assumptions;

1) Chemicals have reached steady-state in the organism

2) Chemicals reach inter-tissue equilibrium (lipid-normalized concentrations)

3) Fluctuation in organism composition over time is insignificant

4) Composition of the diet remains stable over time

3.0 METHODS

The overall approach undertaken for this study involved the following steps. First, the bioaccumulation models described in the previous section were implemented in Excel spreadsheets. The performance of the models was then evaluated by comparing observed BSAFs or BMFs to predicted values. To accomplish this task, an appropriate field study was obtained from the scientific literature. The proposed bioaccumulation models were parameterized to match the site-specific characteristics of the soil and the organisms comprising the food web of the field study. Model performance was also evaluated by conducting Monte Carlo simulations of the model output. These simulations permitted an assessment of the sensitivity of model predictions to changes in input parameters. The models were then applied to; (i) investigate the bioaccumulative potential of chemical substances in terrestrial organisms (ii) estimate BMFs for other species and (iii) to conduct an illustrative hazard assessment of the study site for organisms inhabiting the area.

3.1 Selection of Field Site

A soil—earthworm (*Lumbricus rubellus*)—shrew (*Crocidura russula* and *Sorex araneus*) food-chain in the Netherlands was selected to evaluate model performance as this study contained the most complete and reliable data set that could be located in the literature (Hendriks AJ et al., 1995). Samples of soil, earthworms and shrews were collected from two flood plain areas, Ochten and Gelderse Poort, approximately 10km apart. This field study reported concentrations of both metabolizable and non-

metabolizable PCB congeners as well as other persistent organic contaminants such as DDT. Overall, the study was rigorous however it is important to note the following concerns with the data collected relative to the needs of this project. First, earthworms were purged of ingested soil prior to analysis in this study. While this fact does not affect the predictions of the soil-invertebrate models, the results of bioaccumulation models for terrestrial predators may be affected because measurements of the total concentration of the earthworm together with ingested soil are more reflective of actual diet of the consumer. The other concern with the data collected is that the age, sex and number of each shrew species sampled were not reported. Female animals of reproductive age often have substantially lower body burdens compared to adult males due to maternal transfer of contaminants to offpsring and elimination through lactation.

3.2 Model Parameterization

The models require the physico-chemical properties of modeled substances, the physical characteristics of the soil at each site and the physiological characterisitics of the organisms. Since the physical characteristics of the soil sampled at the Ochten and Gelderse Poort sites were significantly different, each site was modelled separately. The model was developed assuming that earthworms are the only major prey item for shrews. Although shrews are known to consume other prey items such as insects and molluscs (US EPA, 1993), given that earthworms often represent greater than 80% of the total biomass of soil invertebrates (Kreis B et al., 1987, Devliegher W & Verstraete W, 1997), it seems reasonable to assume that they form the majority of the shrew diet. To address the uncertainty associated with this assumption, the effect of changing the diet on predicted BMFs was investigated. It is also important to note that *Crocidura russula* and

Sorex araneus were considered sufficiently similar in physiological terms to be modelled as a single species.

3.2.1 Physico-chemical Properties

The octanol-water partition coefficient (K_{OW}) is a fundamental input for all of the proposed models. Values for K_{OW} were taken from the literature (Hawker DW & Connell DW, 1988) and were assumed to be independent of temperature (see Appendix A). The terrestrial bioaccumulation models also require values for the octanol-air partition coefficient (K_{OA}) and the dimensionless Henry's Law Constant (K_{AW}), otherwise known as the air-water partition coefficient.

Values for K_{OA} were estimated from the following empirical relationship taken from recent literature (Harner T & Macay D,1995, Harner T & Bidleman TF, 1996):

$$\log K_{OA} = \alpha_{OA} + \beta_{OA} / T \quad [47]$$

where T is the temperature (degrees Kelvin) and α_{OA} and β_{OA} are compound specific parameters derived from experiments (see Appendix A). The K_{OA} of chemicals for which values of α_{OA} and β_{OA} are unavailable can be estimated as:

$$K_{OA} = K_{OW} / K_{AW} \quad [48]$$

The air-water partition coefficient (K_{AW}) was calculated according to the following empirically derived equation (Bamford HA et al., 2002):

$$\ln K_{AW} = - H_H / RT + S_H/R \quad [49]$$

where H_H is the enthalpy of the phase change (kJ / mol), R is the gas law constant (kJ · mol^{-1} · K^{-1}), T is the temperature in Kelvin (K) and S_H is the entropy of the phase change (kJ · mol^{-1} · K^{-1}). Calculated values of K_{AW} for PCBs at 10°C, 25°C and 37°C as well as the reported values for H_H and S_H are presented in Appendix B. The terrestrial organism bioaccumulation model used values of K_{AW} at 37oC while the steady-state soil-invertebrate model used values of K_{AW} at 10oC.

K_{AW} can alternatively be estimated as the ratio of K_{OW} and K_{OA}. This method of estimation was also be used in the generic model developed to predict BMFs of hypothetical chemicals as a function of K_{OW} and K_{OA}. The affect of the temperature dependence of K_{OA} and K_{AW} values on predicted BMFs can be addressed by varying the ratio of K_{OA} at 10°C to K_{OA} at 37°C. The temperature dependence of 4 PCB congeners (3,96,118,180) is shown in Figure 3.1.

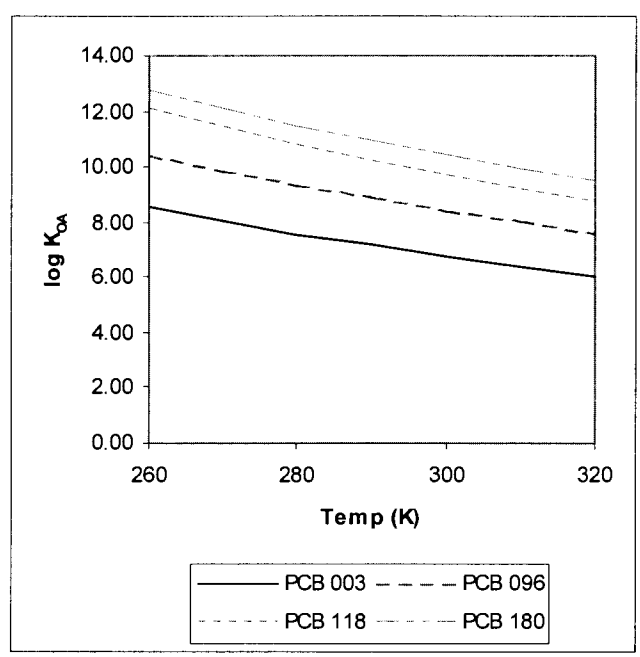


Figure 3-1 – Temperature Dependence of log K_{OA} for PCB3,96,118,180

The ratio of K_{OA} at 10°C to K_{OA} at 37°C of any substance is defined by α_{OA} and β_{OA}. For PCBs, this ratio varies from between approximately 10 to 30. Rather than define a range of α_{OA} and β_{OA} values to vary simultaneously, it is more practical to simply vary the ratio of K_{OA} at 10°C and 37°C to explore the affect of temperature dependence of K_{OA} (and K_{AW}) on model output. The range over which the ratio of K_{OA} at 10°C to K_{OA} at 37°C was varied is discussed in section 3.4.1 of this report.

3.2.2 Soil Properties

The model was parameterized to match the organic matter (%) and moisture content of soil reported in Hendriks AJ et al. (1995) for two sites in Rhine-Meuse Delta floodplains (Ochten and Gelderse-Poort). Organic carbon content (f_{OC}) was assumed to be 58% of the organic matter (Mackay D, 1993). The bulk density of the soil was assumed to be 1500 kg / m^3 (see Table 3-1).

Table 3-1– Mean Organic Matter Content (f_{OM}), Organic Carbon Content (f_{OC}), Moisture Content and Bulk Density of Soils in Ochten and Gelderse Poort

Parameter	Ochten		Gelderse-Poort	
	Mean	SD	Mean	SD
f_{OM}	0.05	Not Reported	0.09	Not Reported
f_{OC}	0.029	Not Reported	0.0522	Not Reported
Moisture (kg / kg)	0.81	0.07	0.73	0.03
Bulk density kg / m^3	1500		1500	

The value for the octanol-OC proportionality constant (X_{OC}) was set at 0.35 (Seth R et al., 1999).

3.2.3 Soil Invertebrates

The EPT soil-to-soil invertebrate bioaccumulation model requires only the lipid and NLOM fraction of the organism and the organic carbon content of the soil. The steady-state bioaccumulation model requires many more input parameters. Estimates for these parameters were based on reported values from the literature or based on the output of submodels (e.g. allometric relationships). The basic physical characteristics of the earthworm to be modeled are presented first followed by an explanation of the parameterization process for each rate constant in the model.

3.2.3.1 Basic Physical Characteristics

The volume of the organism (V_{SI}) was calculated based the average mass (g) reported in growth studies (Lowe CN & Butt KR, 2002, Elvira C & Mato JDS, 1996) and assuming a density of 1000 kg / m^3 (Mackay D, 1993). Lee KE (1986) reported that earthworm populations often have a much larger proportion of subadults compared to adults. Therefore, model simulations were conducted for hatchlings, subadults and adults to reflect this observation and also explore the influence of initial volume on model output. The average lipid content of earthworms collected at each field site was used for the models. Water content was assumed to be 80% and NLOM content was calculated as $1 - F_L - F_W$. These values were assumed to be constant across life stage (i.e. the same for hatchlings, subadults and adults). The value for the octanol-NLOM proportionality constant (X_{NLOM}) was set at 0.035. This value is based on an empirical study which

suggested that the fugacity capacity of lipids is approximately 30 times greater than the fugacity capacity of NLOM (Gobas FAPC et al., 1999). Input parameters for Ochten and Gelderse Poort are summarized in Table 3.3 and 3.4 respectively.

3.2.3.2 Uptake from Air

The rate constant for uptake from water (k_{UA}) requires values for the chemical uptake efficiency from water (E_A) and the volume of air respired per day (G_A). E_A was assumed to be 0.7 for all chemicals (Kelly BC & Gobas FAPC, 2003). G_A was estimated based on a study of respiration of earthworms (*Lumbricus terrestris*) in natural soil (Binet F et al., 1998) and set to 1.2E-06 m^3 / g earthworm

3.2.3.3 Uptake from Water

The rate constant for uptake from water (k_{UW}) requires values for the chemical uptake efficiency from water (E_W) and the rate of water turnover per day (G_W). E_W was estimated as a function of K_{OW} based on empirical studies of bioconcentration that investigated the diffusion of chemicals across the respiratory surface of fish (Gobas FAPC & Mackay D, 1987). Use of this relationship implicitly assumes that diffusion of chemical across the respiratory surface of the worm (i.e. outer skin) is comparable to diffusion across gill membranes. This assumption seems reasonable because the outer skin of the earthworm is moist and highly vascularized (Lee KE, 1986). Based on this assumption, E_W can be estimated as:

$$E_W = 1 / (1.85+(155/K_{ow})) \quad [50]$$

Estimating the rate of water turnover (G_W) for earthworms was challenging. For aquatic species, G_W represents the volume of water gill ventilated by the organism in order to meet oxygen demand. Typically, G_W is estimated using allometric equations for oxygen demand and the dissolved oxygen content of the surrounding water. This approach is not appropriate for earthworms because oxygen demand for these organisms is met via passive diffusion from air and water. However, according to Lee KE (1986), earthworms lose substantial amounts of water through the production of hypotonic urine and the excretion of mucous. Furthermore, earthworms must maintain a moist body surface to facilitate respiration. To avoid desiccation, G_W must therefore be equal to the volume of urine roduced (G_U) plus the volume of water lost through other processes. G_U was estimated as 20% of the volume of the worm (Lee KE, 1986). Based on this information, G_W was then estimated as:

$$G_W = 100.2 * V_{SI} \quad [51]$$

This estimation is based on the assumption that the earthworm loses 100 times its own volume of water per day due to the processes discussed above. It is important to note that the uncertainty associated with this parameter was not expected to significantly affect the results for the compounds being modeled since they are all lipophilic compounds with high K_{OW} values. In aquatic organisms, dietary uptake tends to be the dominant route of exposure for such compounds as the freely dissolved concentrations are extremely low (Mackay D & Fraser A, 2000). Furthermore, the G_W term effectively appears in the expression for k_{UW} and k_{EW} and thus tends to cancel out.

3.2.3.4 Dietary Uptake

The rate constant for dietary uptake requires values for chemical uptake efficiency (E_D) and the amount of food ingested (G_D). E_D can be modeled strictly as a function of K_{OW} if sufficient data are available. However, Ahrens MJ et al (2001) reported that the uptake efficiency of sediment-bound contaminants in the gut of deposit-feeding polychaetes is highly dependent on the composition of the digestive surfactants present in the gut of the organism. For example, the uptake efficiency of HCB (hexachlorobenzene) in *Nereis succinea* is approximately twice that of *Pecinaria gouldii* exposed using the same method. McLachlan MS (1993) suggested that the digestibility of the food may also influence the apparent uptake efficiency and cautioned against extrapolating E_{DIET} values across species. With these considerations in mind, the chemical uptake efficiency was based on information presented in studies of contaminant uptake from soil in earthworms (Belfroid A et al., 1994i,ii, Hendriks AJ et al., 2001) and set to 0.1 for all chemicals, regardless of K_{OW}.

The amount of food ingested (G_D) was estimated following an approach based on Connolly JP (1991) and Thomann RV et al. (1992). Consumption rates are based on the energetic requirements of the organism, the energy content of ingested materials and the energy assimilation efficiency of the ingested materials such that:

$$G_D / V_{SI} = \frac{\varepsilon_{ORG}*(k_{RESP} + k_{GR} + k_{REP})}{\varepsilon_{DIET}*A_F} \quad [52]$$

where ε_{ORG} and ε_{DIET} are the energy contents (kJ / m^3) of the organism and its diet respectively, k_{RESP}, k_{GR}, and k_{REP} are rate constants (day^{-1}) describing the amount of energy required (in tissue equivalents) for normal metabolic function, growth and

reproduction respectively and A_F is the energy assimilation efficiency of the ingested materials. The energy content of the organism (ε_{ORG}) was calculated as:

$$\varepsilon_{ORG} = F_L * \varepsilon_{LIPID} + F_{NLOM} * \varepsilon_{NLOM} \quad (kJ / m^3) \qquad [53]$$

where F_L and F_{NLOM} are the lipid and NLOM content of the organism (%) and ε_{LIPID} and ε_{NLOM} are the energy contents of lipid and NLOM matter (kJ / g) respectively. Values for ε_{LIPID} (39.5 kJ / g) and ε_{NLOM} (20 kJ / g) were taken from Connolly JP & Glaser D (2002) and the calculated value for ε_{ORG} was converted to kJ / m^3 assuming a density of 1000 kg / m^3. Since *Lumbricus rubellus* is an epigeic species that feeds on organic matter in the soil only, the energy content of the diet (ε_{DIET}) was calculated as:

$$\varepsilon_{DIET} = F_{OC} * \varepsilon_{OC} \quad (kJ / m^3) \qquad [54]$$

where F_{OC} is the organic carbon fraction of ingested soil (%) and ε_{OC} is the energy content of organic carbon. The value for ε_{OC} (41.4 kJ / g) was taken from Salonen K et al. (1976) and the calculated value for ε_{DIET} (kJ / g) was converted to kJ / m^3 using the bulk density of the ingested soil.

The value for k_{RESP} (day^{-1}) was estimated using an allometric equation presented in Thomann et al. (1992) which states that:

$$k_{RESP} = 0.036 * Mass_{SI}^{-0.2} \qquad [55]$$

where $Mass_{SI}$ is the mass (g) of the earthworm (hatchling, subadult or adult) (see Table 3.2).

The value for k_{GD} was estimated using growth data over a 28 week period for *Lumbricus rubellus* reported in Lowe CN & Butt KR (2002). Based on data presented in that study, k_{GR} for hatchlings and subadults was calculated by solving the following equation:

$$k_{GD} = [\ln Mass_{SI}(t) - \ln Mass_{SI}(t_0)] / t(day^{-1}) \quad [56]$$

where $Mass_{SI}(t)$ and $Mass_{SI}(t_0)$ represent the mass (g) of the earthworm at the end of the experiment and of the hatchling at the start of the experiment respectively and t is the length of the experiment (days). Based on this data, growth rates for hatchlings and subadults were calculated to be approximately 0.032 per day. According to Lee KE (1986), the growth rate of adult worms is much slower than that of subadults and hatchlings. Therefore, k_{GD} for adult worms was set to 0.005.

