



Probabilistic ecological risk assessment of secondary poisoning from DDT

A case study of the terrestrial ecosystem
at Kolleberga plant nursery

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Abstract

Although prohibited since decades, dichlorodiphenyltrichloroethane (DDT) and its metabolites still remain in the soil and pose a threat to ecosystems, where especially birds are susceptible to toxic effects. In this thesis, a model developed in the 1990s was used and updated in order to estimate the risks of DDT to top predators at a forest-plant nursery site. Unusually high concentrations of DDT have been found at this site and it was therefore of interest to evaluate the potential ecological effects. The model used deals with the fact that species without direct contact with the soil are still exposed to soil contaminants through their prey, a phenomenon called secondary poisoning. Bioaccumulation factors, toxicity data and species-specific diet were combined in order to quantify the maximum permissible concentration in soil (MPC). MPC5 is regarded as the acceptable level, where 95 % of the populations are protected. Red kite, sparrow hawk, kestrel, badger and weasel were selected as species of concern. This study shows that given the soil concentrations of DDT at the site, the risk (probability) of exceeding MPC5 is high, especially for red kite and sparrow hawk. Matter of fact, the probability of exceeding MPC5 for any of the species considered are >64 %. The concentrations of DDT in soil found at the forest-plant nursery are therefore unacceptable for the protection of birds and beasts of prey.

Contents

Abstract 3

Contents 4

Abbreviations 6

Introduction 7

- Ecological risk assessment 8
- Species sensitivity 9
- Case study: plant nursery site with DDT 10
- Secondary poisoning 10

Study aim and research questions 11

Materials & Methods 13

Scope and structure 13

- Probabilistic model for evaluation of secondary poisoning 14
- Software and statistics 16

Hazard assessment 17

- Selection of species of concern 17
- Species sensitivity distributions 18

Exposure assessment 20

- Bioaccumulation weighting through complex food webs 21
- Diet – food choice 22

Risk characterization 24

Results 25

Hazard assessment 26

- Species sensitivity distributions 26

Exposure assessment 29

- Degree of contamination 29
- Bioaccumulation 31

Risk characterization 31

- Risk for the ecosystem based on direct exposure 31
- Risk for the species of concern based on secondary poisoning 32
- Critical food chains 35
- Sensitivity analysis for MPC species of concern 36

Analysis and discussion 37

- Risk for the ecosystem based on direct exposure 37
- Risk for the species of concern based on secondary poisoning 37
- Comparing with other studies 38
- Other measures of vulnerability 40
- Uncertainties 40
- Risk reduction and remedial objectives 41
- Future studies 41

Conclusions 42

Acknowledgements 43

References 44

Appendix

Appendix A – Variables used in model 1

Appendix B – Toxicity data 4

- References toxicity data 8

Appendix C – Soil concentration 10

Appendix D – Diet choice and species of concern 11

- References diet data 12

Appendix E – Bioaccumulation 13

- References bioaccumulation data 14

Appendix F – Maximum permissible concentration 15

- Sensitivity analysis for MPC output 16

Abbreviations

BAF – bioaccumulation factor

BSAF – biota-to-soil accumulation factor

DDD – dichlorodiphenyldichloroethane

DDE – dichlorodiphenyldichloroethylene

DDT – dichlorodiphenyltrichloroethane (see sum-DDT)

DM – dry matter

EC30 – 30% effect concentration

HC5 – hazardous concentration for 5 % of the species in the species sensitivity distribution

KM – sensitive land use, på svenska (sv.): känslig markanvändning

LOEC – lowest observed effect concentration

MKM – less sensitive land use, sv. mindre känslig markanvändning

MPC – maximum permissible concentration

MPC5 or MPC50 – maximum permissible concentration, providing protection for 95 % or 50 % of the species included

NOEC – no observed effect concentration

PAF – potentially affected fraction of species

PNEC – predicted no-effect concentration

RIVM – Dutch National Institute for Public Health and the Environment

RQ – risk quotient

SEPA – Swedish Environmental Protection Agency, Naturvårdsverket

SSD – species sensitivity distribution

sum-DDT – written in text as DDT, which includes p,p'- and o,p'-DDT, p,p'- and o,p'-DDE as well as p,p'- and o,p'-DDD

USEPA – United States Environmental Protection Agency

CCME – Canadian Council of Ministers of the Environment

Introduction

Dichlorodiphenyltrichloroethane (DDT) is probably one of the most famous pesticides ever developed. The effects resulting from this insecticide has been observed across the world, with widely recognized ecological impacts (Chapin et al., 2011). Rachel Carson drew attention to this issue already in the 1960s in her classic book *Silent spring*, almost inevitable to not mention. Although the use have been prohibited for decades (Swedish geotechnical institute (SGI), 2017) it is unfortunately still relevant to talk about DDT, as its long-term persistence causes it and its metabolites to remain in the soil and ecosystems. In Sweden, this is witnessed especially at plant nurseries and garden centres, where the historically use of pesticides have been extensive (ibid.). Here, the most commonly found pesticide in soil is DDT together with metabolites, but quintozone, hexachlorobenzene and aldrin/dieldrin are also frequently found (ibid.).

Pesticides are problematic as they are not entirely selective, meaning that vulnerable species other than the plant pests gets affected (Niesink et al., 1996). Among other things, effects from DDT on liver, nervous system, reproduction and immune system have been shown in animal experiments (Kemakta Konsult AB and Institutet för Miljömedicin, 2016). DDT's long-term persistence and fat solubility cause accumulation in organisms, where critical concentrations can cause reproduction failure, especially in animals feeding on fat-rich species (Chapin et al., 2011; Netherlands National Institute for Public Health and the Environment (RIVM), 2015). For example, effects on the peregrine falcons' eggshell formation, even in remote areas, have caused population decline (Chapin et al., 2011).

From a societal point of view, Swedish national environmental objectives state the importance of ecological sustainability, where persistent pollutants with long-term effects shall be phased out and strictly limited (Naturvårdsverket, 2009b). It is therefore of interest to protect the soil environment from such pollutants (ibid.). A part of this work is achieved through carrying out risk investigations of contaminated land (SGI, 2017).

Ecological risk assessment

An environmental risk assessment is performed in order to examine the effects of a contaminated area on humans, environment or natural resources (Naturvårdsverket, 2009a). Risk is the probability of a negative effect due to a hazard and resulting consequences (De Lange et al., 2010). Effects of chemicals and exposure conditions, together with character of the biotic and abiotic environment is needed to assess the ecological risk from chemicals (De Lange et al., 2010). If the pollutants pose unacceptable risks, measures must be taken to reduce them (Naturvårdsverket, 2009a). A risk assessment usually includes problem formulation, effect and exposure analysis followed by a risk characterization (Naturvårdsverket, 2009a; Iscan, 2004). An ecological risk assessment is usually structured into the following sections (Naturvårdsverket, 2009a; Öberg, 2006):

- Hazard assessment – the hazard is the ability of a chemical to cause harm (Naturvårdsverket, 2009a). By identifying and selecting the environmental values that should be protected, e.g. an ecosystem or bird population, the scope and limitations of the risk assessment can be ruled out (Iscan, 2004). Ecological and toxicological effects can be related to dose by establishing a species sensitivity distribution (SSD) for the selected environmental values (see section below).
- Exposure assessment – quantifications of the size and extent of the exposure (Öberg, 2009). A chemical stressor causes effect only in contact with the assessment endpoint (ibid.). Estimation of transport and relevant aspects such as bioaccumulation potential is therefore needed.
- Risk characterization – a synthesis of the previous steps, usually described in the form of estimates of the occurrence of environmental effects resulting from the exposure (Öberg, 2009). The environmental risk can be expressed through a risk quotient (RQ), where the environmental concentration is divided by the predicted no-effect concentration (PNEC) (Öberg, 2009; Naturvårdsverket, 2009a). When $RQ \leq 1$, no effects are expected to occur (Öberg, 2009).

The extent of a risk assessment varies. In a basic risk assessment, uncertainties are treated with precaution measures in order to avoid underestimation of risk, while a more comprehensive risk assessment addresses the uncertainties by examining them (Naturvårdsverket, 2009a). When conducting a basic risk assessment for a contaminated site in Sweden, contaminant concentrations are compared to guideline values stated by the Swedish Environmental Protection Agency (SEPA)

(Naturvårdsverket, 2009b). These guideline values can either be generic or adjusted to the specific sites and represents the contamination concentration that is regarded as acceptable (ibid.). What is regarded as acceptable depends on the type of land use; less sensitive land use (MKM, sv. mindre känslig markanvändning) and sensitive land use (KM, sv. känslig markanvändning) are based on the protection of either 50 % or 75 % of the soil environment, respectively (Kemakta Konsult AB and Institutet för Miljömedicin, 2016). DDT is expressed as the sum of DDT isomers, in text referred to as simply DDT, and has the guideline values KM: 0.1 mg/kg dry matter (DM), and MKM: 1 mg/kg (DM) (ibid.).

Instead of comparing point values as in the basic risk assessment, a more comprehensive assessment can use a probabilistic approach to quantify the environmental risk (Naturvårdsverket, 2009a). This includes the use of probability distributions that display and clarifies natural variation (variability) and uncertainty, aspects that are otherwise hidden behind point values (Öberg, 2006).

Species sensitivity

In order to characterize and quantify the risk for a specific ecosystem, characterization of the biological community is needed – structure, sensitivity, vulnerability and function (De Lange et al., 2010). It requires consideration of vulnerability at higher organizational levels rather than sensitivity of the individual organisms or species (ibid.). A SSD can be used to extrapolate from single species and laboratory toxicity data to population, community or ecosystem level (ibid.). SSDs characterize variability as it deals with differences that exist in sensitivity between the different species, i.e. interspecies variation (Xu et al, 2015; De Lange et al., 2010). The method is based on statistical extrapolation and can according to guidance from European Commission (2003) be applied in an effect assessment if there is a large dataset with chronic, i.e. long-term studies for different taxonomic groups available.

Many countries (e.g. Canada and the Netherlands) use SSD methods to develop environmental quality thresholds in order to protect the majority of the species (Xu et al, 2015; Traas et al., 1996). The protection of 95% of the species is traditionally used as PNEC, which equals the hazardous concentration for 5% of the species (HC5) (ibid.). The potentially affected fraction (PAF) for different trophic levels, such as microorganisms and vertebrates, can be calculated depending on exposure (Xu et al., 2015; European commission, 2003).

Case study: plant nursery site with DDT

As mentioned before DDT together with metabolites are the most frequently found organic contaminants in soil at plant nurseries in Sweden (SGI, 2017). One of these sites, Kollberga, is located outside Ljungbyhed in Scania (figure 1). At this plant nursery forest plants have been cultivated since the 1950s (Tyréns, 2017). It is about to be decommissioned and the forthcoming land use for the fields is instead planned to be forest (ibid.). As DDT and other pesticides has been used on the fields, a survey and inventory of the area has been carried out with the purpose of determining the extent of contamination and associated risks (ibid.).



Figure 1. Kollberga plant nursery is located in the Scanian countryside, surrounded by farmland and forest. Topografisk webbkarta Visning © Lantmäteriet (Creative commons CC0).

It is quite rare that DDT concentrations exceed SEPAs MKM guideline at plant nurseries (SGI, 2017), but at this site, this limit is continuously exceeded (Tyréns, 2017). A negative impact on the soil environment cannot be ruled out within the field area, planetary ponies and, above all, at the former dipping site that is present in the area (ibid.). This caused the local authorities (Söderåsens miljöförbund) to issue an injunction to obtaining more information about the site through a more comprehensive risk assessment (Tyréns, 2018).

Secondary poisoning

SEPAs guidelines for DDT is based on Dutch evaluations for the protection of soil ecosystem carried out in 2001 by RIVM (Kemakta Konsult AB and Institutet

för Miljömedicin, 2016). However, RIVM argue that effects in the food chain on worm-eaters and predators occur at levels below these guideline values (Smith and Verbuggen, 2015).

Through the process of biomagnification, species without direct contact with the soil is exposed indirectly to DDT, i.e. from secondary poisoning (Jongbloed et al., 1996). In this way, birds and mammals on top of the food chain are exposed to DDT through their prey. Biomagnification result in higher concentrations for each level in a food chain as the dietary absorption is faster than elimination rate (Borgå, et al., 2012; Smith and Verbuggen, 2015); weak detoxification systems causes predator birds to bioaccumulate organic pollutants such as DDTs (Walker et al., 2012). Given the bioaccumulative and persistent properties, it is clear that DDT transport in the food web of predatory birds and mammals should be considered when assessing the effect of DDT. Especially avian carnivores that are top bioaccumulators in many terrestrial food webs are suggested to be important to include in studies of terrestrial systems (Brink et al., 2016).

A probabilistic approach addressing the issue of secondary poisoning was developed by Jongbloed et al. (1994), Jongbloed et al. (1996) and Traas et al. (1996). In Jongbloed et al. (1996), toxicity of and bioaccumulation were treated as stochastic variables, and food webs for specific predator species were used to weight the bioaccumulation potential of DDT depending on diet choice. The model they used yielded the maximum permissible concentration (MPC5) of DDT in soil for the protection of the 5th percentile (5 %) of the specific predator species population, thereby characterizing the transport of DDT between soil and higher trophic levels. MPC is comparable to the PNEC (Smith and Verbuggen, 2015).

Study aim and research questions

The development of a forest area from the former forest plant nursery site can be limited by risks posed by DDT to wildlife, and the exposure should be within an acceptable limit. The objective of this study is to investigate the potential risk of DDT residues in the terrestrial ecosystem connected to Kollleberga plant nursery, focusing on birds of prey and beasts of prey as environmental values to be protected. In order to include uncertainties and variability connected to the risk for predators in the specific area, a probabilistic model incorporates knowledge about exposure, toxicity, bioaccumulation and diet. These components are used to characterize and quantify the risk.

- ⇒ Based on the variability in toxicity for various terrestrial species in the ecosystem, which species group can be identified as sensitive?

Toxicity data for all trophic levels in a terrestrial ecosystem can be displayed as a SSD, where sensitive species and groups can be identified. The sensitivity among species in an ecosystem varies and certain groups, in this case predatory birds and mammals, are species of concern and of interest to investigate, given their position in the food chain and for birds of prey, recognized sensitivity towards DDT.

- ⇒ How is the effect for raptor species of concern related to the concentration of DDT in soil and how does the diet choice influence this?

The species of concern included are raptor species that have been previously observed in the area. Secondary poisoning is taken into account by updating the MPC model developed by Jongbloed et al. (1996) with more data. More data is added as the uncertainties in the estimations of MPC decreases. The effect on a population level for each species is measured by MPC5, the soil concentration with the probability of 5 % that the no-effect-concentration will be exceeded. MPC5 is regarded as the highest acceptable concentration in the soil for the protection of the specific species. The MPC model is also used for specific food chain routes in order to display the influence of diet choice.