The value for k_{RD} was estimated using data on cocoon production presented in Lee KE (1986) and Spurgeon DJ et al. (2000). Based on these sources, cocoon production for *Lumbricus rubellus* was estimated to be approximately 0.3 per day. Given that one hatchling typically emerges from each cocoon (Lee KE, 1986, Pedersen MB & Bjerre A, 1991), it was assumed that each cocoon contains enough energy (in tissue equivalents) for one hatchling to develop. Given that average hatchling mass is known, $k_{RD}(day^{-1})$ can be estimated as:

$$k_{RD} = (Mass_H * 0.3) / Mass_A \quad [57]$$

where $Mass_H$ and $Mass_A$ are the average hatchling and adult mass (g) respectively (see Table 3.2). Based on this equation, k_{RD} for adults was calculated to be 0.0015.

The energy assimilation efficiency (A_{OM}) of earthworms is quite low compared to other organisms. Based on studies of carbon flux in earthworms, Lee KE (1986) reported that the energy assimilation of ingesta is no more than 10-15% in most species. Therefore, A_{OM} was initially set to 0.1. The G_D and associated mg OM / g worm for hatchlings, subadults and adults are presented below in Table 3.2.

Table 3-2 - Estimated Soil Consumption by *Lumbricus rubellus*

Life Stage	OCHTEN		GELDERSE POORT	
	G_D m^3 / day	OM Intake mg OM/ g worm / day	G_D m^3 / day	OM Intake mg OM/ g worm / day
Hatchling	1.62E-08	244	9.03E-09	244
Subadult	2.12E-07	159	1.18E-07	160
Adult	8.99E-07	67	5.00E-07	68

The calculated values for OM intake correspond reasonably well to estimated values in other studies for other earthworm species (Lee KE, 1986).

3.2.3.5 Elimination to Air

No additional information is required to parameterize k_{EA}.

3.2.3.6 Elimination to Water

No additional information is required to parameterize k_{EW} since it is a function of k_{UW} and BCF.

3.2.3.7 Fecal Elimination

The rate constant for fecal elimination (k_{FE}) requires values for the volume of fecal matter excreted (G_F) and the partition coefficient describing the distribution of chemical between the organism and its feces (K_{BF}). These values can be calculated using the information provided in previous sections.

3.2.3.8 Urinary Elimination

All of the information required to calculate the rate constant for urinary elimination (k_{UE}) has already been presented in previous sections.

3.2.3.9 Growth Dilution, Reproduction

The process for parametering the rate constants for growth dilution (k_{GD}) and reproduction (k_{RD}) were discussed in section 3.2.3.2.

3.2.3.10 Metabolism

Metabolism of PCBs and the other compounds was assumed to be negligible and therefore $k_{MT} = 0$.

Summaries of the parameter values used in the steady-state model for *Lumbricus rubellus* from Ochten and Gelderse Poort that do not vary with the specific chemical are presented below in Table 3.3 and Table 3.4 respectively.

Table 3-3 – Summary of Parameter Values For *Lumbricus rubellus* (Ochten)

Parameter	Units	Initial Value		
		Hatchling	Subadult	Adult
Mass	g	0.005	0.1	1
F_L	%	0.0119	0.0119	0.0119
F_{NLOM}	%	0.1881	0.1881	0.1881
F_W	%	0.8	0.8	0.8
X_{NLOM}		0.035	0.035	0.035
X_{OC}		0.35	0.35	0.35
G_A	m^3 / day	6.00E-09	1.20E-07	1.20E-06
G_W	m^3 / day	5.01E-07	1.00E-05	1.00E-04
G_D	m^3 / day	1.62E-08	2.12E-07	1.02E-06
G_F	m^3 / day	1.62E-08	2.11E-07	1.01E-06
G_U	m^3 / day	1.00E-09	2.00E-08	2.00E-07
E_A	%	70	70	70
E_D	%	10	10	10
A_{OM}	%	10	10	10
k_{RESP}	day^{-1}	0.10	0.06	0.04
k_{GD}	day^{-1}	0.032	0.032	0.005
k_{RD}	day^{-1}	0	0	0.0015
k_{MT}	day^{-1}	0	0	0

Table 3-4– Summary of Parameter Values For *Lumbricus rubellus* (Gelderse)

Parameter	Units	Initial Value		
		Hatchling	Subadult	Adult
Mass	g	0.005	0.1	1
F_L	%	0.0123	0.0123	0.0123
F_{NLOM}	%	0.1887	0.1887	0.1887
F_W	%	0.8	0.8	0.8
X_{NLOM}		0.035	0.035	0.035
X_{OC}		0.35	0.35	0.35
G_A	m^3 / day	6.00E-09	1.20E-07	1.20E-06
G_W	m^3 / day	5.01E-07	1.00E-05	1.00E-04
G_D	m^3 / day	9.03E-09	1.18E-07	5.67E-07
G_F	m^3 / day	8.95E-09	1.17E-07	5.62E-07
G_U	m^3 / day	1.00E-09	2.00E-08	2.00E-07
E_A	%	70	70	70
E_D	%	10	10	10
A_{OM}	%	10	10	10
k_{RESP}	day^{-1}	0.10	0.06	0.04
k_{GD}	day^{-1}	0.032	0.032	0.005
k_{RD}	day^{-1}	0	0	0.0015
k_{MT}	day^{-1}	0	0	0

3.2.4 Terrestrial Organisms

The bioaccumulation model for terrestrial organisms also requires many input parameters. Some parameters are based on reported values (e.g. biota lipid content) while others are based either on allometric relationships taken from the literature (e.g. respiration rate) or other types of models. Details of the parameterization process for each variable are organized according to the rate constant they are required for.

3.2.4.1 Basic Physical Characteristics

The average volume of the shrew (V_B) was calculated as a function of BW (kg) and the average density of biota d_B (kg / L). The estimated BW of the common shrew was taken from Stalinski J (1994) and DEFRA (2002). The average density of biota was assumed to be 1000 kg / m^3. The lipid content (F_L) of shrews was assumed to be 7% based on Wijnandts H (1984), water content (F_W) was 70% (Traas TP et al., 1996) and NLOM content was calculated as $1 - F_L - F_W$.

3.2.4.2 Uptake via Inhalation

The volume of air respired per day (G_A) was calculated using the following allometric relationship for mammals (US EPA, 1993).

$$G_A = 0.002173 * BW^{0.8}(g) * 2.5 \quad [58]$$

A factor of 2.5 was included as an adjustment to account for the discrepancy between the volume of air respired by free-living animals versus laboratory animals. The chemical uptake efficiency from air (E_A) was set at 0.7 following the example of Hickie BE et al. (1999) and Kelly BC & Gobas FAPC (2003).

3.2.4.3 Dietary Uptake

The chemical uptake efficiency (E_D) for shrews was based on studies of intestinal absorption and oral bioavailability in a variety of mammals (Tanabe S et al., 1981, Albro PW & Fishbein L, 1988, Owen BA, 1990) and was calculated based on the following empirically-derived relationship:

$$1/E_D = a * K_{OW} + b \quad [59]$$

Values for a and b were determined using a non-linear regression of the available data. The results of these regressions are presented in Appendix C. E_S was estimated as $0.8*E_D$ based on studies of chemical uptake from contaminated soil added to the diet of experimental animals (Fries GF, 1985, Fries GF et al., 1989).

The rate of food intake (G_D) for shrews was calculated using estimated daily energy expenditure (DEE), diet composition and diet item caloric values using empirical relationships and values used by the Department for Environment, Food and Rural Affairs in Great Britain (DEFRA, 2002). This approach is similar to the method used to estimate G_D for earthworms except that the allometric relationships used to estimate metabolic energy needs are specific to mammals.

Daily energy expenditure refers to the amount of energy used by a free-living organism engaged in normal activities such as foraging and is calculated as a function of body size as follows:

$$\log DEE\ (kJ / day) = \log(x) + y * \log BW \quad [60]$$

where x and y are the empirically-derived parameters estimated from mammalian and avian studies reported in DEFRA 2002 and BW is the weight of the animal (wet g). Based on the estimated DEE, daily food intake (DFI) can be calculated as:

$$\text{DFI (wet g / day)} = \text{DEE} / [A\varepsilon * \varepsilon_{PREY} * (1-F_{W-D})] \quad [61]$$

where $A\varepsilon$ is the average energy assimilation efficiency of the diet, ε_{PREY} is the energy content of the diet (kJ / g dry mass) and F_{W-D} is the water content of the diet. Note that because this model only incorporates one prey item, ε_{PREY} is the equal to ε_{ORG} in equation [51].

The amount of soil ingested per day (G_S) was estimated by assuming that the major source of soil in the diet was soil contained by earthworms when consumed. Beyer WN et al (1994) developed a method for estimating soil in diet (% of dry mass) using the acid-insoluble ash of prey items, scat and soil (% of dry mass) and the assumed dry mass digestibility of the diet. Typical estimated values for the fraction of soil in diets range from less than 2% for herbivores such as deer and elk to as high as 30% for sandpipers which feed on sediment-dwelling aquatic invertebrates. Using the Beyer method, Regan HM et al. (2002) reported median dietary soil fractions for short-tailed shrews (*Blarina* brevicauda) and meadow voles (*Microtus* pennsylvanicus) of 0.02 and 0.013 respectively (range 0 – 0.06). While the value for meadow voles is in agreement with other herbivores, the value for the short-tailed shrew is below other soil-invertebrate consumers such as armadillos (*Dasypus novemcinctus,* 0.17), American woodcock (*Scolopax minor,* 0.1) and raccoons (*Procyon lotor,* 0.09) (Beyer WN et al, 1994). Considering that the soil content of earthworms has been estimated at 20 – 30% of dry

mass (Beyer WN et al. 1993), animals feeding predominantly on earthworms, as assumed in the Hendriks AJ et al. (1995) study, are likely to have a fraction of soil in their diet considerably greater than 2%. For the purposes of the proposed model, the ratio of soil (dry mass) to earthworm (dry mass) was assumed to be 25%. Based on these assumptions, the fraction of soil in the shrew diet can be calculated as follows:

$$G_S \text{ (dry g / day)} = \text{DFI (wet g / day)} * P_{WORM} * (1-F_W) * 0.25 \quad [62]$$

where P_{WORM} is the fraction of earthworms in the diet, $1-F_W$ converts the wet g of worm to dry and 0.25 is the assumed ratio of dry soil to dry earthworm. Assuming a diet of 100% earthworm, the DFI for a shrew is approximately 10 g / day. Using an earthworm water content (F_W) of 0.8, the estimated G_S (dry g / day) is 0.5, which corresponds to a dietary soil fraction of about 20% (G_S / [G_S + dry DFI]). G_S (dry g / day) was converted to G_S (wet g / day) using the reported moisture content of the soil and then converted to G_S (m^3 / day) using a bulk soil density of 1500 kg / m^3. Organic matter fractions were also adjusted accordingly.

3.2.4.3 Elimination via Exhalation

No additional information is required to parameterize this elimination route.

3.2.4.4 Urinary excretion

The volume of urine excreted per day (G_U) by shrews was estimated using studies of water exchanges in small mammals (Chew RM, 1951) and set to 5 ml / day.

3.2.4.5 Fecal elimination

As discussed before, the volume of feces excreted per day (G_F) is a function of the assimilation efficiency for dietary lipid, NLOM and water respectively. The amount of soil consumed per day (G_{SOIL}) will also influence fecal elimination to some extent. For shrews, the assimilation efficiency parameters were based on apparent dry mass digestibilities reported for a variety of insectivores and other small, the average fecal water content reported for small mammals and insectivorous bats (Chew RM, 1951, Barclay RMR et al., 1991, Webb PI et al., 1993, Stalinkski J, 1994). Reported assimilation efficiencies for lipids and NLOM such as protein and chitin were also considered (Webb PI et al., 1993). Based on this information, A_L was initially set to 0.98, A_{NLOM} to 0.75 and A_W to 0.85. The assimilation efficiencies of organic matter (A_{OM}) and inorganic soil components (A_S) were assumed to be zero.

3.2.4.6 Biliary elimination

Estimates for the volume of bile excreted per day (G_B) for shrews could not be located in the literature. However, average bile flow rates for rats and rhesus monkeys were both reported to be approximately 40 ml / kg /day (Rozman K et al., 1981). Bile flow rates were assumed to be the same for shrews. The value for β, which reflects the greater solubility of chemical in bile compared to water, was set to 10 following Gobas et al. (2003).

3.2.4.7 Lactation

The rate constant for elimination via lactation (k_{LA}) was set to 0 because the model was initially parameterized to represent adult male organisms (i.e $G_M = 0$).

3.2.4.8 Metabolism

The metabolic transformation rate constant (k_{MT}) was initially set to 0 in order to represent recalcitrant congeners which are either non-metabolizable or metabolized at an insignificant rate.

3.2.4.9 Growth

Elimination via growth dilution (k_G) was set to 0.0001 because the model was initially parameterized to represent adult male organisms with insignificant growth.

3.2.4.10 Parturition / Egg-laying

Elimination via maternal transfer (k_{RD}) was set to 0 because the model was initially parameterized to represent adult male organisms. Summaries of the parameter values used in the steady-state model for the shrew that are not chemical specific are presented below in Table 3.5.

Table 3-5– Summary of Parameter Values For Shrews

Parameter	Units	Initial	
		Ochten	Gelderse Poort
Mass	g	10	10
F_L	%	7	7
X_{NLOM}		0.035	0.035
X_{OC}		0.35	0.35
G_A	m^3 / day	3.43E-02	3.43E-02
G_D	m^3 / day	9.15E-06	9.15E-06
G_S	m^3 / day	3.77E-10	4.18E-10
G_F	m^3 / day	1.53E-06	1.53E-06
G_U	m^3 / day	5.00E-06	5.00E-06
G_B	m^3 / day	4.00E-07	4.00E-07
G_M	m^3 / day	0	0
A_L	%	98	98
A_{NLOM}	%	75	75
A_W	%	85	85
B		10	10
k_{GD}	day^{-1}	0.0001	0.0001
k_{RD}	day^{-1}	0	0
k_{MT}	day^{-1}	0	0

3.3 Model Evaluation

The performance of the proposed models was evaluated in two ways. First, model output, generated using the initial parameter values, was compared to the observed data by calculating the overall model bias (MB). Model bias is defined as:

$$MB = \underset{\text{For } i = 1 \text{ to } n}{[\Sigma \log (V_{Predicted(i)} / V_{Observation(i)})]} / n \qquad [63]$$

where V represents the value of interest (i.e. concentration, BSAF or BMF) and n is the number of observations. A model bias > 0 indicates that the model generally overestimates while a model bias < 0 indicates that the model generally underestimates. The antilog of the model bias represents the average factor by which predictions differ from observations.

Model performance was also evaluated by through the use of Monte Carlo simulations. The purpose of conducting the Monte Carlo simulations was to generate a range of output reflective of the uncertainty associated with key input parameters. Parameter values were assigned distributions or ranges based on available data or reasonable estimates subject to biological constraints. Multivariate Monte Carlo simulations (n = 10 000) were conducted using Crystal Ball (© Decisioneering) and the range of values which captured 95% of the predictions was used to assess the robustness of the model. Table 3.6 to 3.8 detail the parameters varied, the distributions selected and the assigned range for the EPT soil-invertebrate, steady-state soil invertebrate and terrestrial organism models respectively.

Table 3-6 – Soil-invertebrate parameter settings for Monte Carlo simulations (EPT Model)

Parameter	Distribution	Initial Value	Range
F_L	Normal	Table 3.3, 3.4	SD
X_{NLOM}	Uniform	0.035	0.02 - 0.05
X_{OC}	Uniform	0.35	0.14 - 0.89

Table 3-7 – Soil-invertebrate parameter settings for Monte Carlo simulations (Steady-state Model)

Parameter	Distribution	Initial Value	Range
F_L	Normal	Table 3.3, 3.4	SD
X_{NLOM}	Uniform	0.035	0.02 - 0.05
X_{OC}	Uniform	0.35	0.14 - 0.89
Water loss	Uniform	0.1 L / g	0.05 - 0.2
G_U	Uniform	0.2 * V_{SI}	0.1 - 0.4 * V_{SI}
E_{DIET}	Uniform	0.1	0.05 - 0.2
A_{OM}	Uniform	0.1	0.01 - 0.2
Soil Density	Uniform	1500 kg / m^3	1500 - 2500

Table 3-8 – Terrestrial organism parameter settings for Monte Carlo simulations

Parameter	Distribution	Initial Value	Range
F_L	Uniform	0.07	0.04 - 0.1
A_L	Uniform	0.98	0.9 - 1
A_{NLOM}	Uniform	0.75	0.6 - 0.9
E_{DIET}	Normal	Submodel	SD of a and b
X_{NLOM}	Uniform	0.035	0.02 - 0.05
X_{OC}	Uniform	0.35	0.14 - 0.89
$F_{L\text{-}WORM}$	Normal	Table 3.3, 3.4	SD

The influence of diet on predicted BMFs was also explored. The initial parameter settings assume a diet of 100% earthworm including ingested soil. To examine the effect of incorporating different prey items, the steady-state model was simplified to include only dietary uptake. When diet is the only significant route of exposure, the expression for estimating concentrations in biota can be written as:

$$C_B = k_{DIET} * C_{DIET} / k_{\Sigma ELIMINATION} \quad [64]$$

where $k_{\Sigma ELIMINATION}$ is the sum of the elimination rate constants defined previously.

This expression can then be rearranged to estimate BMF as:

$$BMF = C_B / C_{DIET} = k_{DIET} / k_{\Sigma ELIMINATION} \quad [65]$$

Predicted BMFs were converted to lipid-equivalent BMFs using the same lipid and NLOM fractions for earthworms and lipid fractions for beetles and slugs reported in the literature (Van Brummelen TC et al., 1996, Legierse KCHM et al., 1998, Hendriks AJ et al., 2001). The water content of beetles and slugs was assumed to be 70% and NLOM matter content was calculated as before. Simulations were run to compare a diet of 100%

earthworms (with ingested soil), 100% earthworm (no ingested soil) and a mixed diet of 50% earthworms (with ingested soil), 25% beetles and 25% slugs. The daily energy expenditure calculation was also modified to reflect the different diets.

3.4 Model Application

Bioaccumulative potential was investigated by examining the relationship between BMF and key physico-chemical properties. To accomplish this task, BMF was estimated as a function of K_{OW} and K_{OA}. The purpose of this exercise was to examine the appropriateness of the CEPA 1999 bioaccumulation criteria. The effect of metabolism on BMF was also explored by varying k_{MT}.

The steady-state terrestrial organism model was also applied in two other ways. First, a steady-state bioaccumulation model was developed for the little owl (*Athene noctua vidalli*). This bird is considered to be the top predator in Dutch flood plains and feeds mainly on earthworms and insects but has also been observed to consume small rodents (Van den Brink et al., 2001). Unfortunately, no data reporting internal tissue concentrations for PCBs were located in the scientific literature. Therefore, model performance was evaluated simply by comparing predicted BMFs for non-metabolizable chemicals to BMFs reported for other avian species. This exercise was meant to demonstrate the utility of the bioaccumulation model for estimating tissue concentrations in species that can not be sampled due to legislative restrictions (e.g. Species At Risk Act) or practical and ethical considerations.

The other application of the steady-state bioaccumulation model was to use model outputs to conduct a hazard assessment for shrews living in the Ochten

floodplains. This application can also be used to recommend soil remediation targets. The methods for each application are discussed below.

3.4.1 Bioaccumulative Potential and Physico-chemical Properties

The relationship between bioaccumulative potential and physico-chemical properties was investigated by estimating the BMF for shrews as a function of K_{OW} and K_{OA} ranging from 10 to 10^{15}. The original models were modified to represent a general scenario for any organic chemical using the basic soil characteristics of the Ochten site. The soil concentration (C_{SOIL}) was set to 1 ug / m^3 and the corresponding concentrations in interstitial water (C_W, ug / m^3) and air (C_{AIR}, ug / m^3) were estimated as follows:

$$C_W = C_{SOIL} / K_{SW} \quad [66]$$

$$C_{AIR} = C_{SOIL} * K_{AS} \quad [67]$$

C_{AIR} and C_W were calculated assuming an ambient temperature of 10°C.

The steady-state soil-invertebrate bioaccumulation model was modified so that values for K_{AW} were estimated as the ratio of K_{OW} and K_{OA} (at 10°C). The output of this model was used as the concentration in the diet for the shrew (C_{DIET}). The terrestrial organism model was also modified so that K_{AW} was calculated as the ratio of K_{OW} and K_{OA}, however these values were calculated at 37°C. To link the values of K_{OA} at 10°C and 37°C in the model, K_{OA} at 10°C was calculated as:

$$K_{OA}(10°C) = K_{OA}(37°C) * \Phi \quad [68]$$

where Φ represents the ratio of K_{OA} at 10°C to K_{OA} at 37°C. Φ was set to 20 for the base scenario and then varied from 2 to 50. The predicted BMFs were then compared across all values of Φ.

3.4.2 Bioaccumulative Potential and Metabolism

The effect of metabolism on BMF was explored with the same model used in Section 3.4.1. The rate constant for metabolism (k_{MT}) was simply increased incrementally until the lipid EQ-normalized BMF fell below 1 across the range of K_{OW} and K_{OA}.

3.4.3 Steady-state Bioaccumulation Model for the little owl

The steady-state bioaccumulation model for shrews from the Ochten site was re-parameterized to match the characteristics of the little owl. The details of the model are provided below.

3.4.3.1 Basic Physical Characterisitics

The body weight (BW) of the little owl was set to 0.185 kg (Van den Brink NW et al., 2003) and V_B was calculated assuming a density of 1000 kg / m^3. Lipid content (F_L) was set at 12% (Drouillard KG, 2000), water content (F_W) to 70% (Traas TP et al., 1996) and NLOM content was calculated as $1 - F_L - F_W$.

3.4.3.2 Uptake via Inhalation

E_A was set to 0.7 and the volume of air respired per day (G_A) was calculated using the following allometric relationship for non-passerine birds (US EPA, 1993).

$$G_A = 0.002002 * BW^{0.8} * 2.5 \quad [69]$$

3.4.3.3 Dietary Uptake

The feeding rate (G_D) was calculated using the same procedure as for shrews except the diet of the little owl was assumed to be 80% earthworm and 20% shrew. E_D was estimated using equation 55 except that the 'a' and 'b' parameters were estimated by performing a non-linear regression on data from Drouillard KG (2000). E_S was again estimated as 0.8 * E_D.

3.4.3.4 Urinary/Fecal Elimination

In birds, fecal matter and urine are combined in the cloaca prior to excretion. Therefore, a combined volume ($G_U + G_F$) was estimated using data from Drouillard KG (2000). Absorption efficiencies for lipid and NLOM were estimated using data from Drouillard KG (2000), Karasov WH (1990) and DEFRA 2002.

3.4.3.4 Other elimination terms

Elimination via growth dilution, metabolism and reproduction remained at zero and biliary elimination was estimated using the same bile flow rate and ß. Key parameter values are summarized in Table 3.9.

Table 3-9 – Parameter Values for Little Owl

Parameter	Units	Initial Values
Mass	g	185
F_L	%	12
X_{NLOM}		0.035
X_{OC}		0.35
G_A	m^3 / day	2.79E-01
G_D	m^3 / day	7.42E-05
G_S	m^3 / day	2.48E-06
$G_F + G_U$	m^3 / day	5.20E-05
G_B	m^3 / day	7.40E-06
A_L	%	95
A_{NLOM}	%	70
A_W	%	85
B		10
k_{GD}	day^{-1}	0
k_{RD}	day^{-1}	0
k_{MT}	day^{-1}	0

3.4.4 Hazard Assessment

A hazard assessment of the Ochten flood plain soils for shrews was conducted by calculating the Hazard Index (H). The Hazard Index is defined as:

$$H = \frac{\text{Dose (mg / kg / day)}}{\text{RfD (mg / kg / day)}} \qquad [70]$$

where RfD is the oral reference dose. The RfD is based on the No Adverse Effects Level (NOAEL) or Lowest Adverse Effects Level (LOAEL) derived from laboratory toxicity studies. For human exposure assessments, the NOAEL or LOAEL is divided by a safety factor (10 or 100) to account for uncertainties such as inter-species sensitivity. If the Hazard Index is less than 1.0, the exposure level is considered safe.

The Integrated Risk Information System (US EPA) contains RfDs for a large number of chemicals. Unfortunately, RfDs for individual PCB congeners are not available. Therefore, the hazard assessment was conducted for dieldrin. The RfD for dieldrin is $5 * 10^{-5}$ mg / kg / day, based on a long-term feeding study with rats that found a NOAEL of $5 * 10^{-3}$ mg / kg / day. For this exercise, the hazard assessment was conducted with both the RfD and the NOAEL. The daily dose was based on exposure to earthworms and ingested soil using estimated feeding rates (G_D in kg / day), soil ingestion rates (G_S in kg / day), the observed soil concentration (C_{SOIL} in mg / kg), the predicted BSAF and the mass of the shrew (V_B in kg). Using this information, dose can be calculated as:

$$\begin{aligned} \text{Dose} &= (G_S * C_{SOIL} + G_D * C_{DIET}) / V_B \\ &= (G_S * C_{SOIL} + G_D * C_{SOIL} * BSAF) / V_B \end{aligned} \quad [71]$$

If the Hazard Index is greater than 1.0, a soil remediation target can be estimated by setting H to 1 and solving for C_{SOIL} as follows:

$$\begin{aligned} 1.0 &= \text{Dose} / \text{RfD} \quad [72] \\ \text{RfD} &= \text{Dose} \\ \text{RfD} &= (G_S * C_{SOIL} + G_D * C_{SOIL} * BSAF) / V_B \\ \text{RfD} * V_B &= (G_S + G_D*BSAF) * C_{SOIL} \\ C_{SOIL} &= (\text{RfD} * V_B) / (G_S + G_D*BSAF) \end{aligned}$$

4.0 RESULTS AND DISCUSSION

4.1 Bioaccumulation in Soil Invertebrates

Observed and predicted BSAFs are presented in terms of (dry kg soil / wet weight kg). The results of the EPT model for Ochten and Gelderse Poort are presented in Figure 4.1 and 4.2 respectively. Observed BSAFs with 95% confidence intervals and predicted BSAFs are shown with the 95% range of outputs from the Monte Carlo simulations.

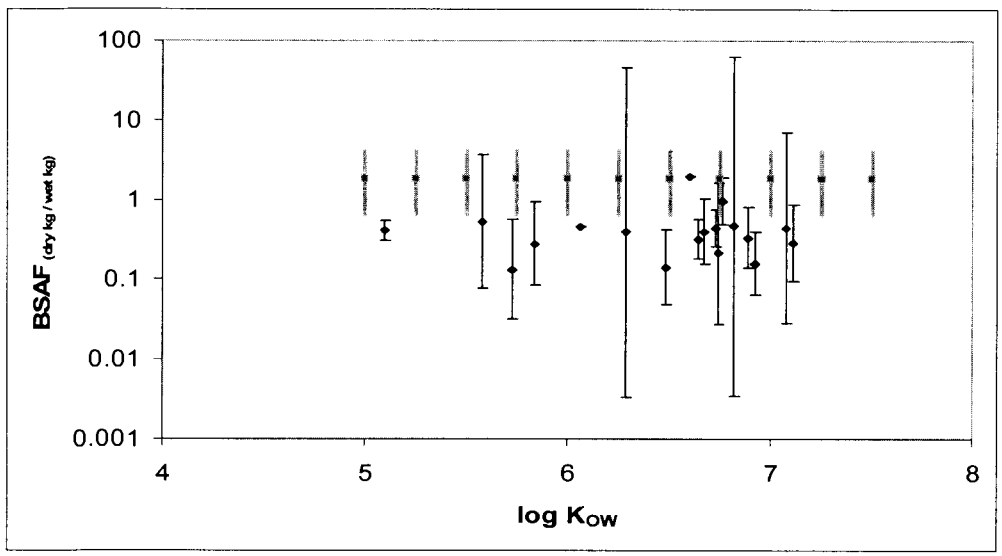


Figure 4-1– Observed (♦) and EPT Predicted (■) BSAFs for Ochten

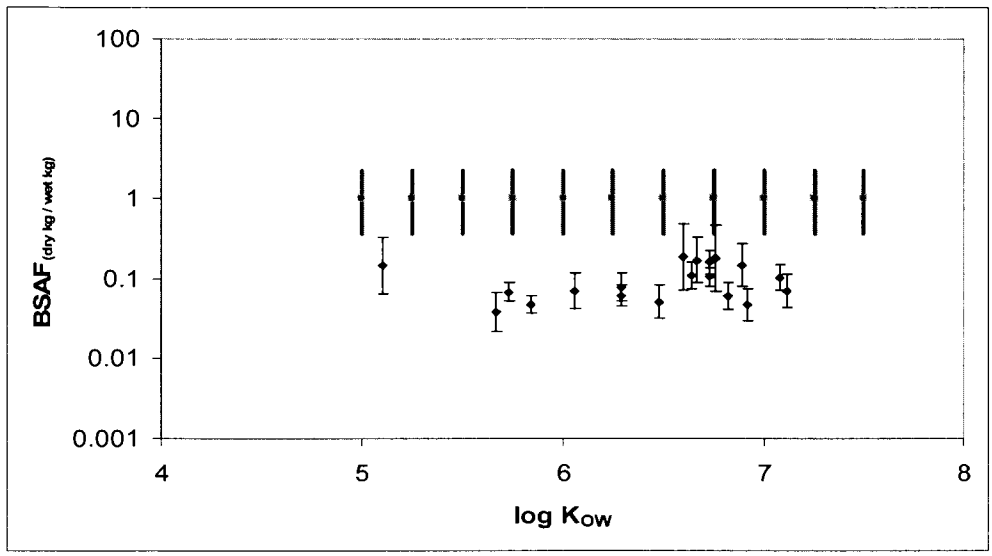


Figure 4-2 – Observed (♦) and EPT Predicted (■) BSAFs for Gelderse Poort

The results of the steady-state model for Ochten and Gelderse Poort are presented in Figures 4.3 – 4.5 and Figures 4.6 – 4.8 respectively. The observed BSAFs are shown with the associated 95% confidence intervals along with the predicted BSAFs estimated and the 95% range of outputs from the Monte Carlo Simulations.