- ⇒ What is the site-specific risk of secondary poisoning for species of concern?

The risk of exceeding the no-effect concentration for the species of concern at the Kollberga site is evaluated using risk quotients (RQ). PAF is given by comparing effect measurements (SSD and MPC distribution) with the DDT concentration in soil at certain percentiles. By using a probabilistic approach, the risk estimation includes a range of possible ecological impacts and the likelihood of them to occur.

Materials & Methods

Scope and structure

Crucial parts of an ecological risk assessment are addressed, however, this thesis is focused on solely the exposure and effects from DDT in the soil and terrestrial biota compartment, thereby excluding contaminated sediment, surface water and ground water. Apart from DDT, dicofol and HCH-beta has been detected in the soil, but these will not be considered due to their low concentrations. Human toxicology is also excluded and the description of the problem associated with the contaminants at the plant nursery is limited to the specific identified species.

The structure follows the sections included in a risk assessment (figure 2) and the endpoint that constitutes the environmental value to be protected are

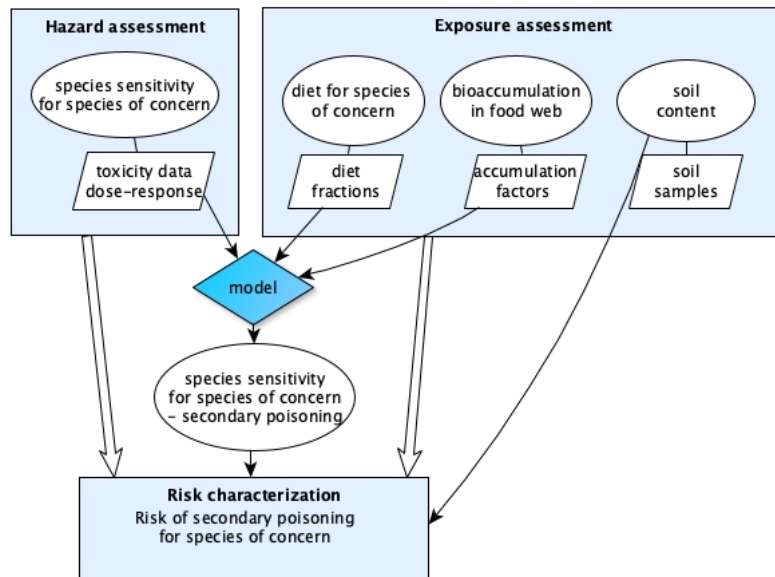


Figure 2. The three sections of a risk assessment and the approach that is used in this case study. Input data (parallelograms) are used in a probabilistic model in order to quantify the risk of secondary poisoning for species of concern in top of the food chain.

vertebrates higher up in the food chain. The risk for these vertebrates is assessed through a probabilistic model that combines knowledge about bioaccumulation, diet choice as well as toxicity, making it possible to compare effect of raptor birds and mammals in relationship to DDT concentration in soil.

The model method used by Jongbloed et al. (1996) was updated with more toxicity and bioaccumulation data. Acquisition of toxicity data was prioritized as the uncertainty analysis conducted by Jongbloed et al. (1996) for the model showed that the toxicity data was the variable causing the highest uncertainties. Ecosystem and species relevant to the forthcoming forest area were studied by site visit to the plant nursery and vicinity area, as well as information from the databases Artdataportalen and Artdatabanken.

Probabilistic model for evaluation of secondary poisoning

In order to incorporate bioaccumulation in the risk assessment for predator species in the top of complex food webs, the probabilistic model presented by Traas et al. (1996) and Jongbloed (1996) was used. The model is based on the calculation of the maximum permissible concentration (MPC) (eq. 1.1).

$$MPC = \frac{NOEC_{soc}}{BAF_{ft}} \quad (1.1)$$

MPC - maximum permissible concentration (mg/kg dry weight soil)

NOEC_{soc} - no-observed-effect concentration in diet for species of concern (mg/kg wet weight prey)

BAF_{ft} - average bioaccumulation factor from soil to diet of species of concern

Due to variability and uncertainty among bioaccumulation factors (BAF) and no effect concentrations (NOECs), these variables are put into the model as stochastic variables, meaning that the variables in eq. 1.1 are expressed as statistical probability distributions. Chronic (long-term exposure) toxicity data for vertebrates were used for establishing NOEC_{soc}. BAFs together with diet choice were used for establishing BAF_{ft}, based on adjustments of the generic food web concept in figure 3. MPCs for specific species of concern as well as for different food chain pathways were calculated using Monte Carlo simulations (2000 iterations). In order to identify the most critical food chain pathways (yielding the highest MPC) irrespective of species, specific food chains were used, e.g. plant and leaves → bird → beast of prey.

To conclude, MPC was calculated for the following scenarios:

- Third trophic level (secondary consumers) birds of prey and beasts of prey, specific for species of concern.
- Third trophic level (secondary consumers) birds of prey and beasts of prey, diet-specific.

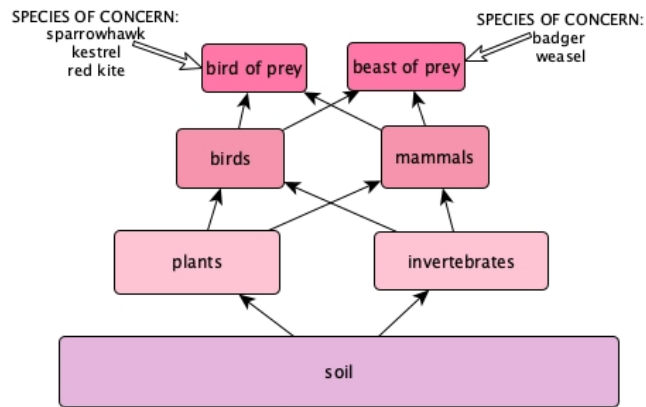


Figure 3. Possible pathways of food web transfer used in the model and relevant predators identified as species of concern that are used in the risk analysis model (modified after Jongbloed et al., 1996). The third trophic level (secondary consumers) prey on the second trophic level (primary consumers), which prey on plants and invertebrates.

Software and statistics

Palisade software @Risk (version 7.6.0), which is an add-in for Microsoft Excel, were used to express variability and uncertainty in toxicity, accumulation and exposure by fitting data sets to statistical probability distributions. This software fits statistical distributions defined by parameters to input data by the maximum likelihood-method. Parametric bootstrap (1000 resamples, 95 % parameter confidence level) was used to express the uncertainties connected to the fit: goodness of fit measures is presented as Anderson-Darling (A-D) test statistic (test-value) and level of significance of the fit (p-value) for each estimated distribution (appendix A). The output result was obtained through Monte Carlo simulations that collect random samples from the input probability distributions in the model, in a repetitive procedure (Öberg and Bergbäck, 2005). The bootstrap resampling generates a two-sided confidence interval for the parameters of the fitted distribution (Öberg, 2009). The confidence interval of 95 % indicates a confidence of 95 % that the parameter has a value within the interval. The simulations yielded the output results presented as probability distributions, mostly displayed as ascending cumulative probability distributions (figure 4).

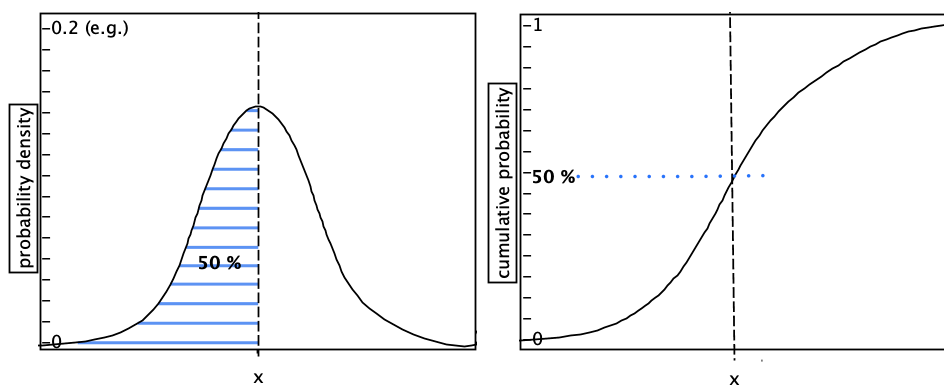


Figure 4. The probability distribution for a variable (x) can be displayed with either a probability density function or a cumulative probability function.

Hazard assessment

Selection of species of concern

Due to the process of biomagnification raptor birds and mammals are regarded as species of concern at the site. Artdatabanken and Artdataportalen gave information about which raptor birds and mammals that could be present in the area and therefore suspected to be exposed to DDT (figure 5). Eurasian sparrowhawk (*Accipiter nisus*, sv. sparvhök), kestrel (*Falco tinnunculus*, sv. tornfalk), and red kite (*Milvus milvus*, sv. röd glada) were chosen as species of concern, as these raptor birds were among those species that had been observed in the area (Artportalen, 2019) and were denoted as carnivore birds present in forest or agricultural areas in Scania (ArtDatabanken, 2019). The query in Artportalen geographically limited the data to birds in vicinity (5 km) to Kolleberga plant nursery. European badger (*Meles meles*, sv. grävling), common weasel (*Mustela nivalis*, sv. småvessla) were also chosen as species of concern, as these raptor mammals were among those species that had been observed in the area (Artportalen, 2019). In this case, the query was limited to mammals within a polygon shaped from the corners Örkelljunga, Tyringe, Norra rorum, Svalöv, Bjuv and Össjö. Observations made from year 2000 to present (2019).



Figure 5. Species of concern used in this risk assessment, from the left: red kite, *Milvus milvus*; kestrel, *Falco tinnunculus*; badger, *Meles meles*; weasel, *Mustela nivalis* and sparrow hawk, *Accipiter nisus*. Photographs from Encyclopædia Britannica ImageQuest: Hamblin, 2009; Arterra, 2018; Benvie, 2016; Eco Images, 2016; Chapman, 2016.

Species sensitivity distributions

In order to evaluate the potential risk for the species at Kollberga, toxicity data for all terrestrial species collected in literature were included to establish a SSD for the whole ecosystem based on both lethal and sublethal effects expressed as lowest observed effect concentration (LOEC) or 30% effect concentration (EC30). For the MPC modelling, SSDs including mammals and birds based on lethal and sublethal effects expressed as NOECs were established.

As toxicity data covers different test conditions and endpoints, various inclusion criteria were applied to homogenize the data set (described below in acquisition sections). Ecotoxicity is evaluated in laboratory experiments in several ways depending on the objectives of the studies (Niesink, 1996). Toxicity can be studied on different levels: biochemical, individual, population, community and ecosystem, which is important to consider upon selecting what toxicity data that should be included (Niesink, 1996). In this study, single-species toxicity data were used. Toxicity data are considered to be a sample from a distribution that can be described mathematically by statistical parameters (Liu et al., 2012). By fitting statistical probability distributions to toxicity data, SSDs for the whole ecosystem, birds and mammals were generated. The log-normal distribution type is recommended by EPA (Xu et al, 2015) whereas other sources assume either a log-normal or log-logistic fit (Wang et al., 2008; Jongbloed et al., 1996). Here, logistic statistical probability distributions were fitted to logarithmic data.

Acquisition of toxicological data for the terrestrial ecosystem

ECOTOX knowledgebase is a database governed by the United States Environmental Protection Agency (USEPA) that provides environmental toxicity data for chemicals. The query and selection of data in ECOTOX database is given in table 1.

Table 1. Query in ECOTOX knowledgebase for acquisition of ecotoxicological data for DDT and metabolites, terrestrial habitat. The dataset given by ECOTOX is further sorted by selection of certain endpoints and appropriate units. Selected data listed in appendix, B6.

Species group	Effect Measurements	Endpoints	Further selection and type of data
Insects/Spiders Amphibians Other Invertebrates Crustaceans Molluscs Worms Birds Mammals	All available, was further selected	No and lowest observed effect data, lethal and effect concentration given in various percentages	Unit: ppm, mg/kg Exposure media: soil, oral capsule, diet Endpoint: LOEC Effects: Mortality, reproduction, growth, morphology

In ECOTOX, toxicity for terrestrial invertebrates are examined and reported in various ways, making it difficult to summarize and pool data: the toxicity is given in ppm, %, mg/mL, kg/ha, µg/organism, µg/g bdwt, or ug/g organism. Moreover, the terrestrial organisms have been exposed to DDT in various ways, ranging from spray, topical, direct apply, oral, or from soil exposure. Only the toxicity as a function of soil exposure is relevant for the specific site, as many invertebrate species, for example earthworms, are directly exposed to the soil. Further literature search outside ECOTOX database were carried out to obtain more data. LOECs and EC30 values were used for the SSD for the whole ecosystem.

Acquisition of toxicological data for birds and mammals and treatment before statistical analysis

Existing toxicity data for terrestrial birds and mammals in the model developed by Jongbloed et al. (1996) and Traas et al. (1996) were updated by collecting data from ECOTOX knowledgebase. The uncertainties expressed as confidence interval around estimated parameters together with probability distributions, can be used in order to compare the original and updated information. The query and selection of data is given in table 2.

Table 2. Query in ECOTOX knowledgebase for acquisition of ecotoxicological data for DDT and metabolites, terrestrial habitat. The data given in ECOTOX is further sorted by selection of certain endpoints and appropriate units. Selected data listed in appendix, B4-B5.

Species group	Effect Measurements	Endpoints	Further selection and type of data
Birds	Mortality, growth, morphology and behavior	No and lowest observed effect toxicity data	Unit: ppm or mg/kg Exposure media: diet or oral via capsule Effects: Mortality, growth, morphology, growth, feeding behaviour
Mammals			Unit: ppm or mg/kg bdwt/d Exposure media: diet or oral via capsule Effects: morphology, growth, mortality

If the same study had reported both NOEC and LOEC, only NOEC data is used. Geometric mean was used for comparable data on same species and endpoint, as suggested by Van Vlaardingen et al. (2007). This was done although the studies were not performed in a similar way. Long exposure durations are prioritized; for species and endpoints with several exposure durations, studies with exposure duration <1 month were not included.

Toxicity values were extrapolated and transformed in order to harmonize the data sets to be expressed as chronic NOECs in mg/kg DM diet. Following the same extrapolation method as Jongbloed et al. (1996), LOECs were divided by a

factor of 2 in order to derive NOEC, and toxicity data with exposure durations <1 month was divided by a factor of 10 in order to extrapolate to longer, chronic exposure durations. Moreover, the NOECs derived are corrected from lab to field conditions according to Jongbloed et al. (1996) and Traas et al. (1996), where the factors are adjusted for different metabolic rates, diet caloric content and food assimilation efficiencies in wild vertebrates (used correction factors in appendix, table A2 and B2). These factors vary from species to species and are used to extrapolate to predators in field from laboratory conditions, yielding lower NOECs. The toxicity data were fitted to statistical distributions representing SSD for birds or mammals separately and used in the model as $NOEC_{SOC}$.