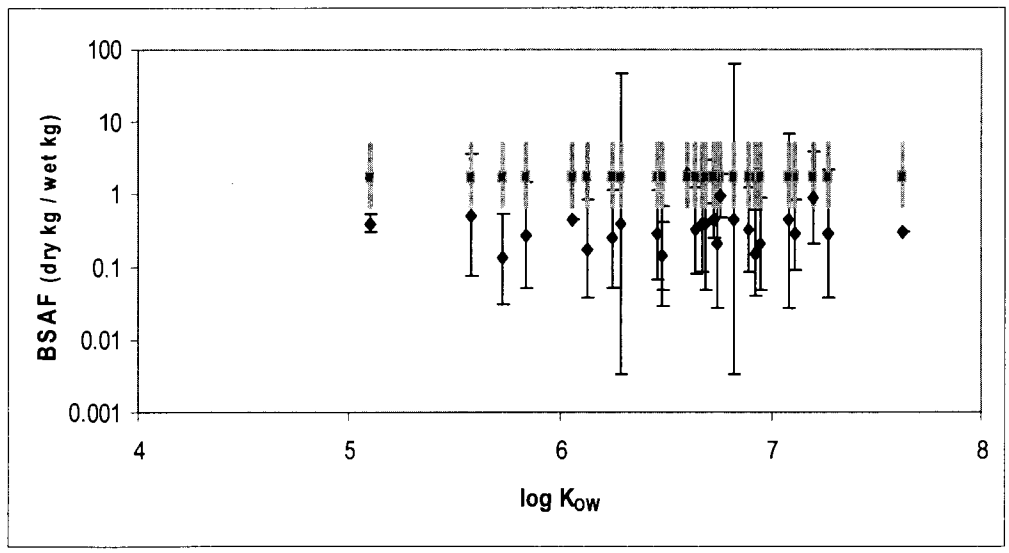


Figure 4-3 – Observed (♦) and SS Predicted (■) BSAFs (Hatchlings) in Ochten

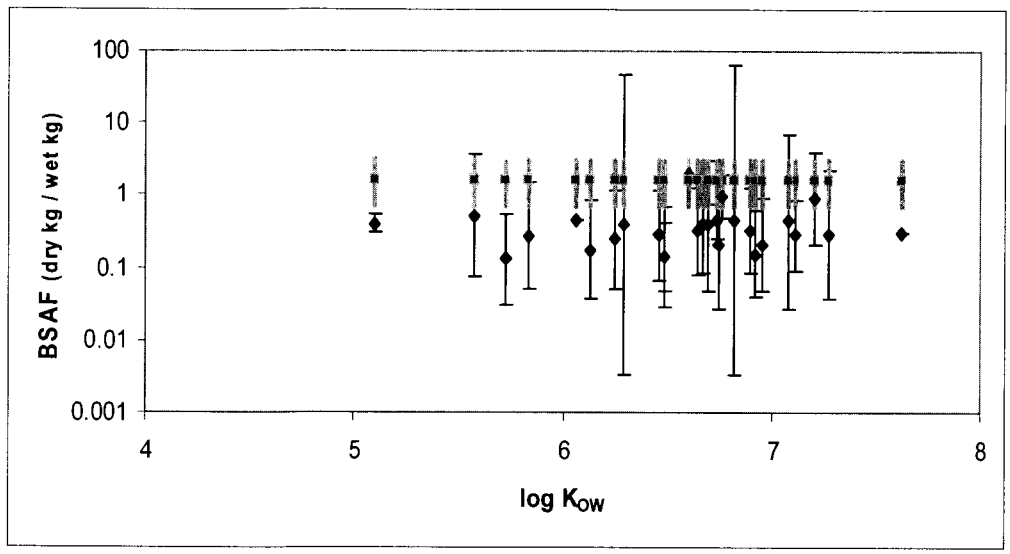


Figure 4-4 – Observed (♦) and SS Predicted (■) BSAFs (Subadults) in Ochten

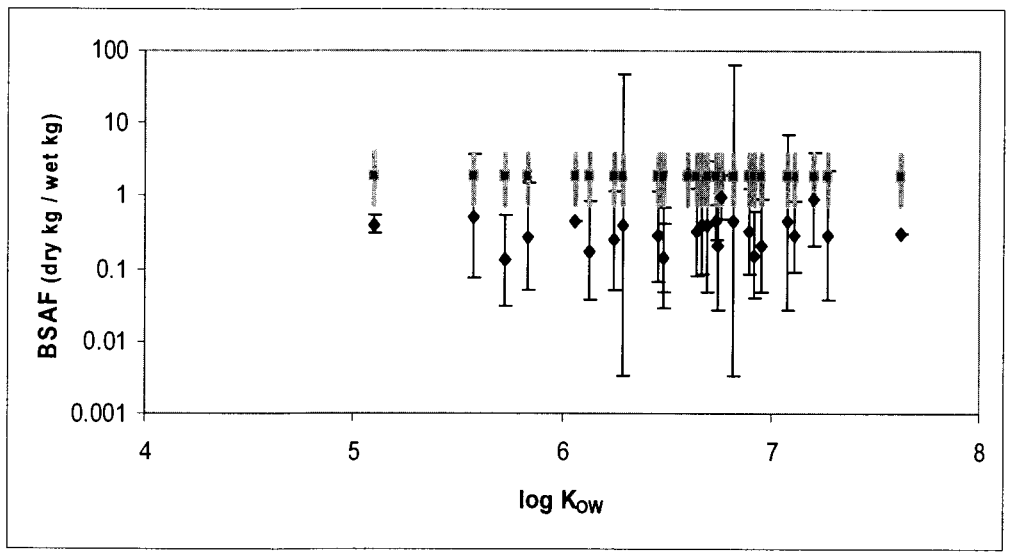


Figure 4-5 – Observed (♦)and SS Predicted(■) BSAFs (Adults) in Ochten

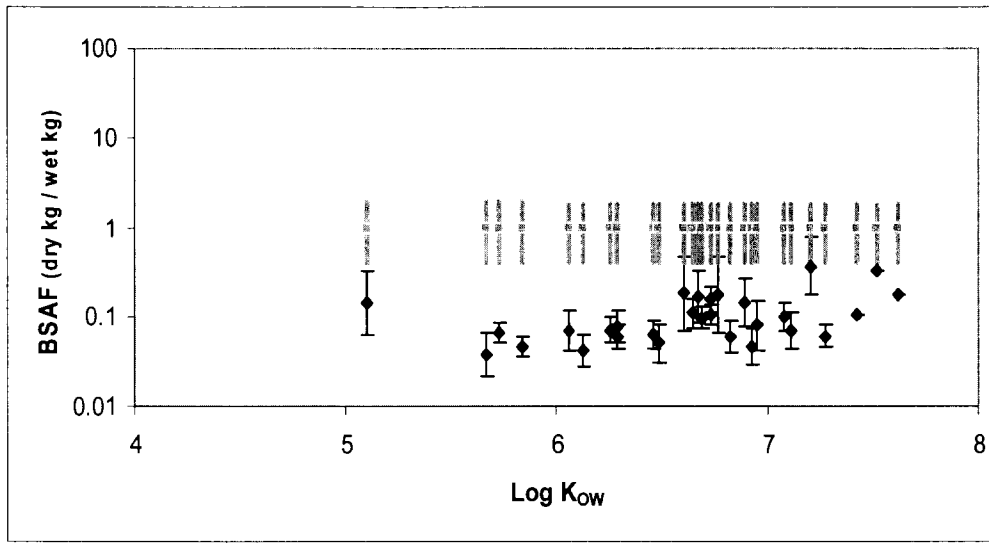


Figure 4-6 – Observed (♦)and SS Predicted (■) BSAFs (Hatchlings) in Gelderse Poort

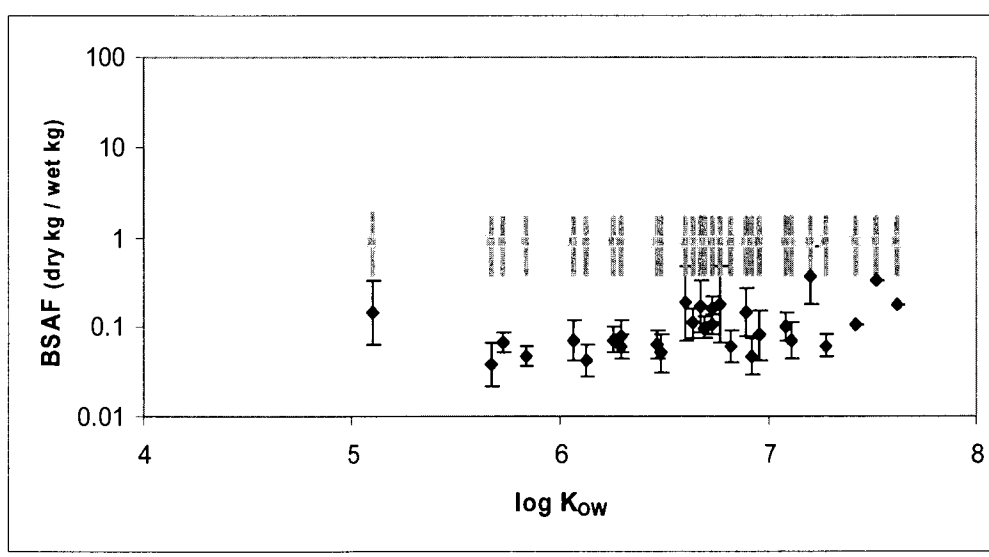


Figure 4-7 – Observed (♦)and SS Predicted (■) BSAFs (Sub-adults) in Gelderse Poort

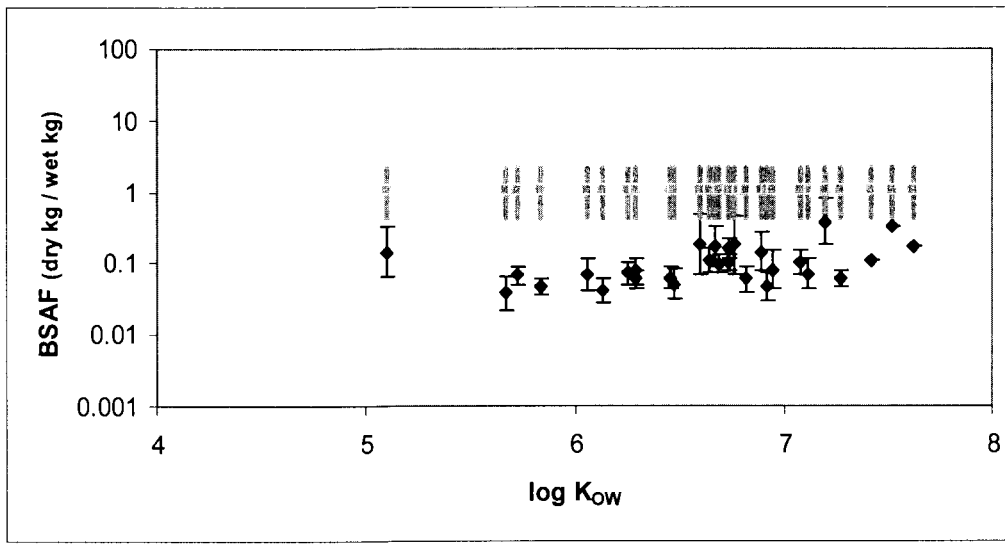


Figure 4-8 – Observed (♦) and SS Predicted (■) BSAFs (Adults) in Gelderse Poort

The original data along with observed BSAFs and predicted BSAFs for the Ochten and Gelderse Poort sites are shown in Table 4.1 and 4.2 respectively. The model bias for the EPT and steady-state models is presented in Table 4.3.

Interpretation of Results

The EPT and steady-state models overestimate observed BSAFs by a factor of approximately 5 and 10 for the Ochten and Gelderse Poort sites respectively. Although the steady-state models perform slightly better, as evidenced by the lower model bias (Table 4.3), the results are still unsatisfactory. The different results obtained for the steady-state model for hatchlings, subadults and adults can be explained by examining the relative rates of uptake and elimination under each set of parameters. For the chemicals modeled in this study (with log K_{OW} from approximately 5 – 8), dietary uptake is the dominant route of exposure while the major elimination routes are fecal elimination

and growth dilution. Although the ratio of k_{UD} to k_{FE} is the same for hatchlings, subadults and adults, the absolute values are highest for hatchlings and lowest for adults. On the other hand, subadults have the highest growth rate constant relative to k_{UD} and k_{FE} while adults have the lowest (even including the reproduction rate constant). The higher relative growth dilution rate constant results in a lower predicted BSAF.

Table 4-1 – Observed vs Predicted BSAFs in Ochten

Chemical	C_{SOIL} ug / kg dry	C_{SI} ug / kg wet	Observed BSAF dry kg/wet kg	EPT BSAF dry kg/wet kg	Steady-state BSAF		
					Hatchling	Subadult	Adult
PCB052	3.90	1.08	0.28	1.82	1.694	1.564	1.794
PCB110	11.00	1.55	0.14	1.82	1.692	1.558	1.792
PCB149	15.00	5.95	0.40	1.82	1.691	1.557	1.792
PCB151	4.50	1.43	0.32	1.82	1.691	1.557	1.792
PCB146	4.30	1.43	0.33	1.82	1.691	1.557	1.792
PCB153	16.00	2.50	0.16	1.82	1.691	1.557	1.792
PCB201	2.50	0.77	0.31	1.82	1.691	1.556	1.792
PCB095(066)	7.40	1.31	0.18	1.82	1.692	1.560	1.793
PCB099/113	4.70	1.31	0.28	1.82	1.692	1.558	1.792
PCB101/090	9.70	2.38	0.25	1.82	1.692	1.559	1.793
PCB123/147	2.60	1.01	0.39	1.82	1.691	1.557	1.792
PCB138/163/164	20.00	4.17	0.21	1.82	1.691	1.557	1.792
PCB170(190)	5.40	1.55	0.29	1.82	1.691	1.556	1.792
PCB182/187	5.50	5.00	0.91	1.82	1.691	1.556	1.792
PCB022	1.80	0.94	0.52	1.82	1.696	1.570	1.795
PCB087	3.00	1.19	0.40	1.82	1.692	1.559	1.793
PCB110	11.00	1.55	0.14	1.82	1.692	1.558	1.792
PCB111	2.00	1.90	0.95	1.82	1.691	1.557	1.792
PCB118	6.70	1.43	0.21	1.82	1.691	1.557	1.792
PCB141	3.60	1.67	0.46	1.82	1.691	1.557	1.792
PCB148	3.00	1.31	0.44	1.82	1.691	1.557	1.792
PCB174	4.60	1.31	0.28	1.82	1.691	1.556	1.792
PCB177	2.60	1.14	0.44	1.82	1.691	1.556	1.792
HCB	18.00	2.38	0.13	1.82	1.695	1.566	1.794
Dieldrin	4.10	1.67	0.41	1.82	1.705	1.594	1.799
p,p'-DDT	6.80	3.09	0.46	1.82	1.693	1.561	1.793
p,p'-DDE	3.20	6.19	1.93	1.82	1.691	1.557	1.792

Table 4-2– Observed vs Predicted BSAFs in Gelderse Poort

Chemical	C_{SOIL} ug / kg dry	C_{SI} ug / kg wet	Observed BSAF	EPT BSAF	Steady-state BSAF		
					Hatchling	Subadult	Adult
PCB028	28.00	1.07	0.04	1.03	0.958	0.885	1.016
PCB052	29.00	1.35	0.05	1.03	0.958	0.883	1.015
PCB149	68.00	11.56	0.17	1.03	0.956	0.879	1.014
PCB151	20.00	2.21	0.11	1.03	0.956	0.879	1.014
PCB146	16.00	2.34	0.15	1.03	0.956	0.879	1.014
PCB148	10.00	1.60	0.16	1.03	0.956	0.879	1.014
PCB153	63.00	2.95	0.05	1.03	0.956	0.879	1.014
PCB193	2.00	0.65	0.33	1.03	0.956	0.879	1.014
PCB201	6.70	1.18	0.18	1.03	0.956	0.879	1.014
PCB095(066)	38.00	1.60	0.04	1.03	0.957	0.881	1.015
PCB099/113	19.00	1.19	0.06	1.03	0.956	0.880	1.014
PCB101/090	46.00	3.32	0.07	1.03	0.957	0.880	1.015
PCB123/147	9.00	0.87	0.10	1.03	0.956	0.879	1.014
PCB138/163/164	82.00	6.64	0.08	1.03	0.956	0.879	1.014
PCB170(190)	24.00	1.48	0.06	1.03	0.956	0.879	1.014
PCB182/187	24.00	8.98	0.37	1.03	0.956	0.879	1.014
PCB192/172	5.70	0.62	0.11	1.03	0.956	0.879	1.014
PCB087	17.00	1.03	0.06	1.03	0.957	0.880	1.015
PCB097	11.00	0.85	0.08	1.03	0.957	0.880	1.015
PCB110	48.00	2.46	0.05	1.03	0.956	0.880	1.014
PCB111	7.60	1.35	0.18	1.03	0.956	0.879	1.014
PCB141	17.00	1.02	0.06	1.03	0.956	0.879	1.014
PCB174	21.00	1.48	0.07	1.03	0.956	0.879	1.014
PCB177	12.00	1.23	0.10	1.03	0.956	0.879	1.014
PCB179	7.40	0.77	0.10	1.03	0.956	0.879	1.014
HCB	80.00	5.41	0.07	1.03	0.958	0.884	1.016
Dieldrin	8.40	1.22	0.14	1.03	0.964	0.901	1.019
p,p'-DDT	14.00	0.98	0.07	1.03	0.957	0.881	1.015
p,p'-DDE	12.00	2.21	0.18	1.03	0.956	0.879	1.014

Table 4-3 – Model Bias for the EPT and Steady-state models

	EPT	Steady-state		
		Hatchling	Subadult	Adult
Ochten				
MB	0.74	0.7	0.67	0.73
Factor	5.45	5.01	4.68	5.37
Gelderse				
MB	1.04	1.01	0.97	1.03
Factor	10.96	10.23	9.33	10.72

It is also important to examine the reasons why the EPT and steady-state models produce such similar results. This observation can be explained by the similarities between the main equations driving the predictions for both models. For the EPT model, predictions are made based on the ratio of BCF/K_{SW}. Given that dietary uptake is the major uptake route, the predictions made by the steady-state model are largely driven by K_{BF}, the partition coefficient describing the distribution of chemical between biota and its fecal material. Because earthworms only consume soil organic matter, BCF/K_{SW} and K_{BF} are actually very similar since K_{BF} is equivalent to BCF /K_{FW}, where K_{FW} is the partition coefficient describing the distribution of chemicals between fecal material and water. In fact, due to digestion of organic carbon in the gut of the earthworm, BCF/K_{FW} is actually greater than BCF/K_{SW}. However, as discussed before, growth dilution and reproduction act to lower the predicted body burden (C_B) and thus the BSAF.

One possible explanation for the performance of the model is that solubilization of chemical in the gut is much more limited than previously thought. The chemical uptake efficiency (E_D), which essentially describes the efficiency of chemical transfer across the gut wall, accounts for both solubilization of chemical in the gut and transfer across the gut wall. It is possible that solubilization of the chemical is limited because chemicals are "sequestered" in a slowly-desorbing fraction of the soil. This phenomenon has been reported in several studies (e.g. Luthy RG et al., 1997, Reid BJ et al., 2000, Kraaij R et al., 2002). As the chemical "ages" in the soil, the bioavailability to soil-dwelling organisms decreases as more chemical becomes sequestered. The fraction of chemical in sediments which is "sequestered" (i.e. subject to slow desorption kinetics) can account for up to 98% of the total (Cornelissen G et al., 2000, Kraaij R et al, 2003)

and is related to the length of time the chemical has been present in the soil. The chemicals analyzed in the Rhine-Meuse Delta study are all historic contaminants suggesting that much of the chemical may be sequestered. To simulate this phenomenon, a 'sequestration' factor was incorporated into the k_{UW} and k_{UD} term to reflect decreased bioavailability from the soil without influencing the chemical uptake efficiencies (E_D, E_W) and fecal elimination rate constant. Table 4.4 shows the performance of the model with 'sequestration' factors of 0.2 and 0.1 for the Ochten and Gelderse Poort sites respectively.

Table 4-4– Model Performance of Steady-state models with 'Sequestration' Factor

	Steady-state		
	Hatchling	Subadult	Adult
Ochten			
MB	0.01	-0.02	0.04
Factor	1.02	0.95	1.10
Gelderse			
MB	0.01	-0.03	0.04
Factor	1.01	0.93	1.10

Although model performance is vastly improved by the addition of the 'sequestration' factor, the utility of the steady-state models has not necessarily improved since the appropriate 'sequestration' factor was deduced from the performance of the model in relation to the observed data and can not be determined *a priori*. Furthermore, although bioavailability of historic contaminants may be limited to some degree, substances that are constantly released into the environment can not be expected to behave in the same way. Without a better sense of the true fraction of contaminant available to soil-dwelling invertebrates, both the EPT and steady-state models can be expected to overestimate BSAFs, particularly for chemicals which have been present in the soil for a long period a

time. Developing methods to assess the actual bioavailability of soil contaminants such as thin-film solid-phase extraction should therefore be a priority.

4.2 Bioaccumulation in Terrestrial Organisms

The performance of the bioaccumulation model for terrestrial organisms was evaluated by comparing observed and predicted lipid-equivalent biomagnification factors (BMFs) for recalcitrant PCBs. Ideally, body burdens in terrestrial organisms would be predicted directly from soil concentrations and estimated BSAFs and compared to observations. However, given the tendency of the BSAF model to over-predict concentrations in soil invertebrates, observed concentrations were used instead. For the purposes of this study, recalcitrant PCBs are congeners that do not have adjacent open meta-para sites on the biphenyl ring as illustrated in Figure 4.12. All 209 PCB congeners are categorized on this basis and the compiled list is presented in Appendix D.

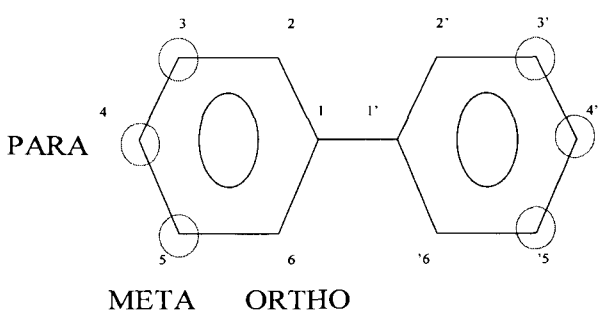


Figure 4-9 – PCB Structure Illustrating Sites of Metabolic Susceptibility

Unfortunately, some of the observed data report combined concentrations of two or more PCB congeners that have "mixed metabolic sensitivity" (e.g one may be recalcitrant, the other readily metabolized). Assuming that metabolism of all congeners in soil invertebrate prey items is negligible, observed BMFs could significantly underestimate

the actual BMF depending on the contribution that the readily metabolized congener makes to the prey item concentration. Two other issues with the observed data complicated the analysis. First, earthworms were starved for 24 hours to remove soil present in the digestive tract (Main Hendriks 1995). In nature, shrews consume earthworms and the soil in the digestive tract. By analyzing only earthworms, the concentration in the diet is artificially lowered, which will result in higher calculated BMFs. The other complicating factor is that the researchers reported the lipid-normalized liver concentrations in the shrews rather than the whole body concentrations. Since the proposed model predicts whole-body concentrations, inter-tissue equilibrium (lipid-equivalent basis) was assumed in order to make comparisons. However, Sigura et al (1975) reported that elimination of both PCB155 (recalcitrant) and PCB065 (readily metabolized) occurs more rapidly from the liver than adipose tissue in mice once dietary exposure ceases suggesting that observed BMFs based on liver concentrations could underestimate BMFs based on whole-body concentrations. Under conditions of constant exposure (as in the environment) though, it is not at all clear if Sigura et al's findings are relevant. Given that field observations (Kelly BC & Gobas FAPC, 2001) and analyses of pharmacokinetic models (Hickie BE et al., 1999) suggest that inter-tissue equilibrium is a valid assumption for certain animals, it seems reasonable to make the same assumption for this study.

Observed and predicted lipid-equivalent BMFs in shrews for recalcitrant and mixed metabolic sensitivity congeners are presented in Figure 4.13 - 4.14 and 4.15 – 4.16 respectively. The original data is presented in Appendix E. The range of predicted values resulting from the Monte Carlo simulations are represented by the thin grey bars.

Where possible, the 95% confidence intervals for the observations are also shown. Note that to be more consistent with the observed data, predicted BMFs were calculated as ratio of predicted shrew and observed worm concentrations (without ingested soil).

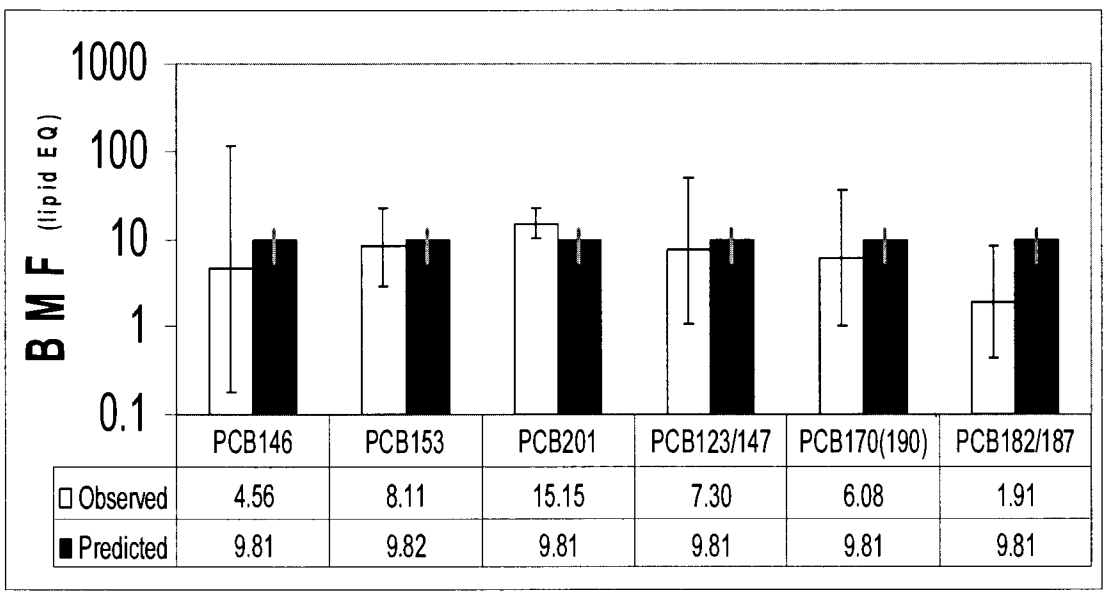


Figure 4-10 – Observed vs Predicted BMFs for Recalcitrant PCBs in Ochten

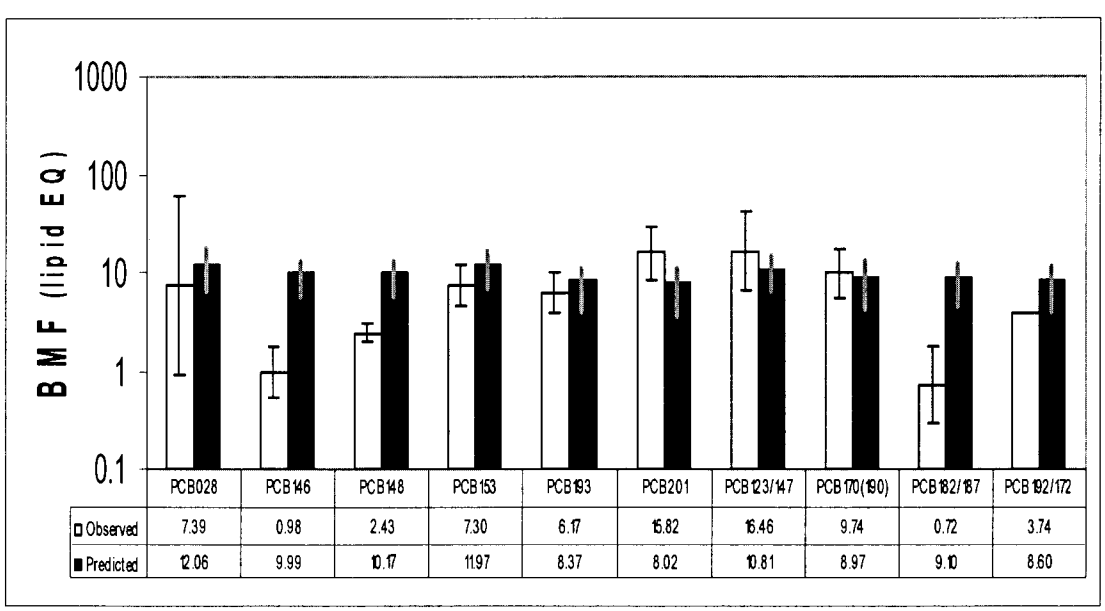


Figure 4-11 – Observed vs Predicted BMFs for Recalcitrant PCBs in Gelderse Poort

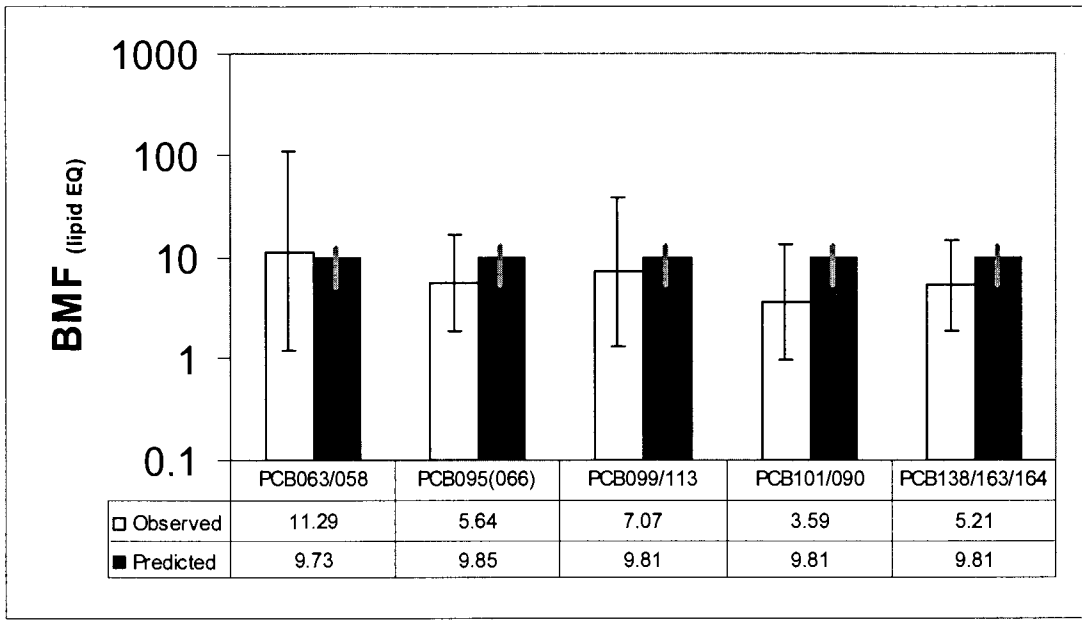


Figure 4-12 – Observed and Predicted BMFs for Mixed Metabolic Sensitivity Coeluted PCBs in Ochten

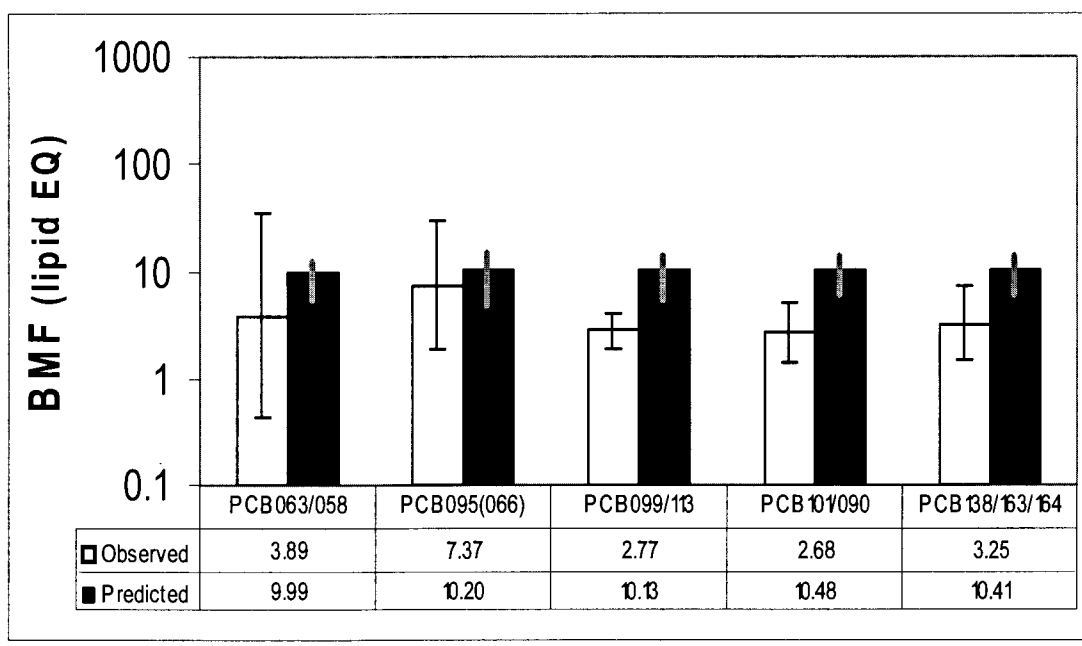


Figure 4-13 – Observed and Predicted BMFs for Mixed Metabolic Sensitivity Coeluted PCBs in Gelderse Poort

The effect of incorporating different diet items on predicted BMFs is shown below in Figure 4.14.