Exposure assessment

The exposure assessment describes the distribution of DDT compounds in soil and also the transport in the food web due to the processes of bioaccumulation (figure 6). DDT in soil at Kollberg plant nursery has already been measured in field as a part of a project conducted by the consultancy company Tyréns. Gathered soil samples (N=18) were analysed and presented as the total sum of DDT (sum-DDT) (appendix C). Fields, plant landfill and plant-dip site are areas with different pollution history but are lumped together and the sampling procedure were not random. The field area is approximately 23 ha (Tyréns, 2017). Exposure data were fitted to a log-normal statistical distribution.

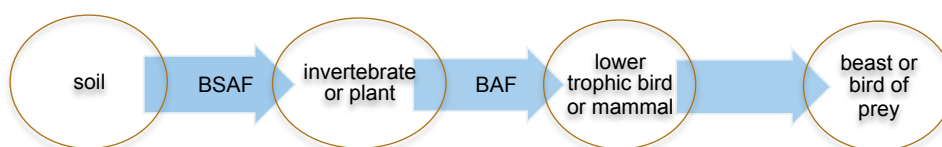


Figure 6. Schematic diagram of the transport process of DDT from soil as a source throughout a food chain. Knowledge about bioaccumulation: biota to soil accumulation factors (BSAF) and bioaccumulation factors (BAF) in each transport step are used to determine the exposure from diet for higher trophic levels.

Bioaccumulation weighting through complex food webs

The average bioaccumulation factor (BAF_{ft}) for a complex food web of the predator species (figure 6) was calculated by weighting each bioaccumulation route according to its fraction in the diet (eq. 1.2).

$$\begin{aligned}
 BAF_{ft} = & DFT_b * BAF_b * \sum_{k=0}^n (DFB_{ipk} * BSAF_{ipk}) \\
 & + DFT_m * BAF_m * \sum_{k=0}^n (DFM_{ipk} * BSAF_{ipk}) \\
 & + \sum_{k=0}^n (DFT_{ipk} * BSAF_{ipk})
 \end{aligned} \tag{1.2}$$

BAF_{ft} = average bioaccumulation factor from soil to diet of species of concern

$BAF_{b//m}$ = BAF of birds or mammals (wet weight tissue of biota)

$BSAF_{ipk}$ = biota-to-soil accumulation factor of the kth type of invertebrate or plant part

$DFT_{b//m}$ = fraction of birds or mammals in diet of top predator

DFT_{ipk} = fraction of the kth type of invertebrates or plant parts in diet of top predator

$DF-M//B_{ipk}$ = fraction of the kth type of invertebrate and plant parts in diet of mammals or birds

n = number of invertebrate and plant parts in the food web of the top predator

Biota to soil accumulation factors (BSAF) and BAF from Traas et al. (1996) were updated with data from literature and fitted to logistic, triangular or uniform statistical probability distributions. Logistic probability distributions were tried out first according to recommendations in Traas et al. (1996). Goodness of fit was low for the estimated logistic distribution relative the input data of BAF for mammals and birds ($p < 0.05$). Therefore, triangular statistical distributions instead of logistic were used for these two variables, defined by the parameters minimum, mean and maximum. A relatively high variability together with scarce data for the accumulation in seeds and tubers resulted in uniform (instead of logistic) statistical distributions for these variables. The parameters minimum and maximum were also set to a wider range than the empirical data range, motivated by uncertainties due to lack of data.

Conversion factors were used to normalize the accumulation data, expressing it on a basis of wet weight whole body/organism content and dry weight soil content (wet/dry). Only BSAF for leaves and fruits, seeds, tubers and soft-bodied invertebrates were added to the already existing data, since more BAF data were difficult to find. Most measurements of DDT residues in bird and

mammal tissue are from field, which makes it difficult to relate the residue content to diet content.

Diet – food choice

Given that the most important uptake route for the transfer of pollutants is from food ingestion especially for vertebrates of higher trophic level (Walker et al., 2012; Brink et al., 2016), the diet is an important factor to include in the risk assessment. The fraction of each diet item in each species of concern's food web (figure 7) is used in the model as the parameters $DFT_{b/m}$, DFT_{ipk} and $DF-M/B_{ipk}$, (eq. 1.2) and are based on a wet weight basis. Fraction of different food items for the species of concern was collected from Traas et al. (1996) and for red kite, through literature search (appendix D). The diet groups were lumped into leaves and fruits, seeds, tubers, soft-bodied invertebrates (earthworms, gastropods, insect larvae), hard-bodied invertebrates (insects, isopods), birds and mammals.

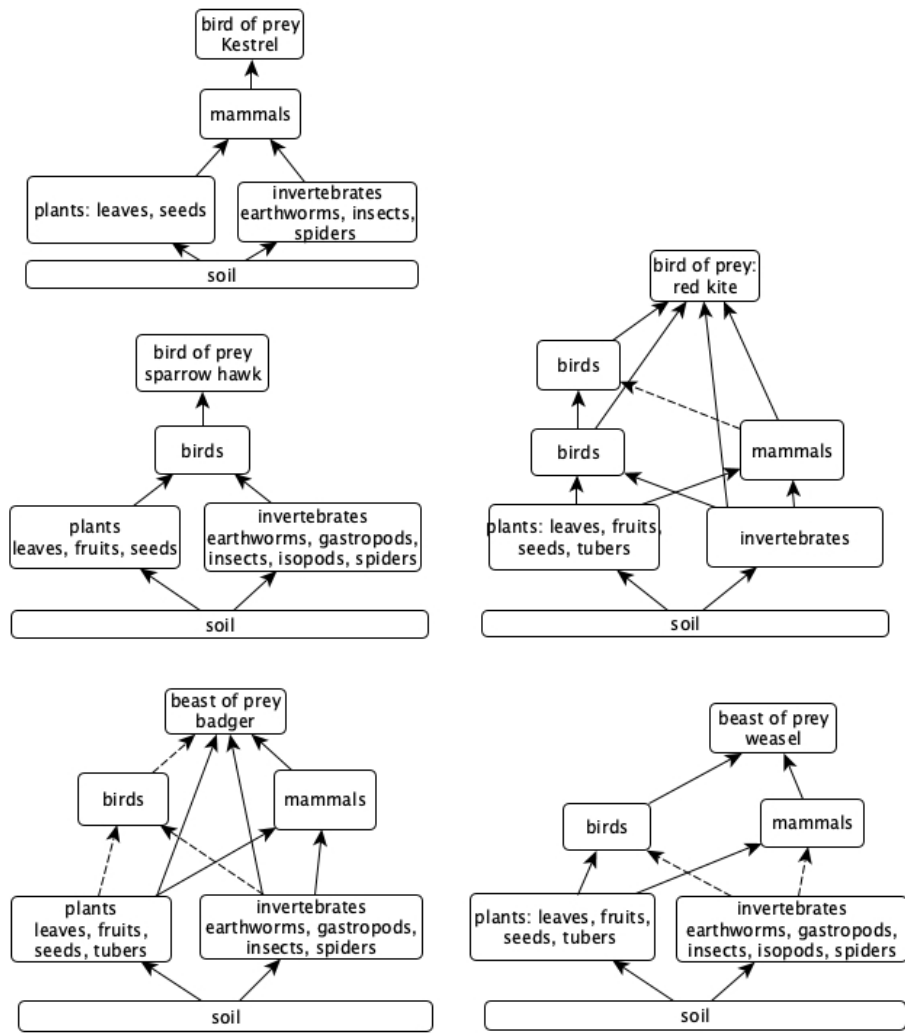


Figure 7. Food webs for species of concern used in model. Dashed lines marks food items of less importance: constituting <10 % of total diet (see Appendix D).

Risk characterization

In order to characterize the risk, calculated MPCs for certain species of concern or food web pathways are related with the exposure situation present in Kollleberga. Risk is estimated by calculating risk quotients (RQ), where the soil concentration is divided by MPC5 (equation 2) (Öberg, 2009; Naturvårdsverket, 2009a). $RQ \leq 1$ for the different species of concern are regarded to be protective.

$$RQ = \frac{\text{soil concentration}}{MPC5} \quad (2)$$

At a given soil concentration were the probability that a species population is affected is 5 % (MPC5), there is a certain corresponding probability that the soil concentration exceeded this concentration. This is the soil concentration were $RQ=1$ for MPC5.

From the SSD and MPC probability distribution graphs, PAF of a species' population (y-axis) corresponds to a certain soil concentration (x-axis). This relationship can be used to investigate how remediation efforts would affect risk.

Results

The input data (table 3) yielding the result of the MPC model simulations (equation 1.1) are expressed as cumulative probability distribution functions. An ascending cumulative probability distribution presents the probability from 0-1 (y-axis) of finding concentrations that are the same or less than the corresponding concentration (x-axis). Moreover, a for example 95th percentile says that in 95 % of the cases the data presented is below this point.

Table 3. General variables used in MPC-model and where to find the input data in Appendix.

Variable abbreviation	Variable	Distribution type	Parameters (defining distribution)	Appendix
BAF _{mammal}	Bioaccumulation factor of mammals (mg/kg wet weight/wet weight diet)	triangular	min, mode, max	Table A1.
BAF _{bird}	Bioaccumulation factor of birds (mg/kg wet weight/ wet weight diet)	triangular	min, mode, max	Table A1.
BSAF _{ip-diet group (ex. seeds)}	Biota-to-soil accumulation for plants or invertebrate (mg/kg wet weight/dry weight soil)	logistic or uniform	α , β or min, max	Table A1.
NOEC _{birds}	No effect concentrations for bird (mg/kg diet)	logistic	α , β	Table A2.
NOEC _{mammal}	No effect concentrations for mammals (mg/kg diet)	logistic	α , β	Table A2.
DFT-x, DFM-x DFB-x	Fraction of diet for different levels in food web	point values	-	Table A3.
Exposure	Exposure from soil content: sum-DDT (mg/kg dry weight soil)	log-normal	μ , σ	Table C2.

Hazard assessment

Species sensitivity distributions

The SSD for a terrestrial ecosystem based on LOEC/EC30 toxicity data (figure 8; data and statistics in appendix, table B6 and B7) characterizes the variability in the sensitivity towards DDT among different species and species groups.

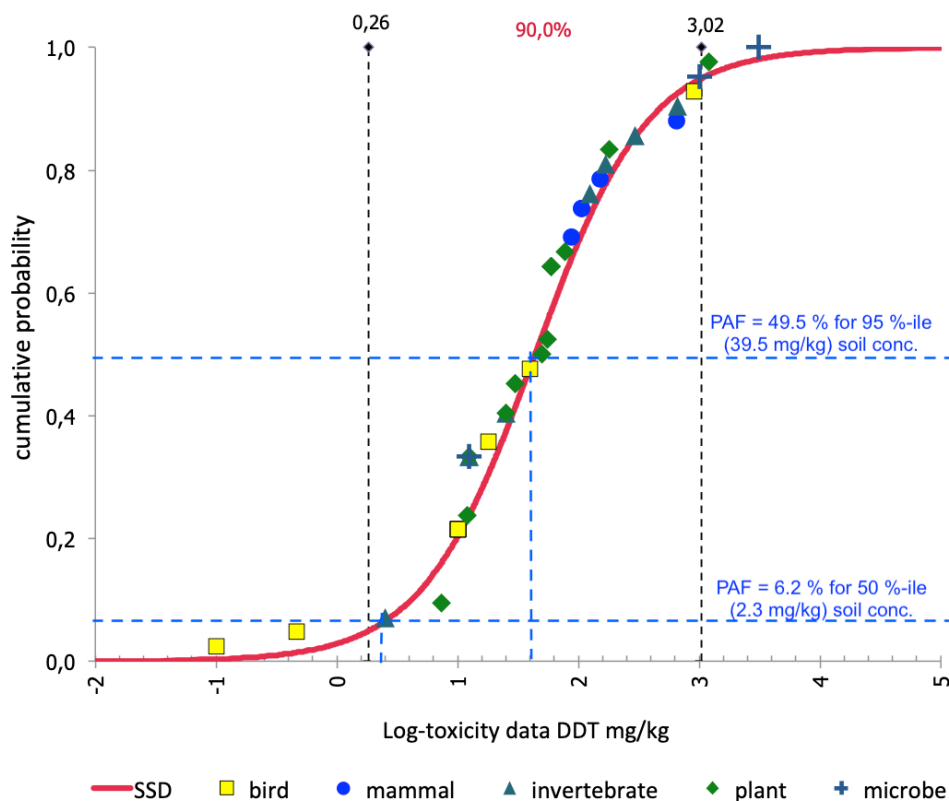


Figure 8. Cumulative species sensitivity distribution (SSD) for terrestrial species obtained by fitting a logistic statistical distribution to logarithmically transformed single-species LOEC/EC30 (mg/kg DM) toxicity data for DDT based on dry soil (invertebrate, plants, soil microbial processes) or diet (mammal and bird) concentrations. The delimiter interval (Log-0.26-3.02, dashed lines) shows the interval that contains 90 % of the SSD data. Potentially affected fraction (PAF) at the 50th (2.3 mg/kg DM) and 95th (39.5 mg/kg DM) percentiles of the soil concentration (see exposure assessment) is marked in the graph (blue dashed lines).

The concentration at the 5th percentile is HC5 for the ecosystem: 1.82 mg/kg (antilog of 0.26). However, note that that the species are exposed to DDT from both soil and diet; the SSD cannot be directly compared against sum-DDT

concentration in soil. Invertebrates (including springtails (*Collembola*), earthworms (*Lumbricidae*) and mites (*Acari*)), plants and microbial processes are exposed to sum-DDT through soil, while mammals and birds are exposed via diet. The species with LOECs below the 5th percentile (HC5) are birds.

The update with more toxicity data for mammals and bird can be compared with Jongbloed et al., 1996 (figure 9 and figure 10; data and statistics in appendix, table B1 and B4-B5). The SSDs expresses the variability of sensitivity towards DDT within these two vertebrate groups.