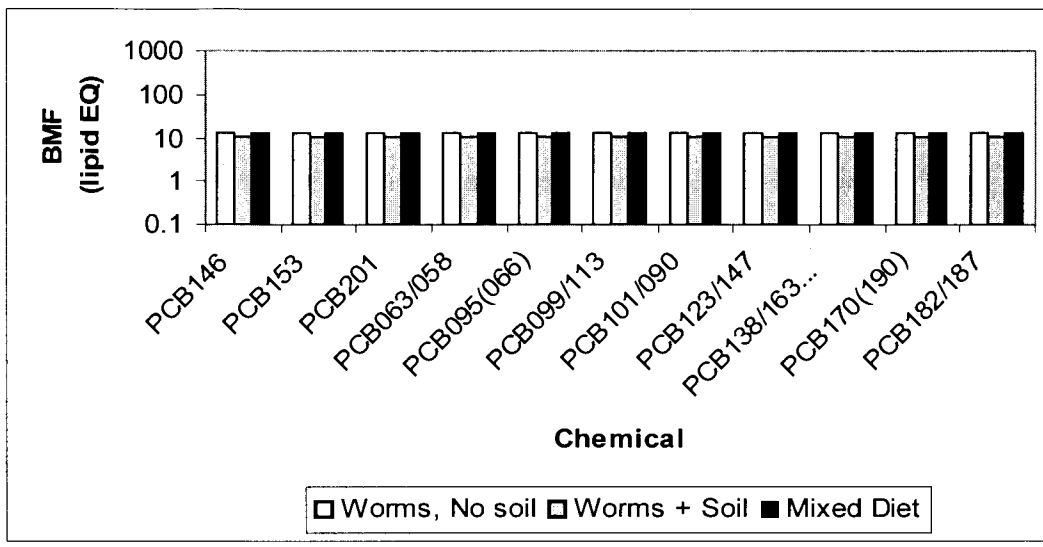


Figure 4-14 – Predicted BMFs as a Function of Diet

Overall, the terrestrial bioaccumulation model for the shrews performed well despite the concerns discussed previously. The calculated model bias (MB) for all congeners modeled in Ochten and Gelderse was 0.21 and 0.35 respectively which indicates that the predictions for the deterministic model were typically within a factor of 1.5 to 2.5 of the observations. The predicted BMFs also fell within the 95% confidence intervals for the majority of observed BMFs. Furthermore, the results of diet change and the Monte Carlo simulations suggest that the model predictions are not overly sensitive to variation of key input parameters. Recalcitrant PCBs with observed BMFs less than 1 (e.g. Gelderse PCB 146 and PCB 182/187) can not be explained by this model nor any current theory of bioaccumulation. These results could be due to analytical error or misidentification of PCB congeners. Coeluted congeners with mixed metabolic sensitivity tended to have lower observed BMFs (Figure 4-12, 4-13) suggesting the possibility that metabolism of susceptible congeners occurs significantly faster in the

shrew compared to earthworms. However, given that the observed BMFs of coeluted congeners with mixed metabolic sensitivity are not significantly different from the BMFs of recalcitrant congeners, there is no statistical basis to conclude that metabolism of certain PCB congeners in the shrew is responsible for this trend. Nevertheless, all researchers should be aware of this potential problem when interpreting coeluted PCB data in organisms with the capability to readily metabolize certain congeners.

4.3 Physico-chemical properties and Bioaccumulative Potential

The relationship between K_{OW}, K_{OA} and BMF was investigated using the terrestrial bioaccumulation model for the male shrew. The results of this analysis are presented in Figure 4.15.

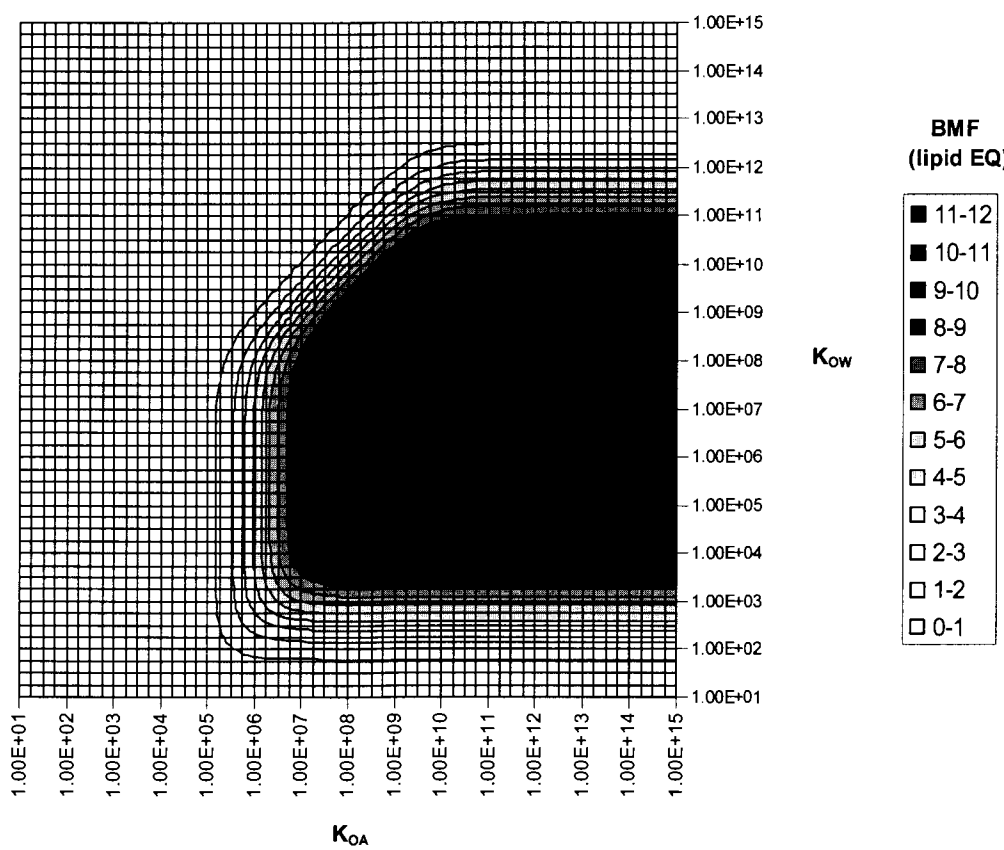


Figure 4-15 – Lipid Equivalent BMFs as a Function of K_{OW} and K_{OA}

The bioaccumulation model suggests that recalcitrant substances with a log K_{OA} of 5 or less will not biomagnify regardless of the value for log K_{OW} due to efficient elimination via exhalation. Substances with log K_{OW} of approximately 1.75 or less will not biomagnify due to efficient elimination, particularly via urine. Superlipophilic chemicals with log K_{OW} greater than 8 will not biomagnify until log K_{OA} is greater than at least 6, indicating that elimination via exhalation is still relatively efficient compared to dietary uptake for chemicals with these physico-chemical properties. Except for these chemicals though, substances with log K_{OW} values greater than 1.75 and log K_{OA} values greater than 5 exhibit BMFs greater than 1, indicating the potential to biomagnify in terrestrial organisms.

The predicted lipid equivalent BMFs were largely insensitive to the value of Φ used to account for the temperature dependence of K_{OA} and K_{AW}. The only significant difference found was in the predicted threshold K_{OA}. The baseline scenario ($\Phi = 20$) predicts that substances with log K_{OA} values less than approximately 5.25 will not biomagnify. While this threshold value remains constant for Φ values from 20 to 50, as Φ is decreased below the baseline value, the threshold log K_{OA} value shifts downward. For example, when $\Phi = 2$, the threshold log K_{OA} value falls slightly below 5. This result can be explained by the fact that elimination via exhalation becomes relatively less efficient in mammals (K_{OA} calculated at 37°C) compared to earthworms (K_{OA} calculated at 10°C) as Φ is decreased.

The results of this analysis are remarkably similar to the results reported by Czub G & McLachlan MS (2004). In that study, the bioaccumulative potential of persistent organic pollutants was explored as a function of K_{OW} and K_{OA} using a bioaccumulation

model that describes chemical transfer through aquatic and agricultural food chains to humans (ACC-HUMAN). The authors concluded that substances with log K_{OW} less than 11 and log K_{OA} greater than 6 have the inherent potential to biomagnify in the human food web. The highest bioaccumulative potential was found for substances with log K_{OW} values from 2 to 11 and log K_{OA} values from 6 to 12. The convergence of results of this study and the Czub G & McLachlan MS study are encouraging and further strengthen the argument that the bioaccumulation criteria need to be re-examined. These results also provide a strong rationale to conduct dietary uptake studies with terrestrial species using persistent chemicals with log K_{OW} values less than 5. Candidate substances for such studies include hexachlorocyclohexanes, endosulfan, atrazine, bis-4-chlorophenyl sulfone (BCPS), tris-chlorophenyl methanol and PFOS as empirical data from a limited number of field studies has already demonstrated the bioaccumulative potential of these substances (Kelly BC et al., 2004).

The generic model can also be used to investigate the relationship between K_{OW}, K_{OA} and BSAF. The results of this analysis are shown in Figure 4.16. The shape of the contour plot is essentially the same as the BMF contour plot except that the magnitude of the BSAFs is lower than the magnitude of the associated BMFs. The BSAF contour plot illustrates that substances with log $K_{OW} > 2$ and < 12 and log K_{OA} values > 6 will generally bioaccumulate in biota to levels that exceed the lipid-equivalent soil concentrations. Substances with physico-chemical properties outside this range will not bioaccumulate to levels in excess of the lipid-equivalent soil concentration due to more efficient elimination. The results of this analysis illustrate that soil remediation targets

for substances with log K_{OW} > 2 and < 12 and log K_{OA} > 6 must account for the inherent potential to bioaccumulate in terrestrial organisms.

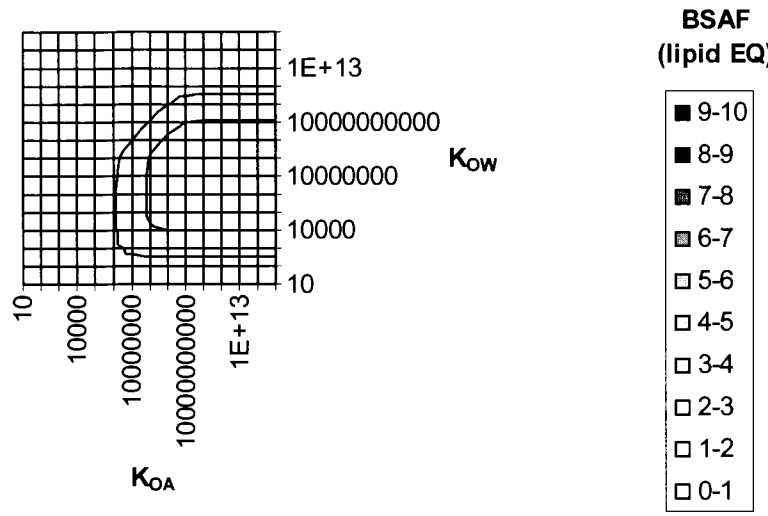
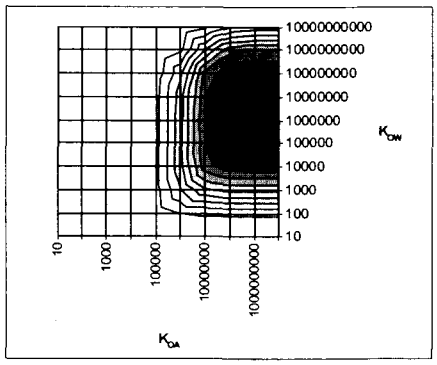


Figure 4-16 – Lipid equivalent BSAFs as a Function of K_{OW} and K_{OA}

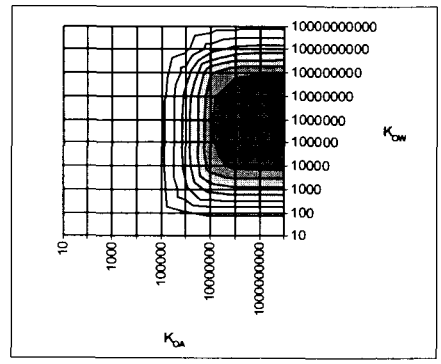
4.4 Metabolism and Bioaccumulative Potential

The terrestrial bioaccumulation model was used to investigate the relationship between metabolism and bioaccumulative potential in order to estimate a threshold metabolic rate constant threshold above which substance do not biomagnify (i.e. BMF = 1 or less). The diet was assumed to be the same as in section 4.3. The results of this analysis are shown in Figure 4.17(a-f).

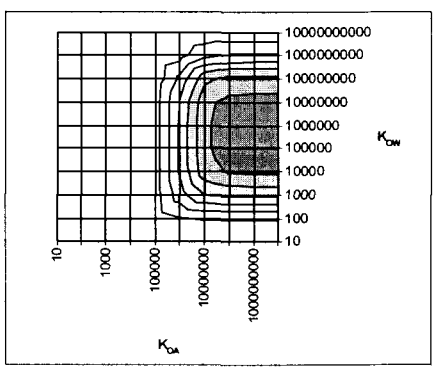
(a) $k_{MT} = 0.001$



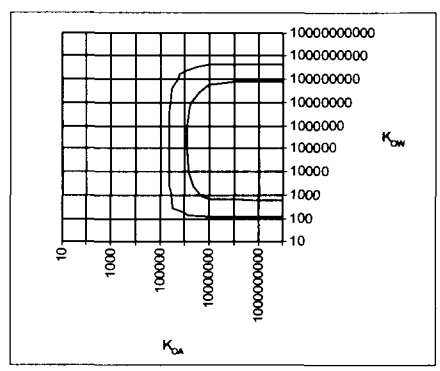
(b) $k_{MT} = 0.005$



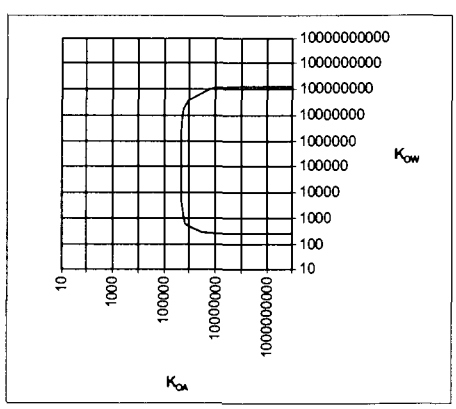
(c) $k_{MT} = 0.01$



(d) $k_{MT} = 0.05$



(e) $k_{MT} = 0.1$



(f) $k_{MT} = 0.2$

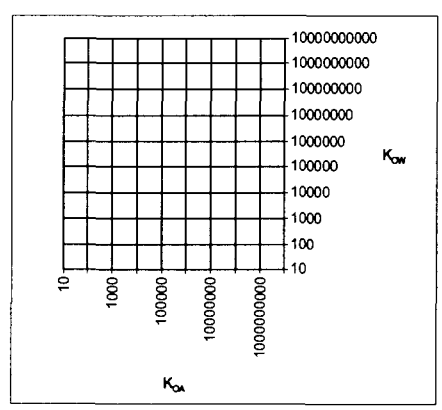


Figure 4-17 (a-f) – Effect of Metabolism on Bioaccumulative Potential

The model suggests that a metabolic rate constant (k_{MT}) of 0.2 d^{-1} or greater effectively negates the bioaccumulative potential of contaminants regardless of their physico-chemical properties. It is important to realize that this threshold value depends on how the model is parameterized. For example, if the lipid or non-lipid organic matter absorption efficiency is increased, the predicted BMFs of chemical substances will increase as well, meaning that the threshold k_{MT} will also be higher. Conversely, if other elimination processes such as growth dilution and maternal transfer (via lactation, parturition, egg-laying) are incorporated into the model, the estimated threshold k_{MT} value will decrease. However, since adult males (no significant growth) may be the most sensitive ecological receptors, it is sensible to consider metabolism as the only additional elimination route for the purposes of establishing a threshold value. As a precautionary measure, estimated metabolic threshold values could be doubled to account for the variability in model output. Alternatively, worst-case scenarios could be used to estimate threshold values. Developing models of other species (e.g. with more efficient digestion or higher dietary lipid content) also seems prudent, especially for organisms which are more sensitive to organic contaminants.