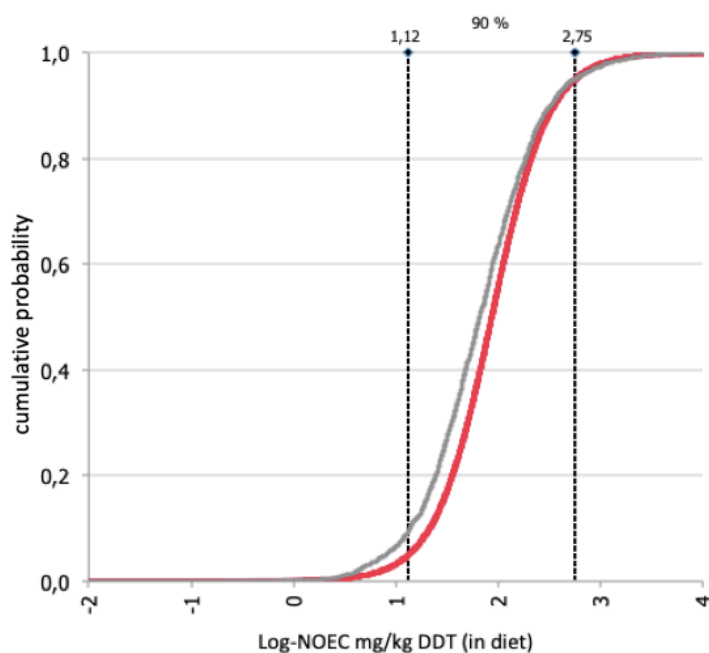


Figure 9. Cumulative species sensitivity distributions (SSD) obtained by fitting logistic statistical distribution to logarithmically transformed single-species no effect concentration (NOEC) toxicity data for mammals (not species-specific corrected here). Grey line based on toxicity data from Jongbloed et al. (1996) (N=6) and red line based on updated toxicity data (N=14) used in the model. The delimiter interval (1.12 - 2.75, dashed lines) shows the interval that contains 90 % of the updated data.

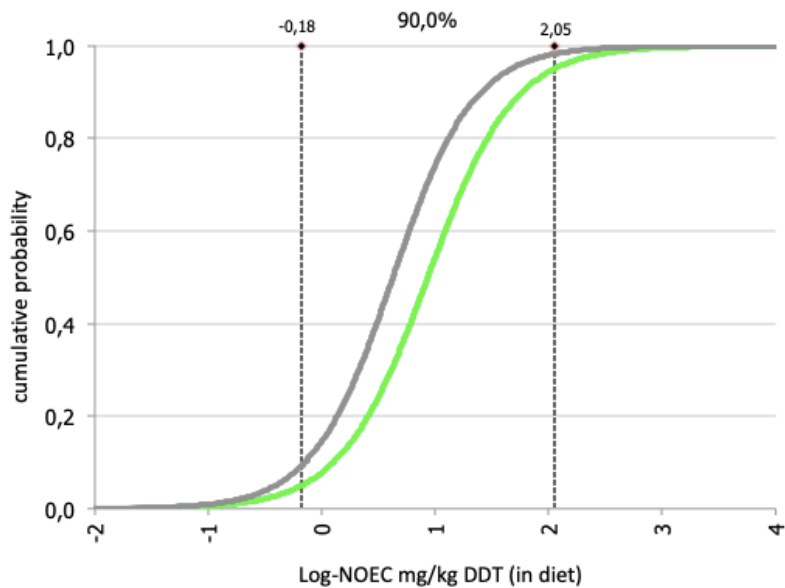


Figure 10. Cumulative species sensitivity distributions (SSD) obtained by fitting logistic statistical distribution to logarithmically transformed single-species no effect concentration (NOEC) toxicity data for birds (not species-specific corrected here). Grey line based on toxicity data from Jongbloed et al. (1996) (N=9) and green line based on updated toxicity data (N=21) used in the model. The delimiter interval (-0.18 - 2.05, dashed lines) shows the interval that contains 90 % of the updated data.

Using species-specific corrected SSDs for birds and mammals, hazardous concentrations based on diet for species of concern could be derived (table 4).

Table 4. Hazardous concentrations (HC) at different percentiles (DDT mg/kg diet). The values are derived from log-logistic probability distributions fitted for no-effect-concentration toxicity data.

Species	Correction factor	5 th percentile (HC5)	50 th percentile (median, HC50)	95 th percentile (HC95)
Kestrel	0.21	0.1	1.8	22.5
Sparrow hawk	0.24	0.2	2.0	25.5
Red kite	0.25	0.2	2.0	25.7
Badger	0.15	2.0	12.9	83.6
Weasel	0.16	2.1	13.8	89.4
Not corrected birds	1	0.7	8.6	113.3
Not corrected mammals	1	13.3	86.4	562.6

Exposure assessment

Degree of contamination

The concentration of DDT in soil at Kollleberga (data in appendix, table C1-C2) is displayed both as a relative frequency distribution (figure 11) and as a descending cumulative probability distribution (figure 12). SEPA's generic MKM guideline (1 mg/kg DM) is continuously exceeded (Tyréns, 2017).

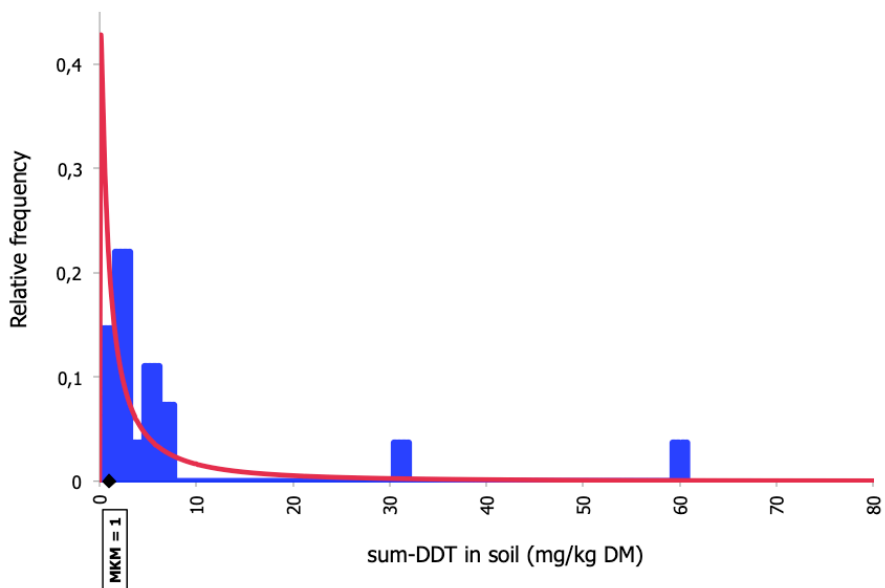


Figure 11. Relative frequency distribution of sum-DDT soil concentrations for input data (N=18, blue bars), and the fitted statistical log-normal probability function (red line) at the site. Generic environmental threshold concentrations according to SEPA is 1 mg/kg DM for less sensitive land use (MKM).

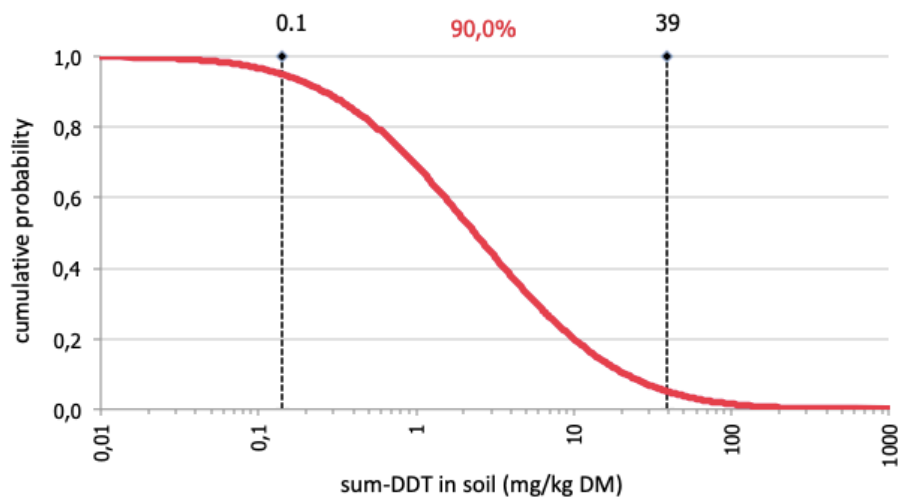


Figure 12. Cumulative descending probability distribution of the total DDT content (sum-DDT) in (collected mixed samples, non representative sampling) from Kollleberga plant nursery. The delimitter interval (dashed lines) shows the interval that contains 90 % of the distribution. The graph shows the probability 1-y of finding concentrations that are the same or that exceed the corresponding (x-axis) concentration. The delimitter interval (0.1 - 39, dashed lines) shows the interval that contains 90 % of the data.

Bioaccumulation

The bioaccumulation probability distributions used in the model are presented in figure 13 (data and statistics in appendix E). BSAF added to the already existing bioaccumulation data used in Jongbloed et al. (1996) is presented in table E4-E5.

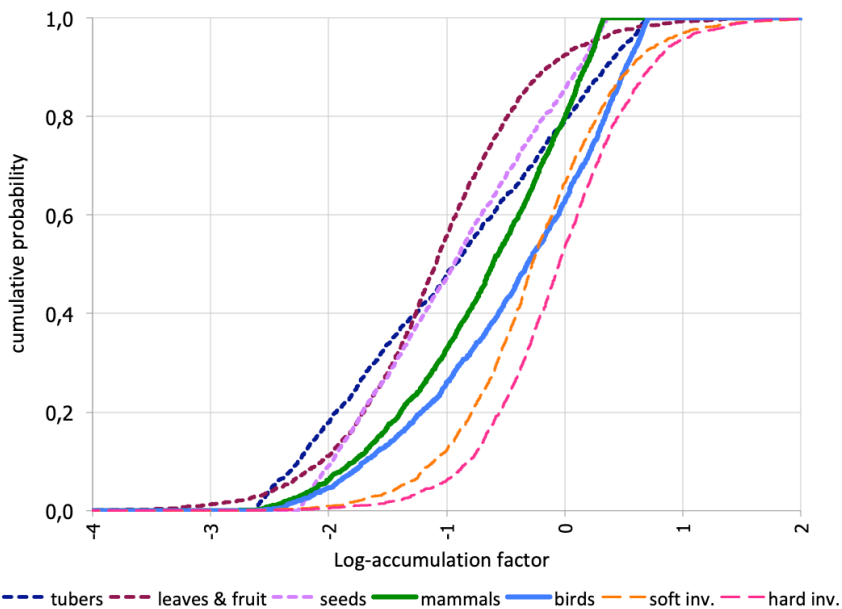


Figure 13. Cumulative probability distribution of bioaccumulation factors (BAF) from diet to mammal or birds and also, biota-to-soil bioaccumulation factors (BSAF) from soil to prey at lower trophic species: soft bodied invertebrates, leaves and fruit, seeds, tubers and hard bodied invertebrates.

Risk characterization

Risk for the ecosystem based on direct exposure

The probability of exceeding SEPAs generic guideline value for less sensitive land use of 1 mg/kg DM of DDT in soil is 68 % at the site (figure 11-12) and the probability of exceeding ecosystem HC5 (1.82 mg/kg given from figure 8, based on the endpoints LOEC and EC30) is 56 %. Below the 95th percentile of the distribution of DDT concentration in soil, approximately 50 % of the ecosystem is potentially affected (figure 8).

Risk for the species of concern based on secondary poisoning

Combining (equation 1.1.) the probability distributions from bioaccumulation and corrected NOEC toxicity together with fraction of each diet item in the model, MPC probability distributions for species of concern (table 5 and figure 14) were calculated. MPCY (x-axis) is the concentration with a corresponding probability of y % that the NOEC for the specific species will be exceeded. The concentration on the x-axis therefore represents the concentration in soil that protects 1-y % of the species included. As stated before, the 5th percentile (5 %) of the modelled MPC distribution, MPC5, is considered as protective for specific species' populations in this risk assessment. Using toxicity data based on NOECs imply that a soil concentration \leq MPC5 should not elicit effects for 95 % of the specific species population.

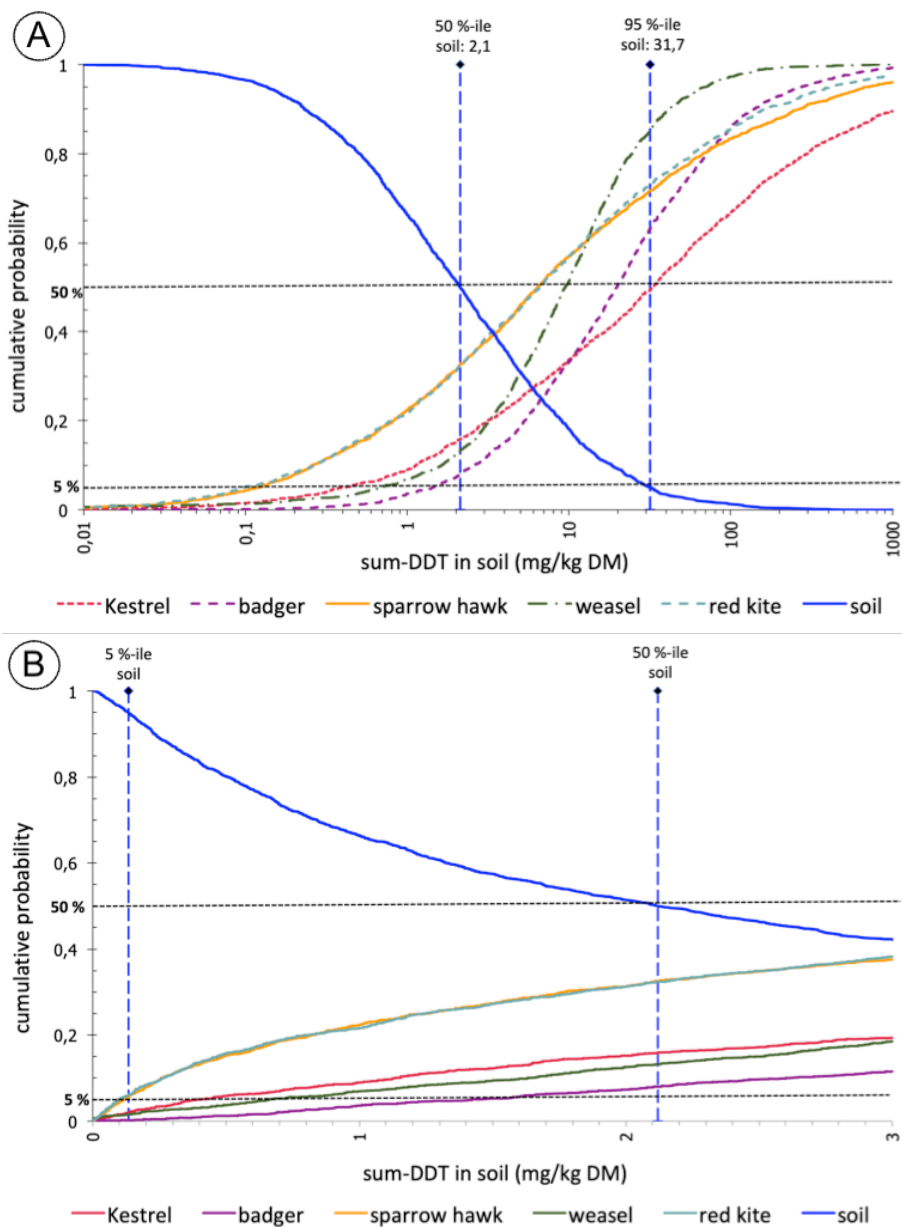


Figure 14. Probability of trespassing the no-effect concentration in beasts of prey and birds of prey depending on the soil concentration, based on species sensitivity distributions and bioaccumulation through species-specific food webs. The graphs show the output from equation 1.1 ($MPC = NOEC_{soc} / BAF_i$) and the probability (y-axis) of exceeding the corresponding maximum permissible concentration (MPC). Limited to the soil concentration intervals 0.01 - 1000 (A) and 0 - 3 (B) sum-DDT. The soil concentration where 5 % of a species population is potentially affected (MPC5) is considered as an acceptable protection level. The 5th, 50th and 95th percentiles of the soil concentration are marked in the graphs with blue dashed line.