4.5 Steady-state Bioaccumulation Model for the Little Owl

Assuming a diet of 80% earthworms and 20% shrews and using the observed concentrations for these organisms, steady-state bioaccumulation model for the little owl predicts a lipid-equivalent BMF of approximately 17 for PCB 146, 153 and 201 (all recalcitrant). The effect of diet on predicted body burdens (C_B) of PCB 146 and BMF was explored by varying the proportion of earthworms in the diet from 0 to 100%. The results of this exercise are presented in Table 4.5.

Table 4-5 – Predicted BMFs as Function of Diet for the Little Owl

Proportion (%)	C_B ug / kg lipid EQ	C_{DIET} ug / kg lipid EQ	BMF
0	9998	757	13.2
10	9507	699	13.8
20	8962	622	14.4
30	8349	554	15.1
40	7660	486	15.8
50	6877	418	16.5
60	5980	350	17.1
70	4940	281	17.6
80	3724	213	17.5
90	2280	145	15.7
100	539	77	7

As shown in Table 4.5, diet does not have a substantial effect on the magnitude of predicted body burdens and BMFs until the proportion of earthworms reaches 100%. Although the magnitude of the predicted body burden falls as the proportion of earthworms in the diet increases, the concentration in the diet also decreases which counteracts this tendency. The substantial drop in predicted BMF when the proportion of earthworms in the diet reaches 100% is related to the low lipid content of earthworms and the resulting high lipid-normalized concentrations in comparison to the Little Owl.

The output of the model was compared to observed lipid-normalized BMFs for herons and herring gulls. In these animals, BMFs were reported to range up to a maximum of 23 and 32 respectively (Kelly BC & Gobas FAPC, in press). The results of the terrestrial model for the little owl are reasonably consistent with these observations as well as with the range of BMFs (10-30) reported by Hendriks AJ (1995) for secondary carnivores. If detailed information about the diet and contaminant levels of prey items is available, the results of the model for shrews and Little Owls suggest that the steady-state terrestrial is a useful tool for assessing the concentrations in predator species. However,

the results of this exercise also indicate that good information on the composition of diet can be important for generating accurate predictions.

4.6 Hazard Assessment and Remediation of Contaminated Sites

The hazard assessment for dieldrin in shrews inhabiting the Ochten flood plains was conducted using the observed soil concentrations and observed BSAF assuming a diet of 100% earthworms. The results of the assessment using the NOAEL and the RfD are shown in Figure 4.18 and 4.19 respectively.

Substance	Dieldrin	
RfD	5.00E-05	mg/kg/d
NOAEL	5.00E-03	mg/kg/d
Mass	0.01	kg
Feeding	0.01	kg / day
Soil Ingestion	0.00051	kg / day
C_{SOIL}	4.1	ug/kg
	0.0041	mg / kg
BSAF	0.4	
C_{DIET}	0.00164	mg / kg
DOSE	0.0018491	mg / kg / day
H	0.37	
Remediated		
C_{SOIL}	Not Required	ug / kg dry

Figure 4-18 – Hazard Assessment for Dieldrin using the NOAEL

Substance	Dieldrin	
RfD	5.00E-05	mg/kg/d
NOAEL	5.00E-03	mg/kg/d
Mass	0.01	kg
Feeding	0.01	kg / day
Soil Ingestion	0.00051	kg / day
C_{SOIL}	4.1	ug/kg
	0.0041	mg / kg
BSAF	0.4	
C_{DIET}	0.00164	mg / kg
DOSE	0.0018491	mg / kg / day
H	36.98	
Remediated		
C_{SOIL}	0.111	ug / kg dry

Figure 4-19 – Hazard Assessment for Dieldrin using the RfD

The results of the hazard assessment depend on the choice of reference dose. If the hazard assessment is conducted using the NOAEL from a laboratory study on rats, then the contaminant levels in Ochten are not considered to present any danger to shrews inhabiting the area. On the other hand, if the RfD is used, as it would be for a human exposure assessment, then dieldrin contamination levels do present a hazard ($H > 1$). According to the assessment, dieldrin levels in the soil would continue to present a danger until soil concentrations were reduced to approximately 0.1 ug / kg dry soil.

The choice of reference point is controversial. It can be argued that the NOAEL determined through long-term toxicity studies on rats is the more appropriate measure for a hazard assessment of another rodent species. In other words, the safety factors applied

to the NOAEL are too conservative and inter-species sensitivity differences are unlikely to be relevant. This conclusion may be reasonable for shrews but may not be for other species that may differ in sensitivity to the contaminant. As an example, a hazard assessment for the little owl was conducted using the NOAEL for dieldrin. Exposure was calculated using estimated feeding rates, the observed BSAF for earthworms and a predicted BMF (on a wet-weight basis). The diet was assumed to be 80% earthworms and 20% shrews and the results are presented in Figure 4.20. Using the NOAEL as a reference point, H is approximately 0.98 which indicates that the levels of dieldrin in the soil present no danger to the Little Owl. In this case however, it is much more difficult to argue in favour of using the NOAEL given the lack of knowledge regarding inter-species sensitivity to contaminants. If a safety factor of 2 is applied to the NOAEL, the hazard assessment will then conclude that Little Owls are at risk. While the merits and limitations of the hazard assessment methodology could be debated more thoroughly, a further discussion is beyond the scope of this project.

Mass	0.185	kg
Feeding	0.0671	kg / day
Soil Ingestion	0.00187	kg / day
C_{SOIL}	4.1	ug / kg dry
BSAF	0.4	kg dry / kg wet
C_{WORM}	1.64	ug / kg wet
C_{SHREW}	65.6	ug / kg wet
BMF	40	kg wet / kg wet
EXPOSURE	0.0049	mg / kg / day
H	0.98	

Figure 4-20 – Hazard Assessment for the Little Owl

5.0 CONCLUSIONS

This study has demonstrated the potential of a relatively simple mechanistic model to predict biomagnification factors in a terrestrial mammal with reasonable accuracy. The most important finding of this project related to the model development is that the current screening level criteria for bioaccumulative potential are inadequate for properly identifying bioaccumulative substance in terrestrial organisms. Recalcitrant substances with log K_{OW} values greater than 2 and log K_{OA} values greater than 5 were shown to biomagnify in certain terrestrial organisms, particularly those with high digestive efficiencies (e.g. carnivorous animals, humans). The model output should be validated for substances with these physico-chemical properties as soon as possible. If these results are confirmed, the number of substances on the DSL that are considered bioaccumulative could expand significantly. However, as demonstrated by the BMF model, biomagnification will not occur if a threshold metabolic rate is exceeded, regardless of physico-chemical properties. Unfortunately, data on metabolic sensitivities is not abundant. This issue is also complicated by the dependence of the exact threshold value on diet and digestive capabilities of the organism. However, metabolic threshold values for indicator species could be estimated from model outputs using Monte Carlo or 'worst-case' scenarios. Comparisons with existing empirical data would also be extremely useful. Since the purpose of the screening level criteria is to identify substances with the potential to be of concern, the issue of bioaccumulative potential in

terrestrial organisms and the potential of metabolism to negate biomagnification should be of great interest to officials and scientists involved in the DSL categorization process.

The proposed models for estimating the bioaccumulation of chemicals in soil invertebrates were not as successful. Both the EPT and steady-state approach overestimate observed BSAFs by a factor of up to an order of magnitude. This degree of model bias prevents the use of these models to characterize chemical concentrations in biota throughout a food-chain based solely on measured soil concentrations. Given an accurate measure of the actual bioavailable fraction of chemical however, it is reasonable to assume that the performance of the proposed models will improve. It is also interesting to note that the EPT and steady-state models are likely to result in similar predictions for organisms that consume soil organic matter. For such animals, the EPT approach, calibrated with an appropriate sequestration factor, may be sufficient to accurately predict bioaccumulation. For organisms such as insects that consume living plant material, the steady-state model is likely to be more useful. Considering the number of mammal and avian species that consume insects, developing and evaluating a steady-state model for insects would be a worthwhile endeavour, assuming an appropriate data set can be located.

APPENDIX A : K_{OW} AND K_{OA} OF MODELLED COMPOUNDS

Table A1 – Octanol-water Partition Coefficient of Modelled Compounds

Chemical	log K_{OW}
PCB028	5.67
PCB052	5.84
PCB110	6.48
PCB149	6.67
PCB151	6.64
PCB146	6.89
PCB153	6.92
PCB201	7.62
PCB095(066)	6.13
PCB099/113	6.46
PCB101/090	6.25
PCB123/147	6.69
PCB138/163/164	6.95
PCB170(190)	7.27
PCB182/187	7.20
PCB022	5.58
PCB087	6.29
PCB110	6.48
PCB111	6.76
PCB118	6.74
PCB141	6.82
PCB148	6.73
PCB174	7.11
PCB177	7.08
HCB	5.73
Dieldrin	5.10
p,p'-DDT	6.06
p,p'-DDE	6.60

Table A2 – Octanol-air Partition Coefficients for Modelled Compounds at 10°C, 20°C and 37°C

Congener	Substitution Pattern	α	β	$\log K_{OA}$ 10°C	$\log K_{OA}$ 20°C	$\log K_{OA}$ 37°C
3	4	-4.82	3470	7.44	7.02	6.37
15	4,4'	-5.06	3792	8.34	7.88	7.17
29	2,4,5	-4.77	3792	8.63	8.17	7.46
49	2,2',4,5	-4.96	3981	9.11	8.63	7.88
53	2,2',5,6'	-5.26	3965	8.75	8.27	7.53
61	2,3,4,5	-2.89	3464	9.35	8.93	8.28
66	2,3',4,4'	-3.82	3827	9.70	9.24	8.53
77	3,3'4,4'	-3.14	3828	10.39	9.92	9.21
95	2,2',3,5',6	-4.3	3904	9.50	9.02	8.29
96	2,2',3,6,6'	-4.6	3913	9.23	8.75	8.02
101	2,2',4,5,5'	-3.82	3841	9.75	9.29	8.57
105	2,3,3',4,4'	-5.68	4678	10.85	10.29	9.41
118	2.3',4,4',5	-5.92	4693	10.66	10.10	9.22
126	3,3',4,4',5	-5.98	4870	11.23	10.64	9.73
138	2,2',3,4,4',5'	-5.57	4584	10.63	10.08	9.22
153	2,2',4,4',5,5'	-6.02	4695	10.57	10.00	9.13
155	2,2',4,4',6,6'	-2.21	3954	11.76	11.28	10.54
171	2,2',3,3',4,4',6	-5.71	4757	11.10	10.53	9.64
180	2,2',3,4,4',5,5'	-4.7	4535	11.32	10.78	9.93

APPENDIX B : TEMPERATURE DEPENDENCE OF AIR-WATER PARTITION COEFFICIENT

Table B1 – Temperature Dependence of the Air-water Partition Coefficient (K_{AW})

Chemical	H_H	S_H	ln K_{AW}			K_{AW}		
			10°C	25°C	37°C	10°C	25°C	37°C
PCB028	33	0.0700	-5.6056	-4.8997	-4.3841	0.0037	0.0074	0.0125
PCB052	31	0.0700	-4.7556	-4.0925	-3.6082	0.0086	0.0167	0.0271
PCB149	46	0.1200	-5.1169	-4.1328	-3.4142	0.0060	0.0160	0.0329
PCB151	37	0.1000	-3.6974	-2.9059	-2.3278	0.0248	0.0547	0.0975
PCB146	59	0.1700	-4.6281	-3.3660	-2.4442	0.0098	0.0345	0.0868
PCB148	47	0.1300	-4.3391	-3.3337	-2.5994	0.0130	0.0357	0.0743
PCB153	66	0.1900	-5.1976	-3.7857	-2.7546	0.0055	0.0227	0.0636
PCB193	140	0.4300	-7.7816	-4.7867	-2.5994	0.0004	0.0083	0.0743
PCB201	145	0.4600	-6.2984	-3.1965	-0.9311	0.0018	0.0409	0.3941
PCB095(066)	21	0.0400	-4.1139	-3.6647	-3.3366	0.0163	0.0256	0.0356
PCB099/113	16	0.0200	-4.3944	-4.0521	-3.8022	0.0123	0.0174	0.0223
PCB101/090	30	0.0200	-10.3443	-9.7025	-9.2338	0.0000	0.0001	0.0001
PCB123/147	56	0.1500	-5.7586	-4.5607	-3.6858	0.0032	0.0105	0.0251
PCB138/163/164	87	0.2600	-5.7034	-3.8423	-2.4830	0.0033	0.0214	0.0835
PCB170(190)	54	0.1400	-6.1114	-4.9562	-4.1125	0.0022	0.0070	0.0164
PCB182/187	97	0.3000	-5.1424	-3.0673	-1.5519	0.0058	0.0465	0.2118
PCB192/172	149	0.4600	-7.9983	-4.8109	-2.4830	0.0003	0.0081	0.0835
PCB087	33	0.0700	-5.6056	-4.8997	-4.3841	0.0037	0.0074	0.0125
PCB097	30	0.0700	-4.3306	-3.6889	-3.2202	0.0132	0.0250	0.0399
PCB110	38	0.0900	-5.3251	-4.5122	-3.9185	0.0049	0.0110	0.0199
PCB111	56	0.1500	-5.7586	-4.5607	-3.6858	0.0032	0.0105	0.0251
PCB141	70	0.2000	-5.6949	-4.1974	-3.1038	0.0034	0.0150	0.0449
PCB174	113	0.3500	-5.9286	-3.5113	-1.7459	0.0027	0.0299	0.1745
PCB177	112	0.3400	-6.7063	-4.3104	-2.5606	0.0012	0.0134	0.0773
PCB179	62	0.1800	-4.7004	-3.3741	-2.4054	0.0091	0.0342	0.0902

APPENDIX C : DIETARY UPTAKE EFFICIENCY FOR TERRESTRIAL MAMMALS

Table C1 – Observed Dietary Uptake Efficiency Data

Compound	$\log K_{OW}$	K_{OW}	E_D	$1/E_D$	Species	SOURCE
PCB004	4.65	44668.36	0.96	1.04166667	RAT	Tanabe et al, 1981
PCB009	5.06	114815.4	0.94	1.06382979	RAT	Tanabe et al, 1981
PCB007	5.07	117489.8	0.95	1.05263158	RAT	Tanabe et al, 1981
PCB008	5.07	117489.8	0.93	1.07526882	RAT	Tanabe et al, 1981
PCB015	5.3	199526.2	0.95	1.05263158	RAT	Tanabe et al, 1981
PCB019	5.02	104712.9	0.93	1.07526882	RAT	Tanabe et al, 1981
PCB018	5.24	173780.1	0.925	1.08108108	RAT	Tanabe et al, 1981
PCB017	5.25	177827.9	0.925	1.08108108	RAT	Tanabe et al, 1981
PCB016/027	5.3	199526.2	0.93	1.07526882	RAT	Tanabe et al, 1981
PCB032	5.44	275422.9	0.925	1.08108108	RAT	Tanabe et al, 1981
PCB026/034	5.66	457088.2	0.925	1.08108108	RAT	Tanabe et al, 1981
PCB025	5.67	467735.1	0.91	1.0989011	RAT	Tanabe et al, 1981
PCB020/028	5.62	416869.4	0.91	1.0989011	RAT	Tanabe et al, 1981
PCB033	5.6	398107.2	0.9	1.11111111	RAT	Tanabe et al, 1981
PCB037	5.83	676083	0.89	1.12359551	RAT	Tanabe et al, 1981
PCB050	5.63	426579.5	0.91	1.0989011	RAT	Tanabe et al, 1981
PCB052/043	5.8	630957.3	0.91	1.0989011	RAT	Tanabe et al, 1981
PCB048/049	5.82	660693.4	0.87	1.14942529	RAT	Tanabe et al, 1981
PCB059/069	6	1000000	0.885	1.1299435	RAT	Tanabe et al, 1981
PCB075/044	5.9	794328.2	0.885	1.1299435	RAT	Tanabe et al, 1981
PCB042/064	5.85	707945.8	0.885	1.1299435	RAT	Tanabe et al, 1981
PCB040/041	5.67	467735.1	0.885	1.1299435	RAT	Tanabe et al, 1981
PCB070	6.2	1584893	0.885	1.1299435	RAT	Tanabe et al, 1981
PCB076	6.13	1348963	0.865	1.15606936	RAT	Tanabe et al, 1981
PCB055	6.11	1288250	0.85	1.17647059	RAT	Tanabe et al, 1981
PCB077	6.36	2290868	0.89	1.12359551	RAT	Tanabe et al, 1981
PCB095	6.14	1380384	0.85	1.17647059	RAT	Tanabe et al, 1981
PCB084	6.04	1096478	0.865	1.15606936	RAT	Tanabe et al, 1981
PCB092	6.35	2238721	0.835	1.19760479	RAT	Tanabe et al, 1981
PCB101	6.38	2398833	0.835	1.19760479	RAT	Tanabe et al, 1981
PCB099	6.39	2454709	0.815	1.22699387	RAT	Tanabe et al, 1981
PCB087/097	6.29	1949845	0.83	1.20481928	RAT	Tanabe et al, 1981
PCB082/110	6.34	2187762	0.84	1.19047619	RAT	Tanabe et al, 1981
PCB107	6.71	5128614	0.8	1.25	RAT	Tanabe et al, 1981
PCB118	6.74	5495409	0.8	1.25	RAT	Tanabe et al, 1981
PCB105	6.65	4466836	0.82	1.2195122	RAT	Tanabe et al, 1981
PCB136	6.22	1659587	0.85	1.17647059	RAT	Tanabe et al, 1981
PCB135	6.64	4365158	0.805	1.24223602	RAT	Tanabe et al, 1981
PCB148/151	6.69	4897788	0.8	1.25	RAT	Tanabe et al, 1981
PCB134	6.55	3548134	0.82	1.2195122	RAT	Tanabe et al, 1981
PCB132	6.58	3801894	0.82	1.2195122	RAT	Tanabe et al, 1981
PCB146	6.89	7762471	0.785	1.27388535	RAT	Tanabe et al, 1981
PCB153/141	6.87	7413102	0.78	1.28205128	RAT	Tanabe et al, 1981
PCB130	6.8	6309573	0.795	1.25786164	RAT	Tanabe et al, 1981
PCB138	6.83	6760830	0.78	1.28205128	RAT	Tanabe et al, 1981
PCB128	6.74	5495409	0.8	1.25	RAT	Tanabe et al, 1981
PCB167	7.27	18620871	0.84	1.19047619	RAT	Tanabe et al, 1981
PCB156	7.18	15135612	0.79	1.26582278	RAT	Tanabe et al, 1981
PCB179	6.73	5370318	0.79	1.26582278	RAT	Tanabe et al, 1981