Risk can be expressed as the probability of exceeding MPC5. The risk that soil concentrations exceed MPC5 given the soil concentrations at Kolleberga plant nursery (table 5) is when $RQ \geq 1$ (table 5, figure 15), based on equation 2. The risk is $>64\%$ for all species included.

Table 5. Relating the content of DDT in soil at Kolleberga plant nursery with the maximum permissible concentrations at different protection levels (MPC5 and MPC50, for the protection of 95 and 50 % of the species, respectively) for species of concern that are likely to be present in the area. The risk is expressed as the probability of soil concentrations exceeding MPC5 or MPC50 (risk quotient ≥ 1). Numbers given in parenthesis is the reported value from Jongbloed et al. (1996).

Species of concern	MPC ₅ (mg/kg DW)	RISK (%) OF $RQ \geq 1$	MPC ₅₀ (mg/kg DW)	RISK (%) OF $RQ \geq 1$
Kestrel	0.40 (0.25)	85	22.74	9
Sparrow hawk	0.12 (0.015)	96	5.13	32
Red kite	0.09	97	5.32	32
Badger	1.30 (0.75)	64	17.07	11
Weasel	0.66 (1.6)	77	7.88	23

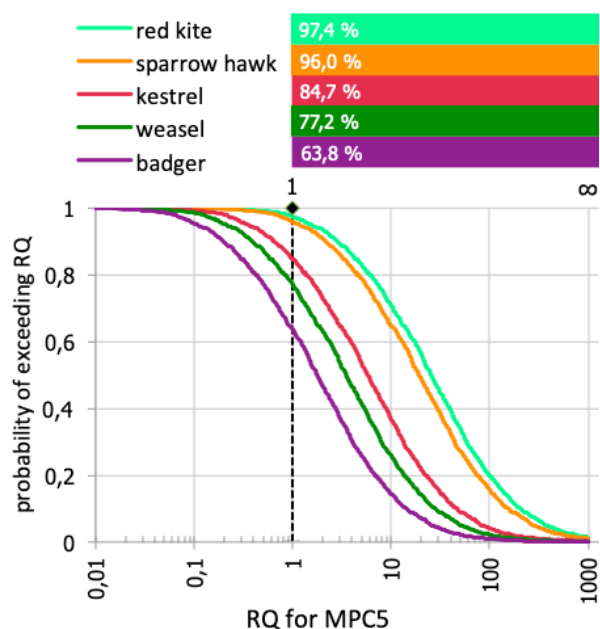


Figure 15. Probability of exceeding species-specific risk quotients (RQ) for MPC5 at the plant nursery site.

Critical food chains

Figure 16 and figure 17 show the model result using single specific diet routes, indicating how the type of diet influence the risk of secondary poisoning for secondary consumers. The most critical route for both birds of prey and beasts of prey were soil→ hard-bodied invertebrates → bird (data for MPC5 and MPC50 in appendix, table F1-F2). MPC5 for beast of prey and birds of prey were in this case 0.61 and 0.063 mg/kg DM, respectively. Although not in focus in this risk assessment, second trophic level birds and mammals are also susceptible to be affected by DDT (table F4-F5 compared to F2-F3).

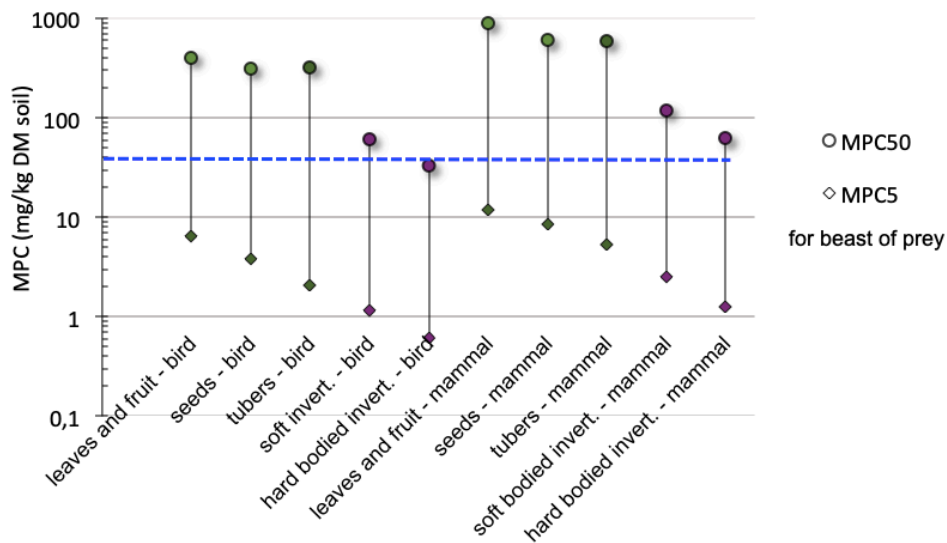


Figure 16. Maximum permissible concentration (MPC) for sum-DDT in soil for secondary poisoning modelled for specific routes through the food web, indicating how beast of prey diet choice influence the risk of getting effected by DDT. Each category denotes one specific route in the food chain: soil→ leaves and fruit, seeds, tubers, soft bodied invertebrates or hard bodied invertebrates →bird or mammal→ beast of prey. The points using plant diet are marked green and the points using invertebrate diet are marked purple. The 95th percentile of the soil concentration (39.5 mg/kg DM) is marked in the figure (blue dashed line).

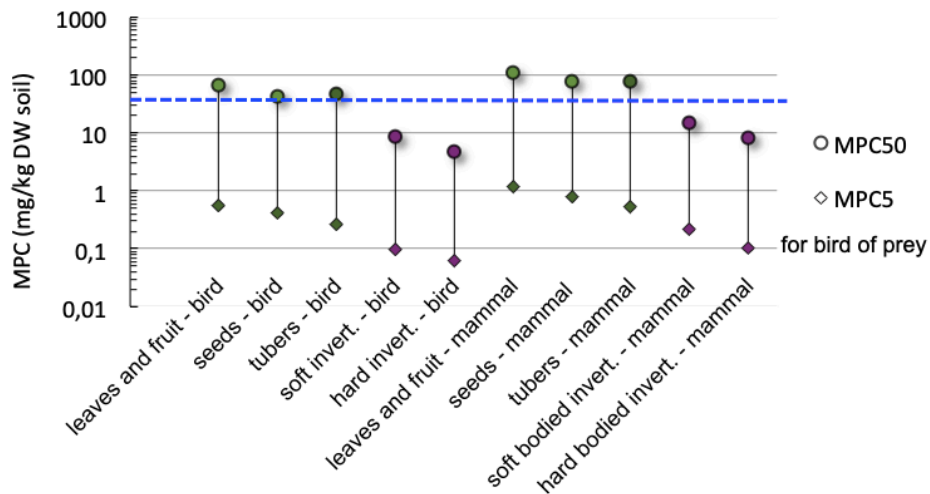


Figure 17. Maximum permissible concentration (MPC) for DDT in soil for secondary poisoning modelled for specific routes through the food web, indicating how bird of prey diet choice influence the risk of getting effected by DDT. Each category denotes one specific route in the food chain: soil→ leaves and fruit, seeds, tubers, soft bodied invertebrates or hard bodied invertebrates →bird or mammal→ bird of prey. The points using plant diet are marked green and the points using invertebrate diet are marked purple. The 95th percentile of the soil concentration (39.5 mg/kg DM) is marked in the graph (blue dashed line).

Sensitivity analysis for MPC species of concern

The sensitive analysis (Spearman Rank) identified BAF_{bird} as the input distribution with highest influence on the MPC output for birds of prey, although $NOEC_{bird}$ also had a high impact (Appendix F, table F5). The most influencing input distribution on MPC output for beasts of prey were the $NOEC_{mammal}$. In general, the variation in modelled species specific MPCs is mostly contributed by variation in toxicity and bioaccumulation from invertebrates or plants to bird or mammal. Another aspect that influences the result is the choice of statistical probability distributions type (table F6).

Analysis and discussion

Risk for the ecosystem based on direct exposure

Given the exposure situation at Kolleberga, the risk (i.e. probability) that more than half (49.5 %) of the species in the whole ecosystem is affected through direct exposure is 5 % (100-95) and the risk that the most sensitive species (6.2 % of the species) in the ecosystem are affected through direct exposure is 50 % (from PAF - blue dashed lines figure 8). However, the effect assessment is based on LOEC and not on NOECs, which otherwise is recommended (Naturvårdsverket, 2009b).

Given the SSD, the risks on the site cannot be regarded as negligible. However, it can be discussed whether the risk for invertebrates and plants is lower in the field, given that the toxicity data is usually from laboratory tests with more or less freshly spiked soil (Jensen and Pedersen, 2006). Time aspects that is likely to have an influence on the toxicity include both the decrease in bioavailability due to soil aging, and also the tendency that invertebrates build up resistance towards DDT (Jensen and Pedersen, 2006; National Research Council, 1986). Resistance implies that species develop a genetically reduced susceptibility to the toxicity (Walker et al., 2012). Resistance in vertebrates are more unusual to find (National Research Council, 1986), which can be added as another reason why mammals and birds are of concern to investigate.

It is difficult to draw informed conclusions about the risk posed to the whole ecosystem; more knowledge about especially invertebrate toxicity is needed. This is known problem and is for example discussed by Smith and Verbuggen (2015) and Jongbloed (1996).

Risk for the species of concern based on secondary poisoning

Through the hazard assessment, birds were identified as the most sensitive group (figure 8) and birds of prey and beasts of prey were of interest to investigate further, given their top position in the food chain and subsequent potential risk of biomagnification. For sparrow hawk, red kite, badger and weasel, the biomagnification aspects included in the model lead to lower MPC5 (soil based) than HC5 (diet based) (table 4 and table 5). This confirm that indirect exposure (secondary poisoning) from the soil have to be regarded when assessing the risk

for top predators, as Jongbloed et al. (1996) among others previously stated. However, this was not the case for Kestrel.

Given the concentrations at the site, the risk of exceeding MPC5 for bird species of concern is high (>85 %, table 5 and figure 15). The probability that half of the red kite population is potentially affected is 32 %. The effects reported for birds mainly involve mortality and reproduction (appendix B). For beasts of prey, effects reported mainly include mortality, growth and reproduction and the risk is relative to birds of prey lower (>77 %). This shows that mammals are less sensitive to DDT.

Effects such as reproduction, growth and behaviour affect species on a populational level (Naturvårdsverket, 2009b). Given the result of this study, it is possible that DDT act as a chemical stressor that combined with other population limiting factors, determines the health and density of the populations. DDT might locally be responsible for restraining e.g. population abundance for the species investigated. However, without validation, it cannot be ruled out whether the risk is responsible for effects, especially as population density might already be limited by other factors.

Given the BAFs (figure 13) and species-specific food chains (figure 7; Appendix D), the resulting probability distributions of MPC make sense: sparrow hawk and red kite have lower MPC5 compared to kestrel, as the later feed on herbivorous (plant eating) mammals, which accumulate DDT in a lower extent. The relatively high fraction of hard-bodied invertebrates consumed by birds eaten by sparrow hawk and red kite makes them vulnerable to DDT; the probabilities of $RQ \geq 1$ are higher for red kite and sparrow hawk relative the other species.

Red kite, as oppose to the other species of concern, is partly feeding on birds of prey, which is one of the reasons it's the most sensitive species of the ones included. Badger on the other hand is more omnivorous, partly feeding on invertebrates and plants, which increase MPC5.

Comparing with other studies

The update of toxicity data to Jongbloed's et al. MPC-model from 1996 resulted in higher HC5 for especially birds, but also mammals (figure 9-10). Adding more toxicity data decreased the uncertainties associated with the parameter estimations from the toxicity data, indicated by smaller confidence intervals (table B3). The updated data caused an increase in MPC5 for the species of concern (except for weasel) relative to Jongbloed.

The effect of updated bioaccumulation data is a bit more complicated to estimate; it's not always clear what type of probability distributions that was used in the model from 1996. However, both mean values and standard deviation for the updated diet items (leaves and fruits, tubers, seeds, soft bodied invertebrates)

decreased (table E1). On the other hand, quite wide range (between minimum and maximum) uniform distributions were used here for tubers and seeds, motivated by the lack of data and a high variability. This study used a more conservative approach than in Jongbloed et al. (1996) where BSAF for especially tubers were assumed to be low. This partly explains the decrease in MPC5 for weasel (relative to 1996), as this species feed on birds and mammals eating seeds and tubers (appendix D, table D1).

Plant parts tend to have a lower bioaccumulation potential relative to invertebrates and mammals and birds. The most critical food chain is soil → hard-bodied invertebrates → bird → beast or bird of prey (figure 16 and 17), which is in line with Jongbloed et al. (1996), where the critical food chain were found to be soil → insect → bird → beast or bird of prey.

Although not in focus in this risk assessment, second trophic level (primary consumers in figure 3) birds and mammals are also susceptible to be affected by DDT (table F4-F5 compared to F2-F3). The outcome of the MPC calculation varies depending on what type of toxicity correction factor that is used. Which correction factor that is suitable for species at the second trophic level is not evaluated and it is therefore difficult to draw any conclusions from this. Nevertheless, the trend is the same as for raptor species; birds and mammals feeding on invertebrates are more sensitive to DDT in soil. This was also investigated by Jongbloed et al. (1996), who found that worm eating birds and mammals had a factor of approximately 11 and 3 higher MPC5, respectively, compared to the lowest MPC5 beast of prey and birds of prey.