Compound	$\log K_{OW}$	K_{OW}	E_D	$1/E_D$	Species	SOURCE
PCB176	6.76	5754399	0.795	1.25786164	RAT	Tanabe et al, 1981
PCB178	7.14	13803843	0.78	1.28205128	RAT	Tanabe et al, 1981
PCB187	7.17	14791084	0.75	1.33333333	RAT	Tanabe et al, 1981
PCB174/183	7.15	14125375	0.78	1.28205128	RAT	Tanabe et al, 1981
PCB177	7.08	12022644	0.755	1.32450331	RAT	Tanabe et al, 1981
PCB171	7.11	12882496	0.765	1.30718954	RAT	Tanabe et al, 1981
PCB172	7.33	21379621	0.75	1.33333333	RAT	Tanabe et al, 1981
PCB180	7.36	22908677	0.755	1.32450331	RAT	Tanabe et al, 1981
PCB170	7.27	18620871	0.76	1.31578947	RAT	Tanabe et al, 1981
PCB202	7.24	17378008	0.66	1.51515152	RAT	Tanabe et al, 1981
PCB201	7.62	41686938	0.735	1.36054422	RAT	Tanabe et al, 1981
PCB200	7.27	18620871	0.73	1.36986301	RAT	Tanabe et al, 1981
PCB196	7.65	44668359	0.79	1.26582278	RAT	Tanabe et al, 1981
PCB194	7.8	63095734	0.77	1.2987013	RAT	Tanabe et al, 1981
PCB052	5.84	691831	0.913	1.09529025	RAT	Fries et al, 1989
PCB101	6.38	2398833	0.861	1.16144019	RAT	Fries et al, 1989
Benzene	2.15	141.2538	0.99	1.01010101	RABBIT	Owen 1990
Methylene chloride	1.25	17.78279	0.99	1.01010101	Unknown	Owen 1990
Naphthalene	3.37	2344.229	0.99	1.01010101	RAT	Owen 1990
Toluene	2.69	489.7788	0.99	1.01010101	RABBIT	Owen 1990
Xylene	3.15	1412.538	0.99	1.01010101	Unknown	Owen 1990
PCB001	4.46	28840.32	0.984	1.01626016	RAT	Albro & Fishbein 1972
PCB002	4.69	48977.88	0.973	1.02774923	RAT	Albro & Fishbein 1972
PCB003	4.69	48977.88	0.964	1.0373444	RAT	Albro & Fishbein 1972
PCB010	4.84	69183.1	0.949	1.05374078	RAT	Albro & Fishbein 1972
PCB004	4.65	44668.36	0.982	1.01832994	RAT	Albro & Fishbein 1972
PCB007	5.07	117489.8	0.971	1.02986612	RAT	Albro & Fishbein 1972
PCB006	5.08	120226.4	0.979	1.02145046	RAT	Albro & Fishbein 1972
PCB008	5.07	117489.8	0.976	1.02459016	RAT	Albro & Fishbein 1972
PCB013	5.29	194984.5	0.971	1.02986612	RAT	Albro & Fishbein 1972
PCB015	5.3	199526.2	0.974	1.02669405	RAT	Albro & Fishbein 1972
PCB018	5.24	173780.1	0.943	1.06044539	RAT	Albro & Fishbein 1972
PCB034	5.66	457088.2	0.95	1.05263158	RAT	Albro & Fishbein 1972
PCB035	5.82	660693.4	0.903	1.10741971	RAT	Albro & Fishbein 1972
PCB028	5.67	467735.1	0.94	1.06382979	RAT	Albro & Fishbein 1972
PCB052	5.84	691831	0.96	1.04166667	RAT	Albro & Fishbein 1972
PCB061	6.04	1096478	0.973	1.02774923	RAT	Albro & Fishbein 1972
PCB077	6.36	2290868	0.918	1.08932462	RAT	Albro & Fishbein 1972
PCB101	6.38	2398833	0.951	1.05152471	RAT	Albro & Fishbein 1972
PCB153	6.92	8317638	0.953	1.04931794	RAT	Albro & Fishbein 1972

APPENDIX D : METABOLIC SUSCEPTIBILITY OF PCB CONGENERS

Table D1 – Metabolic Susceptibility of PCB Congeners

Congener	Adjacent meta, para Hs?	Metabolic Susceptibility
1	YES	Metabolizable
2	YES	Metabolizable
3	YES	Metabolizable
4	YES	Metabolizable
5	YES	Metabolizable
6	YES	Metabolizable
7	YES	Metabolizable
8	YES	Metabolizable
9	YES	Metabolizable
10	YES	Metabolizable
11	YES	Metabolizable
12	YES	Metabolizable
13	YES	Metabolizable
14	YES	Metabolizable
15	NO	Recalcitrant
16	YES	Metabolizable
17	YES	Metabolizable
18	YES	Metabolizable
19	YES	Metabolizable
20	YES	Metabolizable
21	YES	Metabolizable
22	YES	Metabolizable
23	YES	Metabolizable
24	YES	Metabolizable
25	YES	Metabolizable
26	YES	Metabolizable
27	YES	Metabolizable
28	NO	Recalcitrant
29	YES	Metabolizable
30	YES	Metabolizable

Congener	Adjacent meta, para Hs?	Metabolic Susceptibility
31	YES	Metabolizable
32		Recalcitrant
33	YES	Metabolizable
34	YES	Metabolizable
35	YES	Metabolizable
36	YES	Metabolizable
37	NO	Recalcitrant
38	YES	Metabolizable
39	NO	Recalcitrant
40	YES	Metabolizable
41	YES	Metabolizable
42	YES	Metabolizable
43	YES	Metabolizable
44	YES	Metabolizable
45	YES	Metabolizable
46	YES	Metabolizable
47	NO	Recalcitrant
48	YES	Metabolizable
49	YES	Metabolizable
50	YES	Metabolizable
51	YES	Metabolizable
52	YES	Metabolizable
53	YES	Metabolizable
54	YES	Metabolizable
55	YES	Metabolizable
56	YES	Metabolizable
57	YES	Metabolizable
58	YES	Metabolizable
59	YES	Metabolizable
60	NO	Recalcitrant
61	YES	Metabolizable
62	YES	Metabolizable
63	NO	Recalcitrant
64	YES	Metabolizable
65	YES	Metabolizable
66	NO	Recalcitrant
67	YES	Metabolizable
68	NO	Recalcitrant
69	YES	Metabolizable
70	YES	Metabolizable
71	YES	Metabolizable
72	YES	Metabolizable

Congener	Adjacent meta, para Hs?	Metabolic Susceptibility
73	YES	Metabolizable
74	NO	Recalcitrant
75	NO	Recalcitrant
76	YES	Metabolizable
77	NO	Recalcitrant
78	YES	Metabolizable
79	NO	Recalcitrant
80	NO	Recalcitrant
81	NO	Recalcitrant
82	YES	Metabolizable
83	YES	Metabolizable
84	YES	Metabolizable
85	NO	Recalcitrant
86	YES	Metabolizable
87	YES	Metabolizable
88	YES	Metabolizable
89	YES	Metabolizable
90	NO	Recalcitrant
91	YES	Metabolizable
92	YES	Metabolizable
93	YES	Metabolizable
94	YES	Metabolizable
95	YES	Metabolizable
96	YES	Metabolizable
97	YES	Metabolizable
98	YES	Metabolizable
99	NO	Recalcitrant
100	NO	Recalcitrant
101	YES	Metabolizable
102	YES	Metabolizable
103	YES	Metabolizable
104	YES	Metabolizable
105	NO	Recalcitrant
106	YES	Metabolizable
107	NO	Recalcitrant
108	NO	Recalcitrant
109	YES	Metabolizable
110	YES	Metabolizable
111	NO	Recalcitrant
112	YES	Metabolizable
113	YES	Metabolizable
114	NO	Recalcitrant

Congener	Adjacent meta, para Hs?	Metabolic Susceptibility
115	NO	Recalcitrant
116	YES	Metabolizable
117	NO	Recalcitrant
118	NO	Recalcitrant
119	NO	Recalcitrant
120	NO	Recalcitrant
121	NO	Recalcitrant
122	YES	Metabolizable
123	NO	Recalcitrant
124	YES	Metabolizable
125	YES	Metabolizable
126	NO	Recalcitrant
127	NO	Recalcitrant
128	NO	Recalcitrant
129	YES	Metabolizable
130	NO	Recalcitrant
131	YES	Metabolizable
132	YES	Metabolizable
133	NO	Recalcitrant
134	YES	Metabolizable
135	YES	Metabolizable
136	YES	Metabolizable
137	NO	Recalcitrant
138	NO	Recalcitrant
139	NO	Recalcitrant
140	NO	Recalcitrant
141	YES	Metabolizable
142	YES	Metabolizable
143	YES	Metabolizable
144	YES	Metabolizable
145	YES	Metabolizable
146	NO	Recalcitrant
147	NO	Recalcitrant
148	NO	Recalcitrant
149	YES	Metabolizable
150	YES	Metabolizable
151	YES	Metabolizable
152	YES	Metabolizable
153	NO	Recalcitrant
154	NO	Recalcitrant
155	NO	Recalcitrant
156	NO	Recalcitrant
157	NO	Recalcitrant

Congener	Adjacent meta, para Hs?	Metabolic Susceptibility
158	NO	Recalcitrant
159	NO	Recalcitrant
160	YES	Metabolizable
161	YES	Metabolizable
162	NO	Recalcitrant
163	NO	Recalcitrant
164	YES	Metabolizable
165	NO	Recalcitrant
166	NO	Recalcitrant
167	NO	Recalcitrant
168	NO	Recalcitrant
169	NO	Recalcitrant
170	NO	Recalcitrant
171	NO	Recalcitrant
172	NO	Recalcitrant
173	YES	Metabolizable
174	YES	Metabolizable
175	NO	Recalcitrant
176	YES	Metabolizable
177	NO	Recalcitrant
178	NO	Recalcitrant
179	YES	Metabolizable
180	NO	Recalcitrant
181	NO	Recalcitrant
182	NO	Recalcitrant
183	NO	Recalcitrant
184	NO	Recalcitrant
185	YES	Metabolizable
186	YES	Metabolizable
187	NO	Recalcitrant
188	NO	Recalcitrant
189	NO	Recalcitrant
190	NO	Recalcitrant
191	NO	Recalcitrant
192	NO	Recalcitrant
193	NO	Recalcitrant
194	NO	Recalcitrant
195	NO	Recalcitrant
196	NO	Recalcitrant
197	NO	Recalcitrant
198	NO	Recalcitrant
199	NO	Recalcitrant
200	NO	Recalcitrant
201	NO	Recalcitrant
202	NO	Recalcitrant
203	NO	Recalcitrant
204	NO	Recalcitrant
205	NO	Recalcitrant
206	NO	Recalcitrant
207	NO	Recalcitrant
208	NO	Recalcitrant
209	NO	Recalcitrant

APPENDIX E : OBSERVED EARTHWORM, SHREW AND BMF DATA WITH STANDARD DEVIATIONS

Table E1 – Observed Earthworm (C_{SI}), Shrew (C_B) and BMF data (geometric means) with standard deviations (geometric SD) in Ochten

	C_{SI} (ug / kg lipid EQ)		C_B (ug / kg lipid EQ)		BMF (lipid EQ)	
Chemical	Mean	SD	Mean	SD	Mean	SD
PCB052	58.59	1.52	156.56	1.00	2.67	1.52
PCB110	83.70	1.47	234.83	3.96	2.81	4.17
PCB149	321.91	1.39	939.33	1.00	2.92	1.39
PCB151	77.26	1.22	336.59	1.22	4.36	1.33
PCB146	77.26	1.35	352.25	4.94	4.56	5.09
PCB153	135.20	1.38	1095.89	1.49	8.11	1.67
PCB201	41.85	1.00	634.05	1.22	15.15	1.22
PCB063/058	90.13	1.44	1017.61	2.91	11.29	3.09
PCB095(066)	70.82	1.48	399.22	1.47	5.64	1.73
PCB099/113	70.82	1.41	500.98	2.17	7.07	2.33
PCB101/090	128.76	1.48	461.84	1.70	3.59	1.93
PCB123/147	54.72	2.30	399.22	1.60	7.30	2.60
PCB138/163/164	225.34	1.39	1174.17	1.48	5.21	1.67
PCB170(190)	83.70	2.11	508.81	1.62	6.08	2.43
PCB182/187	270.40	1.39	516.63	1.95	1.91	2.10

Table E2 - Observed Earthworm (C_{SI}), Shrew (C_B) and BMF data (geometric means) with standard deviations (geometric SD) in Gelderse Poort

Chemical	C_{SI} (ug / kg lipid EQ)		C_B (ug / kg lipid EQ)		BMF (lipid EQ)	
	Mean	SD	Mean	SD	Mean	SD
PCB028	56.71	1.22	418.92	2.83	7.39	2.88
PCB052	71.70	1.09	251.35	1.23	3.51	1.25
PCB149	612.73	1.38	837.85	1.09	1.37	1.40
PCB151	117.33	1.20	373.22	1.39	3.18	1.46
PCB146	123.85	1.36	121.87	1.00	0.98	1.36
PCB148	84.74	1.11	205.65	1.00	2.43	1.11
PCB153	156.44	1.24	1142.52	1.10	7.30	1.26
PCB193	34.55	1.00	213.27	1.27	6.17	1.27
PCB201	62.58	1.00	990.19	1.36	15.82	1.36
PCB063/058	156.44	1.19	609.34	2.94	3.89	2.98
PCB095(066)	84.74	1.21	624.58	1.94	7.37	2.00
PCB099/113	63.23	1.20	175.19	1.00	2.77	1.20
PCB101/090	176.00	1.19	472.24	1.33	2.68	1.40
PCB123/147	46.28	1.11	761.68	1.58	16.46	1.60
PCB138/163/164	352.00	1.43	1142.52	1.21	3.25	1.50
PCB170(190)	78.22	1.12	761.68	1.30	9.74	1.33
PCB182/187	475.85	1.43	342.76	1.33	0.72	1.59
PCB192/172	32.59	1.00	121.87	1.00	3.74	1.00

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