A compilation of different material used for establishing environmental guideline values for DDTs in soil, shows that there is a rather large variation of concentrations when effects are expected to occur and when bioaccumulation is considered (Kemakta Konsult AB and Institutet för Miljömedicin, 2016). Values from Canadian and American organizations (USEPA and CCME) range from 0.093-0.7 mg/kg DM for birds and 0.21-2 mg/kg DM for mammals (irrespective of trophic level), while the Dutch organization RIVM estimates that no negative effects are expected at 0.02 and 0.002 mg/kg DM for worm-eaters and predators, respectively (ibid.). RIVM also estimates that serious (over 50% of species or processes affected) effects are expected at 3.8 and 0.38 mg/kg DM for worm-eaters and predators (ibid.). RIVMs guideline value for predators that are assumed to eat small meshes' (worm eating) birds was obtained applying the safety factor 10 (Smith and Verbuggen, 2015). The MPC5s obtained through this risk assessment are compared with the guideline values from USEPA and CCME quite similar (0.093-0.7 compared to 0.11-0.41 for birds; 0.21-2 compared to 0.62-1.28 for mammals). RIVMs estimations are a factor of 32 lower than what was found through here (comparing RIVM: 0.002 and the lowest critical food chain MPC5 in this study: 0.063 mg/kg DM). However, all of the mentioned

studies have been derived in various ways, using various extrapolation and assessments factors, and cannot be directly compared to this study.

Other measures of vulnerability

Apart from toxicological sensitivity and bioaccumulation other factors may be relevant to determine and speculate about effects from chemical stressors on ecosystem and species groups. The result shows that birds are more sensitive to DDT relative mammals, but mammals are, relative to birds, on the other hand more vulnerable to soil pollution as population resilience generally is lower (De Lange et al., 2010). Including other ecological traits such as population recovery and habitat preference could further widen the ecological risk assessment (De Lange et al., 2010). Migration and size of the home range for species are probably important factors that influence the exposure. It is not very likely that raptor species prey on organisms from the same contaminated area (Kemakta Konsult AB and Institutet för Miljömedicin, 2016).

The biodiversity in Scania is affected by the fragmentation of habitats, overexposure, supply of nutrients, other pesticides and climate change (Berlin and Rosquist, 2014). When it comes to raptor birds in Sweden, population curves' lowest points was witnessed in the 1970s (Otvall et al., 2009). Since this decline, the numbers of raptor birds breeding in Sweden have generally increased, a recovery likely caused by a reduction from stressors such as hunting and pollution (Otvall et al., 2009). Swedish bird population (including all species monitored) trends in Sweden show that there are more birds in decline than that are increasing, although the majority of bird populations are stable (Otvall et al., 2009; Green et al., 2018). The bird populations are also controlled by prey availability, for example, the insectivorous Honey Buzzard is one of the raptor bird population that are decreasing, which can probably partly be connected to the decline in insects populations (Otvall et al., 2009).

Uncertainties

Although using probability distributions includes variability and uncertainties in the model, there are other sources of uncertainties connected to this risk assessment. Some of these uncertainties are described and quantified, such as the goodness of fit and sensitivity analysis whereas some are not included. Extrapolation and correction factors, quality of data and discrepancy between model and reality (validation) are uncertainties that are not dealt with.

There is also a balance between being realistic and on the other hand, express large uncertainties when data is scarce. This is the case for e.g. tubers and

seeds, where a large interval (minimum-maximum) defines the chosen input probability distributions (appendix, table E2). Comparing scenario A and B (table F6), it seems like the effect of interval size is influencing MPC (appendix, table F6), although the effect of this is minor. Instead, the variables NOEC_{soc} and BAF for birds and mammals have the major influence on the modelled (sensitivity analysis in appendix, table F5). A critical part in this assessment was also choosing, i.e. assuming type of statistical distribution when fitting data (appendix, table F6).

Risk reduction and remedial objectives

This study has provided knowledge about how risk for raptor populations varies depending on the concentrations of DDT in soil. Although the assessment includes uncertainties, the result can provide information about how much the stressor DDT must be reduced to reach acceptable effects. Given the concentrations at the site, it is clear that the DDT content is exceeding the acceptable limit, defined as the protection of 95 % of the specific populations. By using the probability distributions of MPC (figure 14), other limits than MPC₅ can be used to estimate the risk at certain soil concentrations. For example if the aim is set to a protection level of 75 % (MPC₂₅) or 50 % (MPC₅₀). The highest risk reduction for especially badger and weasel would be given by removing the upper 50th percentile of the soil DDT concentrations, reducing the risk for these species to < 20 %. The probability distribution of MPC can be used in order to rule out how measures to decrease the DDT concentrations in the soil would affect the probability of affecting beast of prey and birds of prey present at the site. However, as this risk assessment is generated as a thesis with learning as main purpose, it should be used with precaution in decision-making.

Future studies

For future studies, lower trophic species could also be included in the risk assessment, as primary consumers also are susceptible of secondary poisoning. This could be motivated by the fact that many bird species other than raptors are in decline (see section above). Given the sensitivity analysis, toxicity data together with BAF for mammals and birds should be prioritized to collect in order to further decrease the uncertainties connected to the estimated risks. For the specific site, more soil sampling would reduce the uncertainties connected to the exposure scenario. Also, to find out the actual risks for invertebrates, field studies should be carried out, given the scarcity of laboratory data and effect of time factors.

Conclusions

Updating the MPC-model developed by Jongbloed et al. (1996) with more data decreased the uncertainties connected to the hazard assessment. Although the same patterns observed in the study from 1996 were also shown here, the MPC for both birds and mammals were increased in this study. This means that the sensitivity towards DDT is regarded as lower in this risk assessment.

Given the measured DDT concentrations at the site, the bioaccumulation potential and the relatively high toxicological sensitivity among birds of prey, the risk of exceeding MPC5 for kestrel, sparrow hawk and red kite is high. The same goes for the beasts of prey badger and weasel, but not in the same extent, as mammals are less sensitive to DDT. Looking at the species of concern evaluated here, it is evident that the higher position in the food web, the higher the risk (comparing badger and red kite). Furthermore, raptor species that feed on birds or mammals that feed on invertebrates are more susceptible to risks. Especially hard-bodied invertebrates are known to bioaccumulate DDT, which was already shown in the model from 1996.

The results indicate that DDT have the potential to act as a chemical stressor that combined with other population limiting factors determines the health and density of these raptor populations. This study shows that neither the ecosystem nor specific raptor populations are exposed to acceptable DDT concentrations. However, what is regarded as acceptable is defined as the protection of 95 % of the populations in this risk assessment, and other levels can be used. What is regarded as acceptable is more of a political question than scientific.

Acknowledgements

I would like to express my gratitude to my supervisors Olof Berglund and David Hagerberg for helpful suggestions and discussions throughout the process. It's been interesting and motivating to deal with a real site and I hope that the results can bring knowledge about important aspects to consider when assessing the risks connected to the plant nursery.

I would also like to thank the members of the group supervising meetings, for giving support and philosophical advices. And not to forget, my friends for their encouragement and support throughout this spring!

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Appendix

Appendix A – Variables used in model

Table A1. Bioaccumulation variables used in model (logarithmically transformed indata). Expressed as biota to soil accumulation factors (BSAF) and bioaccumulation factors (BAF). Anderson-Darling (A-D) and p-value measures the goodness of fit between the statistical distribution and the input data distribution, a high p-value indicate a good fit.

Variable abbreviation	Variable	Distribution type	Parameters (defining distribution)	A-D; p-value
BAF _m	Bioaccumulation factor of mammals	triangular	min: -2.7333 mode: 0.70415 max: 0.70415	not reported
BAF _b	Bioaccumulation factor of birds	triangular	min: -2.8242 mode: 0.33122; max:0.33122	not reported
BSAF _{fip-leaves-fruits}	Biota-to-soil accumulation factor for leaves and fruits	logistic	α : -1.0995 β : 0.42708	0.5187; 0.1290
BSAF _{fip-seeds}	Biota-to-soil accumulation factor for seeds	uniform	min: -2.2608 max: 0.36078	0.2499; 0.9240
BSAF _{fip-tubers}	Biota-to-soil accumulation factor for tubers	uniform	min: -2.6289 max: 0.68879	0.4; 0.3970
BSAF _{fip-soft-inverteb}	Biota-to-soil accumulation factor for soft-bodied invertebrates (gastropods, larvae of insects, earthworms)	logistic	α : -0.25876 β : 0.38048	0.3164; 0.4980
BSAF _{fip-hard-inverteb}	Biota-to-soil accumulation factor for hard-bodied invertebrates (insects, isopods)	logistic	α : -0.026219 β : 0.37181	0.4858; 0.1730

Table A2. Toxicity variables used in model (ppm or mg/kg wet weight prey, using logarithmically transformed indata from appendix B). Anderson-Darling (A-D) and p-value measures the goodness of fit between the statistical distribution and the input data distribution, a high p-value indicate a good fit. Confidence interval for parameter estimations in table B2.

Variable abbreviation	Variable	Distribution type	Parameters (defining distribution)	A-D; p-value
NOEC _{birds}	No effect concentrations for bird, no correction factor	Logistic	α : 0.93435; β : 0.37883	0.4121; 0.2270
NOEC _{mammal}	No effect concentrations for mammal, no correction factor	Logistic	α : 1.93651; β : 0.27647	0.3524; 0.3740
NOEC _{bird KESTREL}	No effect concentrations for Kestrel correction factor 0.21	Logistic	α : 0.25206; β : 0.37409	0.4121; 0.2270
NOEC _{bird SPARROW HAWK}	No effect concentrations for sparrow hawk correction factor 0.24	Logistic	α :0.31005; β : 0.37409	0.4121; 0.2270
NOEC _{bird RED KITE}	No effect concentrations for red kite correction factor 0.25	Logistic	α : 0.31005; β : 0.37409	0.4121; 0.2270
NOEC _{mammal BADGER}	No effect concentrations for badger correction factor 0.15	Logistic	α : 1.1126; β : 0.27647	0.3524; 0.3740
NOEC _{mammal WEASEL}	No effect concentrations for weasel correction factor 0.16	Logistic	α : 1.14063; β : 0.27647	0.3524; 0.3740

Table A3. Fraction of diet for top predators used as variables in model (eq. 1.2). More information in Appendix D.

FOR KESTREL:		Fraction of species group in diet:
DFTbird	fraction of birds in diet of top predator	0
DFTmammal	fraction of mammals in diet of top predator	1
DFMip-leaves-fruits	fraction of leaves and fruits in diet of mammals	0.952
DFM-ip-seeds	fraction of seeds in diet of mammals	0.029
DFM-ip-soft-inv.	fraction of soft bodied invertebrates in diet of mammals	0.015
DFM-ip-hard-inv.	fraction of hard bodied invertebrates in diet of mammals	0.004
FOR BADGER:		
DFTbird	fraction of birds in diet of top predator	0.02
DFTmammal	fraction of mammals in diet of top predator	0.12
DFB-ip-leaves and fruits	fraction of leaves and fruits in diet of birds	0.006
DFB-ip-seeds	fraction of seeds in diet of birds	0.004
DFB-ip-soft bodied invert.	fraction of soft bodied invertebrates in diet of birds	0.005
DFB-ip-hard bodied invert.	fraction of hard bodied invertebrates in diet of birds	0.006
DFM-ip-leaves and fruits	fraction of leaves and fruits in diet of mammals	0.046
DFM-ip-seeds	fraction of seeds in diet of mammals	0.018
DFM-ip-soft bodied invert.	fraction of soft bodied invertebrates in diet of mammals	0.04
DFM-ip-hard bodied invert.	fraction of hard bodied invertebrates in diet of mammals	0.009
DFM-ip-tubers	fraction of tubers in diet of mammals	0
DFT-ip-leaves and fruits	fraction of leaves and fruits in diet of badger	0.16
DFT-ip-seeds	fraction of seeds in diet of badger	0.19
DFT-ip-soft bodied invert.	fraction of soft bodied invertebrates in diet of badger	0.28
DFT-ip-hard bodied invert.	fraction of hard bodied invertebrates in diet of badger	0.18
FOR SPARROW HAWK:		Fraction of species group in diet:
DFTbird	fraction of birds in diet of top predator	1.00
DFTmammal	fraction of mammals in diet of top predator	0.00
DFB-ip-leaves and fruits	fraction of leaves and fruits in diet of birds	0.24
DFB-ip-seeds	fraction of seeds in diet of birds	0.36
DFB-ip-soft bodied invert.	fraction of soft bodied invertebrates in diet of birds	0.18
DFB-ip-hard bodied invert.	fraction of hard bodied invertebrates in diet of birds	0.22
FOR WEASEL:		Fraction of species group in diet:
DFTbird	fraction of birds in diet of top predator	0.30
DFTmammal	fraction of mammals in diet of top predator	0.70
DFB-ip-leaves and fruits	fraction of leaves and fruits in diet of birds	0.10
DFB-ip-seeds	fraction of seeds in diet of birds	0.08
DFB-ip-soft bodied invert.	fraction of soft bodied invertebrates in diet of birds	0.03
DFB-ip-hard bodied invert.	fraction of hard bodied invertebrates in diet of birds	0.05
DFB-ip-tubers	fraction of tubers in diet of birds	0.04
DFM-ip-leaves and fruits	fraction of leaves and fruits in diet of mammals	0.55
DFM-ip-seeds	fraction of seeds in diet of mammals	0.08
DFM-ip-soft bodied invert.	fraction of soft bodied invertebrates in diet of mammals	0.04
DFM-ip-hard bodied invert.	fraction of hard bodied invertebrates in diet of mammals	0.01
DFM-ip-tubers	fraction of tubers in diet of mammals	0.02
FOR RED KITE:		Fraction of species group in diet:
DFTbird	fraction of birds in diet of top predator	0.82
DFTmammal	fraction of mammals in diet of top predator	0.18
DFB-ip-leaves and fruits	fraction of leaves and fruits in diet of birds	0.31
DFB-ip-soft bodied invert.	fraction of soft bodied invertebrates in diet of birds	0.26
DFB-ip-hard bodied invert.	fraction of hard bodied invertebrates in diet of birds	0.15

DFB-bird ((som i sin tur ätit bytesdjur, bildar ytterligare trofisk nivå))	fraction of lower trophic birds in diet of birds	0.19
DFB-mammal (som i sin tur ätit bytesdjur)	fraction of lower trophic levels mammals in diet of birds	0.08
DFB-bird-ip-leaves and fruits	fraction of leaves and fruits in diet of lower trophic birds	0.27
DFB-bird-ip-seeds	fraction of seeds in diet of lower trophic birds	0.19
DFB-bird-ip-soft-invert.	fraction of soft invertebr in diet of lower trophic birds	0.22
DFB-bird-ip-hard-invert	fraction of hard invertebr in diet of lower trophic birds	0.31
DFB-bird-ip-tubers	fraction of tubers in diet of lower trophic birds	0.00
DFB-mammal-ip-leaves and fruits	fraction of leaves and fruits in diet of lower trophic mammals	0.45
DFB-mammals-ip-seeds	fraction of seeds in diet of lower trophic mammals	0.22
DFB-mammals-ip-soft invert	fraction of soft invertebr in diet of lower trophic mammals	0.21
DFB-mammals-ip-hard invert	fraction of hard invertebr in diet of lower trophic mammals	0.08
DFB-mammals-ip-tubers	fraction of tubers in diet of lower trophic mammals	0.04
DFM-ip-leaves and fruits	fraction of leaves and fruits in diet of mammals	0.71
DFM-ip-seeds	fraction of seeds in diet of mammals	0.17
DFM-ip-tubers	fraction of tubers in diet of mammals	0.13

Appendix B – Toxicity data

Table B1. Collected toxicity data for birds and mammals, based on diet concentrations (mg/kg). Longer more comprehensive information in table B2 and B3.

BIRDS tox. Data (not species-specific corrected)	MAMMALS tox. Data (not species-specific corrected)
0.5	20.0
3.3	25.0
3.3	28.4
5	100.0
5	200.0
10	400.0
10	75.0
17	53.5
100	53.5
50	62
5.6	44.1
2.8	215.8
50	325
5.8	650
0.23	
5	
5	
20	
9	
200	
34.6	

Table B2. Correction factors for standardization of NOECs for predators depending on metabolic rate, caloric content of food and food assimilation efficiency, resulting in a total correction factor, calculated by Jongbloed et al. (1996).

Top predator		Total correction factor
Birds of prey:	Bird eater (ex. sparrow hawk)	0.24
	Mammal eater (ex. kestrel)	0.21
Beast of prey:	Bird eater	0.17
	Mammal eater (ex. badger)	0.15

Table B3. Comparison between goodness of fit measurements between Jongbloed et al. (1996) data and updated data (table B3 and B4 below) used in this study (logarithmic data fitted). Bootstrap yielded confidence interval (CI) around the fitted value of the parameters α and β . Anderson-Darling (A-D) and p-value measures the goodness of fit between the statistical distribution and the input data distribution, a high p-value indicate a good fit.

	Parameter defining logistic distribution	Fitted value and 95 % lower and upper limit CI	CI width	A-D; p-value
Bird toxicity data only Jongbloed data	α	0.6272 0.2022-1.0399)	0.8376	0.2375; 0.7370
	β	0.8376 (0.1707-0.5505)	0.3797	
Bird toxicity data updated data (used in model)	α	0.9298 (0.6583-1.2259)	0.5676	0.4121; 0.2770
	β	0.3741 0.2415-0.5131)	0.2715	
Mammal toxicity data only Jongbloed data	α	1.8157 (1.3829-2.2552)	0.8723	0.3948; 0.2800
	β	0.3067 (0.108-0.3918)	0.3918	
Mammal toxicity data update (used in model)	α	1.9365 (1.676-2.1897)	0.5137	0.3524; 0.370
	β	0.2765 (0.1606-0.3894)	0.2287	

Table B4. Chronic dietary toxicity data for birds (oral exposure). The data from Jongbloed et al. (1996) is updated with toxicity data from ECOTOX knowledgebase. For data collected from ECOTOX: for the same study, the geometric mean is reported. When several studies have evaluated the same effect parameter and have similar exposure periods, a geometric mean of these studies are used.

Species	Effect parameter	Exposure period	Reported value	Converted value (NOEC, mg/kg)	Conversion comment	Reference, as written in Jongbloed et al. (1996)	Reference ECOTOX knowledgebase
<i>Streptopelia risoria</i>	reproduction	8 days	10 (LOEC)	0.5	1, 2	Peakall (1970)	
<i>Molothrus ater</i>	mortality	13 Days	<100 (LOEC)	3.3	1, 2	Van Velzen et al. (1972)	
<i>Anas platyrhynchos</i>	reproduction	2 Years	3.3	3.3		Heath et al. (1969)	
<i>Anas platyrhynchos</i>	mortality	106 days	10 (LOEC)	5	1		Vangilder and Peterle (1980)
<i>Anas platyrhynchos</i>	growth	106 days	10 (LOEC)	5	1		Vangilder and Peterle (1980)
<i>Coturnix c. japonica</i>	reproduction	12 Weeks	10	10		Davison et al. (1976)	
<i>Coturnix c. japonica</i>	morphology	21 days	100	10	2		Bernstein and Johnson (1973)
<i>Colinus virginianus</i>	mortality	63 Days	50	17	2	Coburn and Treichler (1946)	
<i>Colinus virginianus</i>	morphology		50	100			Geometric mean for the two studies below
	morphology	121 days	50				Hurst et al. (1974)
	morphology	242 days	150				Lehman et al. (1974)
<i>Phasianus colchicus</i>	reproduction	8 Weeks	<100	50	1	Genelly and Rudd (1956)	
<i>Falco sparverius</i>	reproduction			5.6		Geometric mean for the three studies below	
		5.5 Months	0.3	3	3	Lincer (1975)	
		Not reported	<3	6	3	Peakall et al. (1973)	
		>2 Years	<2.6	10	3	Wiemeyer and Porter (1970)	
<i>Otus asio</i>	reproduction	>1 Year	2.8	2.8		McLane and Hall (1972)	
<i>Gallus domesticus</i>	feeding behaviour	196 days	50	50			Lillie et al. (1972)
<i>Gallus domesticus</i>	mortality			5.8			Geometric mean for the three studies below
	mortality	196 days	78.3	78.3			Lillie et al. (1972)
	mortality	196 days	50	50			Lillie et al. (1972)
	mortality	70 days	0.1	0.05	1		Sauter and Steele (1972)

Gallus domesticus	Reproduction	70 days	0.46 (LOEC)	0.23	1		Sauter and Steele (1972)
Anas rubripes	Mortality	152 days	10 (LOEC)	5	1		Longcore and Samson (1973)
Anas rubripes	Reproduction	1095 days	10 (LOEC)	5	1		Longcore and R.C. Stendell (1977)
Anas sp.	morphology	45 days	40 (LOEC)	20	1		Lundholm (1990)
Columba livia	morphology	56 days	18 (LOEC)	9	1		Jefferies and French (1972)
Galliformes	mortality	154 days	200	200			DeWitt (1955)
Passer domesticus	growth			34.6			Geometric mean for the two studies below
	growth	5 days	1500	75	1, 2		Hill (1972)
	growth	5 days	320	16	1, 2		Hill et al. (1971)

(1) a factor of 2 were applied for LOEC toxicity data to derive NOEC.

(2) a factor of 10 were applied to toxicity value to compensate for short (<1 month) studies

(3) Jongbloed et al. (1996) have derived NOEC by extrapolating a level of 20% egg shell thinning.

Table B5. Chronic dietary toxicity data for mammals (oral exposure). The data from Jongbloed et al. (1996) is updated with toxicity data from ECOTOX knowledgebase. For data collected from ECOTOX: for the same study, the geometric mean is reported.

Species	Effect parameter	Exposure period	Reported value	Converted value (NOEC, mg/kg)	Conversion comment	Reference, as written in Jongbloed et al. (1996)	Reference ECOTOX knowledgebase
Rattus norvegicus	reproduction	7 Months	20	20		Clement and Okey (1974)	
Mus musculus	reproduction	6 generations	25	25		Keplinger et al. (1970)	
Saimura sciureus	mortality	6 Months	5 (3)	28.4		Cranmer et al. (1972)	
Microtus pennsylv.	mortality	31 Days	1000	100	1	Coburn and Treichler (1946)	
Macaca mulatta	mortality, growth	7.5 Years	200	200		Durham et al. (1963)	
Canis domesticus	mortality	4 Years	400	400		Lehman (1965)	
Myotis lucifugus	Mortality	40	150 (LOEC)	75	1		Clark and Stafford (1981)
Tadarida brasiliensis	Mortality	40	107 (LOEC)	53.5	1		Clark and Kroll (1977)
Tadarida brasiliensis	Growth	40	107 (LOEC)	53.5	1		Clark and Kroll (1977)
Ovis aries	Growth	94	62	62			Wilson et al. (1946)
Oryctolagus cuniculus	Morphology	57	2.67 (mg/kg bdwt/d) LOEC	44.055	1, 4		Street and Sharma (1975)
Oryctolagus cuniculus	Growth	57	6.54 (mg/kg bdwt/d)	215.82	4		Street and Sharma (1975)
Canis familiaris	Morphology	32	50 (mg/kg bdwt/d)	325	1, 4		Copeland and Cranmer (1974)

			(LOEC)				
Canis familiaris	Growth	32	50 (mg/kg bdwt/d)	650	4		Copeland and Cranmer (1974)

(1) a factor of 2 were applied for LOEC toxicity data to derive NOEC.

(2) a factor of 10 were applied to toxicity value to compensate for short (<1 month) studies

(3) Jongbloed et al. (1996) have derived NOEC by extrapolating a level of 20% egg shell thinning.

(4) NOEC derived by applying approximate conversion factors (from NZEPA, 2012), relating concentration in diet (mg/kg) to dietary intake (mg/kg bw/day) rabbit: 1 mg/kg bw/day = 33 mg/kg of diet; dog: 1 mg/kg bw/day = 13 mg/kg of diet.

Table B6. Toxicity data used for the species sensitivity distribution (SSD) for the whole ecosystem. For data collected from ECOTOX: for the same study, the geometric mean is reported. When several studies have evaluated the same effect parameter and have similar exposure periods, a geometric mean of these studies is used.

Scientific or common name	Effect parameter	LOEC/EC30 (mg/kg dw soil)	Species group	Reference
Eisenia fetida	reproduction	294	invertebrate	Cavanagh and Munir, 2016
Folsomia candida	reproduction	167	invertebrate	Cavanagh and Munir, 2016
Phaseolus vulgaris	growth	25	plant	Cavanagh and Munir, 2016
Lolium perenne	root length	1 209	plant	Cavanagh and Munir, 2016
Chlorococcum meneghini	growth density	7	plant	Cavanagh and Munir, 2016
Abruzzi rye	tops yeidl (ww)	60	plant	Cavanagh and Munir, 2016
Balbo rye	tops yield (ww)	60	plant	Cavanagh and Munir, 2016
Black Valentine beans	vine yield	12	plant	Cavanagh and Munir, 2016
Buckwheat	yield (aerial portion)	78	plant	Cavanagh and Munir, 2016
Green beans	yield	55	plant	Cavanagh and Munir, 2016
Mustard	seedling height	50	plant	Cavanagh and Munir, 2016
Netted Gem potatoes	tuber yield	30	plant	Cavanagh and Munir, 2016
Onions	yield (bulbs)	180	plant	Cavanagh and Munir, 2016
Peanut	seedling height	13	plant	Cavanagh and Munir, 2016
Perfection peas	plant & seed yield	30	plant	Cavanagh and Munir, 2016
Purple top white Globe turnips	tops yield	60	plant	Cavanagh and Munir, 2016
Rutgers tomatoes	plant yield	60	plant	Cavanagh and Munir, 2016
Stringless Black Valentine beans	plant yield	60	plant	Cavanagh and Munir, 2016
Microarthropods (mites etc)	mortality	25	invertebrate	Cavanagh and Munir, 2016
Microarthropods (Collembola, Cryptopygus (Rhodanella) fasciatus	mortality	125	invertebrate	Cavanagh and Munir, 2016
Hyperiodrylus spp.	casting activity	13	invertebrate	Cavanagh and Munir, 2016
Eudrilus spp.	casting activity	13	invertebrate	Cavanagh and Munir, 2016
Earthworms	reduction in biomass	3	invertebrate	Cavanagh and Munir, 2016
Microbes	ammonification	3125	microbe	Cavanagh and Munir, 2016
Microbes	nitrate production	13	micorbe	Cavanagh and Munir, 2016
Microbes	nitrification/inhibition	1000	microbe	Cavanagh and Munir, 2016
Folsomia fimetaria springtail	reproduction	663.8	invertebrate	Jensen and Pedersen, 2006
		LOEC (mg/kg, diet)		
Streptopelia risoria	reproduction	10	bird	Jongbloed, 1996; Peakall (1970)
Anas platyrhynchos	mortality	10	bird	ECOTOX: Vangilder and Peterle (1980)
Anas platyrhynchos	growth	10	bird	ECOTOX: Vangilder and Peterle (1980)
Gallus domesticus	mortality	0.1	bird	ECOTOX: Sauter, E.A., and E.E. Steele
Gallus domesticus	reproduction	0.5	bird	ECOTOX: Sauter, E.A., and E.E. Steele

Anas rubripes	mortality	10	bird	ECOTOX: Longcore and Samson (1973)
Anas rubripes	reproduction	10	bird	ECOTOX: Longcore and Samson (1973)
Anas sp.	morphology	40	bird	ECOTOX: Lundholm (1990)
Columba livia	morphology	18	bird	ECOTOX: Jefferies and French (1972)
Passer domesticus	growth	910	bird	ECOTOX: Hill (1972); Hill, Dale, and Miles (1971)
Myotis lucifugus	mortality	150	mammal	ECOTOX: Clark and Stafford (1981)
Tadarida brasiliensis	mortality	107	mammal	ECOTOX: Clark and Stafford (1981)
Tadarida brasiliensis	growth	107	mammal	ECOTOX: Clark and Stafford (1981)
Oryctolagus cuniculus	morphology	88.1	mammal	ECOTOX: Street and Sharma (1975)
Canis familiaris	morphology	650	mammal	ECOTOX: Copeland and Cranmer (1974)

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Table B7. Goodness of fit statistics for the ecosystem species sensitivity distribution (data from table B6). Bootstrap yielded confidence interval (CI) around the fitted value of the parameters α and β . Anderson-Darling (A-D) and p-value measures the goodness of fit between the statistical distribution and the input data distribution, a high p-value indicate a good fit.

	Parameter defining logistic distribution	Fitted value and 95 % lower and upper limit CI	CI width	A-D; p-value
Toxicity data whole ecosystem	α	1.6436 (1.3923; 1.8704)	0.4781	0.4188; 0.2700
	β	0.4648 (0.3409; 0.5688)	0.228	

Appendix C – Soil concentration

Table C1. Soil concentration values at Kollberga forest plant nursery (Tyréns, 2017).

Location on site	Soil concentration sum-DDT (mg/kg DM)
Field	0.36
Field	6.2
Field	4.58
Field	5.53
Field	2.33
Field	5.58
Field	4.73
Field	1.04
Field	2.09
Field	1.68
Field	2
Dipping site	31.03
Dipping site	60.74
Dipping site	0.084
Dipping site	0.048
Plant land fill	1.97
Plant land fill	7.57
Plant land fill	1.8

Table C2. Parameter confidence interval for the log-normal distribution fit for soil concentration values (sum-DDT mg/kg DM). Bootstrap yielded confidence interval (CI) around the fitted value of the parameters μ and σ . Anderson-Darling (A-D) and p-value measures the goodness of fit between the statistical distribution and the input data distribution, a high p-value indicate a good fit.

parameters	fit value	95% lower limit	95 % upper limit	confidence interval width	A-D; p-value
μ	10.186	2.999	33.69	30.691	0.6340
σ	42.757	5.342	361.035	355.694	0.0872

Appendix D – Diet choice and species of concern

Table D1. Diet choice for species of concern used in the model expressed as fractions of total diet. Data taken from Jongbloed et al. (1996), where also more comprehensive information regarding the diets can be found.

	Sparrow hawk		Kestrel		Weasel		Badger		
	Route via birds	Route via mammals	Route via birds	Route via mammals	Route via birds	Route via mammals	Route via birds	Route via mammals	Direct route via invertebrates and plants
Leaves	1	0	0	95.1	4.7	51.2	0.1	4.4	14
Fruits	23	0	0	0.1	5.1	3.7	0.5	0.2	2
Seeds	36	0	0	2.9	8	8.2	0.4	1.8	19
Earthworms	8.8	0	0	0.6	1.4	3.2	0.3	3.2	27
Gastropods	3.2	0	0	0	0.7	0	0.1	0	1
Insect larvae	6	0	0	0.9	0.8	0.8	0.1	0.8	0
Caterpillars	5.8	0	0	0.1	1.2	0.2	0.1	0.2	0
Insects	15.2	0	0	0.1	3.1	0.6	0.3	0.3	18
Isopods	0.1	0	0	0	0.2	0	0	0	0
Spiders	0.8	0	0	0.2	0.5	0.5	0.2	0.4	0
Tubers	0	0	0		4.4	1.5	0	0.6	0
Total	100	0	0	100	30	70	2	12	81

Table D2. Diet choice for red kite, fractions of either the total bird route or total mammal route. Semiquantitative data from Kjellen (1998) and qualitative data from Artdatabanken, SLU (2019a-2019c).

		Route via birds	Route via mammals
Leaves & fruits		30.5	70.8
Seeds		0.0	16.7
Soft-bodied invertebrates (gastropods, larva of insects, earthworms)		26.4	0.0
Hard-bodied invertebrates (adult insecta, isopods, spiders, caterpillars)		15.3	0.0
Tubers		0.0	12.5
Birds (lower trophic)	Leaves & fruits	19.4	0
	Seeds		
	Soft-bodied invertebrates (gastropods, larva of insects, earthworms)		
	Hard-bodied invertebrates (adult insecta, isopods, spiders, caterpillars)		
	Tubers		
Mammals (lower trophic)	Leaves & fruits	8.3	0
	Seeds		
	Soft-bodied invertebrates (gastropods, larva of insects, earthworms)		
	Hard-bodied invertebrates (adult insecta, isopods, spiders, caterpillars)		
	Tubers		

References diet data

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Appendix E – Bioaccumulation

Table E2, E3 and E4 give biota-to-soil accumulation factors (BSAF) that are used in the model, as an update to the already existing bioaccumulation data in Jongbloed et al. (1996). Geometric mean and standard deviation for all data (Jongbloed combined with new data) available in table E1.

Table E1. Geometric mean, numbers of data points (N) and standard deviation for bioaccumulation factors used in model. Reported for Jongbloed et al. (1996) and from update (containing data from both Jongbloed et al. and new data). Not logarithmic presented here.

	Leaves and fruits	Seeds	Tubers	Soft-bodied invertebrates	Hard-bodied invertebrates	Birds	Mammals
Jongbloed geometric mean	0.15 (N=16)	0.84 (N=1)	0.17 (N=4)	0.65 (N=16)	0.83 (N=24)	0.52 (N=20)	0.47 (N=19)
Update geometric mean	0.08 (N=27)	0.12 (N=5)	0.07 (N=6)	0.52 (N=29)			
Standard deviation Jongbloed	0.39	-	0.67	2.38	1.68	1.59	0.76
Standard deviation update	0.33	0.34	0.59	1.99			

Table E2. Goodness of fit measurements for bioaccumulation data used in the model (logarithmic data fitted). Bootstrap yielded confidence interval (CI) around the fitted value of the parameters α and β . Anderson-Darling (A-D) and p-value measures the goodness of fit between the statistical distribution and the input data distribution, a high p-value indicate a good fit.

Diet item	Parameter defining logistic distribution	Fitted value and 95 % lower and upper limit CI	CI width
leaves and fruits	α	-1.0995 (-1.3726; -0.8237)	0.5489
	β	0.4271 (0.2943; 0.5706)	0.2763
seeds	min	-2.2608 (-2.8428; -1.0665)	1.7762
	max	0.3608 (-0.7294; 0.9295)	1.659
tubers	min	-2.6289 (-3.228; -1.4443)	1.7836
	max	0.6888 (-0.4578; 1.2699)	1.7276
soft bodied invertebrates (gastropods, larvae of insects, earthworms)	α	-0.2588 (-0.501; -0.0216)	0.4794
	β	0.3805 (0.2674; 0.5027)	0.2353
hard bodied invertebrates (insects, isopods)	α	-0.0262 (-0.2819; 0.2437)	0.5256
	β	0.3718 (0.2527; 0.5037)	0.251
mammals	min	-2.7333 (-3.1537; -1.5983)	1.5554
	mode (most likely)	0.7042 (-1.6799; 0.7021)	2.382
	max	0.7042 (0.3929; 1.2124)	0.8195
birds	min	-2.8242 (-3.2084; -1.7395)	1.4689
	mode (most likely)	0.3312 (-1.9088; 0.3293)	2.2381
	max	0.3312 (0.0268; 0.8081)	0.7814

Table E3. Bioconcentration factors (BCF) used as biota-to-soil accumulation factors (BSAF) for DDTs in the edible parts of different crop species, geometric means from Li et al. (2018).

Group	Species	DDT/DDE	BFC	Wet weight/dry weight (WW/DW)	BCF (WW)
fruit	Asparagus bean	DDTs	0.093	WW	0.09
fruit	Maize	DDTs	0.005	WW	0.01
fruit	Peanut	DDTs	0.114	WW	0.11
fruit	Soybean	DDTs	0.236	WW	0.24

leaves	Bok choy	DDTs	0.258	DW (93 % water content)	0.018
leaves	Cauliflower	DDTs	0.026	WW	0.03
leaves	Celery	DDTs	0.007	WW	0.01
leaves	Chinese cabbage	DDTs	0.149	DW (95 % water content)	0.007
leaves	Chinese chives	DDTs	0.008	WW	0.01
leaves	Spinach	DDTs	0.013	WW	0.01
leaves	Violet	DDTs	0.156	WW	0.16
seed	Gingili	DDTs	0.606	WW	0.61
seed	Mustard	DDTs	0.015	WW	0.02
seed	Rice	DDTs	0.123	WW	0.12
seed	Wheat	DDTs	0.025	WW	0.03
tuber	Carrot	DDTs	0.016	WW	0.02
tuber	Turnip	DDTs	0.007	WW	0.01

Table E4. BSAF for soft bodied invertebrates, Lumbricidae (earthworms) spp. (lipid weight /organic carbon). From Vermeulen et al. (2010), transformed according to method in Jongbloed et al. (1996).

Organ/ tissue	field/lab	soil type	Csoil (mg/kg)	BSAF	WW or DW	% OC soil	% lipid content earthworms	BSAF (wet whole body, soil)
fat	field	grassland	0.00927	0.56 lw/OC	dw soil	2.58	6.34	0.23
fat	field	open woodland	0.00212	1.70 lw/OC	dw soil	2.32	6.31	0.63
fat	field	grassland	0.00129	0.49 lw/OC	dw soil	2.15	6.16	0.17
fat	field	open woodland	0.00285	0.48 lw/OC	dw soil	1.5	6.96	0.10

Table E5. BSAFs for sum-DDT in worms for soils, expressed as whole body weight, summary of field data from Smith and Verbuggen (2015).

Group	BSAF (kgdwt soil/kgwwt worm sum-DDT)
soft bodied invertebrates	0.72
soft bodied invertebrates	0.29
soft bodied invertebrates	0.59
soft bodied invertebrates	0.69
soft bodied invertebrates	0.6
soft bodied invertebrates	0.33
soft bodied invertebrates	0.48
soft bodied invertebrates	0.41

References bioaccumulation data

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Appendix F – Maximum permissible concentration

Table F1. Maximum permissible concentration (MPC) for DDT in soil (mg/kg DM) for secondary poisoning modelled for specific routes through the food web, indicating how beast of prey diet choice influence the risk of getting effected by DDT. Each category denotes one specific route in the food chain: soil → leaves and fruit, seeds, tubers, soft bodied invertebrates *or* hard bodied invertebrates → bird *or* mammal → beast of prey. Most critical food chain underlined. MPC is for this table modelled with a correction factor of 0.15, which is the lowest for mammal used in this study.

FOR BEASTS OF PREY	leaves and fruit-bird	seed-bird	tuber-bird	soft invert-bird	hard invert-bird	leaves and fruit-mammal	seed-mammal	tuber-mammal	soft invert-mammal	hard invert-mammal
MPC5	6.49	3.84	2.05	1.16	0.61	11.72	8.5	5.25	2.53	1.25
MPC50	405.57	313.82	321.41	61.51	32.67	899.54	602.75	587.77	119.21	62.22

Table F2. Maximum permissible concentration (MPC) for DDT in soil (mg/kg DM) for secondary poisoning modelled for specific routes through the food web, indicating how bird of prey diet choice influence the risk of getting effected by DDT. Each category denotes one specific route in the food chain: soil → leaves and fruit, seeds, tubers, soft bodied invertebrates *or* hard bodied invertebrates → bird *or* mammal → bird of prey. Most critical food chain underlined. MPC is for this table modelled with a correction factor of 0.21, which is the lowest for birds used in this study.

FOR BIRDS OF PREY	leaves and fruit-bird	seed-bird	tuber-bird	soft invert-bird	hard invert-bird	leaves and fruit-mammal	seed-mammal	tuber-mammal	soft invert-mammal	hard invert-mammal
MPC5	0.547	0.42	0.26	0.0963	0.0625	1.19	0.79	0.54	0.22	0.105
MPC50	68.93	43.29	46.75	8.69	4.69	112.01	80.55	78.14	15.37	8.43

Table F3. Maximum permissible concentration (MPC) for DDT in soil (mg/kg DM) for second trophic level mammals, modelled for specific routes through the food web, indicating how mammals (second trophic level) diet choice influence the risk of getting effected by DDT. Each category denotes one specific route in the food chain: soil → leaves and fruit, seeds, tubers, soft bodied invertebrates *or* hard bodied invertebrates → mammal. The MPC is given as an interval, where the lower value is modelled with a toxicity correction factor of 0.15 (the lowest correction factor for beasts of prey used in this study, although not representative for lower trophic birds (Traas et al., 1996)), and the higher value is modelled without correction factor.

MAMMALS	leaves and fruit	seed	tuber	soft bodied invert.	hard bodied invert.
MPC5	4.9-38.0	7.6-47.6	5.31-36.9	1.01-5.51	0.69-4.5
MPC50	157.6-1103.1	86.8-602.8	112.6-837.8	22.8-175.5	14.2-101.7

Table F4. Maximum permissible concentration (MPC) for DDT in soil (mg/kg DM) for second trophic level bird, modelled for specific routes through the food web, indicating how birds (second trophic level) diet choice influence the risk of getting effected by DDT. Each category denotes one specific route in the food chain: soil → leaves and fruit, seeds, tubers, soft bodied invertebrates *or* hard bodied invertebrates → bird. The MPC is given as an interval, where the lower value is modelled with a toxicity correction factor of 0.21 (the lowest correction factor for birds of prey used in this study, although not representative for lower trophic birds (Traas et al., 1996)), and the higher value is modelled without correction factor.

BIRDS	leaves and fruit	seed	tuber	soft bodied invert.	hard bodied invert.
MPC5	0.5-2.4	0.6-2.7	0.5-1.9	0.08-0.5	0.06-0.3
MPC50	23.3-103.0	12.7-57.9	16.0-79.0	3.5-15.2	2.0-10.1

Sensitivity analysis for MPC output

A sensitivity analysis identifies and ranks the input distributions depending on their influence on the output. Using Spearman rank correlation coefficient, a high correlation between input and output imply a more significant impact on the output's value (table F5).

Table F5. Ranking of inputs by correlation coefficients, indicating the impact on output maximum permissible concentration (MPC) for species of concern using correlation (Spearman's Rank). The numbers are ranked, with the input parameter with the highest influence first and underlined.

Ranked input parameter	MPC Kestrel	Ranked input parameter	MPC Sparrow hawk	Ranked input parameter	MPC Red kite	Ranked input parameter	MPC Badger	Ranked input parameter	MPC Weasel
<u>BAF bird</u>	-0.676	<u>BAF bird</u>	-0.687	<u>BAF bird</u>	-0.683	<u>NOECbadger</u>	0.707	<u>NOECweasel</u>	0.879
NOECKestrel	0.55	NOECsparrow hawk	0.552	NOECred kite	0.577	BSAF hard inv	-0.394	BSAF hard inv	-0.168
BSAFleaves fruit	-0.386	BSAF hard inv	-0.253	BSAF hard inv	-0.216	BSAF soft inv	-0.378	BAF mammals triang	-0.155
BSAF hard inv	-0.088	BSAF soft inv	-0.15	BSAF soft inv	-0.2	BSAF seed	-0.118	BSAFleaves fruit	-0.149
BSAF seed	-0.06	BSAF seed	-0.092	BSAFleaves fruit	-0.122	BSAFleaves fruit	-0.096	BAF bird	-0.129
BSAF soft inv	-0.06	BSAFleaves fruit	-0.091	BAF mammals triang	-0.097	BSAF tuber	-0.029	BSAF seed	-0.094
				BSAF seed	-0.04	BAF bird	0.025	BSAF soft inv	-0.093
						BAF mammals triang	0.019	BSAF tuber	-0.041

Table F6. Variation of MPC5 and MPC50 depending on parameter and probability distribution type for the bioaccumulation variables. Scenario A is the output using the present probability distributions and parameters. In scenario B, the probability distributions types are the same as in scenario A, but the parameters defining the uniform probability distributions for seed and tuber are more narrow (min: -1,6; max: -0,076 and min: -2,15; max: 0,215, respectively). In the last scenario C, all probability distribution types are logistic ($p < 0.05$ for the fit in the case for bird and mammal bioaccumulation factors here).

	MPC5 Kestrel	MPC5 badger	MPC5 sparrow hawk	MPC5 weasel	MPC5 red kite	MPC50 Kestrel	MPC50 badger	MPC50 sparrow hawk	MPC50 weasel	MPC50 red kite
Scenario A	0.40	1.3	0.12	0.66	0.09	31.83	20.26	7.27	9.44	7.19
Scenario B	0.47	1.42	0.14	0.78	0.12	32.58	22.02	6.55	9.47	6.31
Scenario C	0.11	1.27	0.05	1.68	0.02	20.93	19.72	4.53	65.65	3.35



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