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Methodology proposal for the derivation of Soil Guideline Values for Plant Protection Product residues

Part 1 - Review and comparison of international methodologies

Commissioned by the Federal Office for the Environment (FOEN)

February 2023

Imprint

Publisher

Swiss Centre for Applied Ecotoxicology, 8600 Dübendorf / 1015 Lausanne, Switzerland

Commissioned by

FOEN, Federal Office for the Environment, Soil and Biotechnology Division, Soil Section, 3003 Bern, Switzerland

Coordinators of the Measure 6.3.3.7 of the Action Plan for Plant Protection Products

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Acknowledgement

This project was funded by the Federal Office for the Environment. The authors would like to acknowledge Gudrun Schwilch and Bettina Hitzfeld from the FOEN and Michael Zimmermann and Katja Knauer from the Federal Office for Agriculture (FOAG) for the discussions along the project and for their valuable comments on the report. The authors would like to thank all the persons listed under scientific support for the exchange we had and the advice that we received.

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Citation Proposal

Mireia Marti-Roura, Gilda Dell'Ambrogio, Sophie Campiche, Janine Wong, Marion Junghans, Mathieu Renaud, Benoit J.D. Ferrari. 2023 Methodology proposal for the derivation of Soil Guideline Values for Plant Protection Product residues. Part 1 - Review and comparison of international methodologies. Swiss Centre for Applied Ecotoxicology, Dübendorf and Lausanne, Switzerland; 156 pp.

Cover Photo

Gilda Dell'Ambrogio, Swiss Centre for Applied Ecotoxicology

Summary

The Ecotox Centre, EnviBioSoil and the Swiss Soil Monitoring Network (NABO) were commissioned to develop a long-term monitoring of PPP residues in soil as a task of the measure 6.3.3.7 of the *Action Plan for the reduction and sustainable use of Plant Protection Products in Switzerland*. The NABO is in charge of the exposure monitoring of Plant Protection Product (PPP) residues in the soils and the Ecotox Centre and EnviBioSoil on the development of bioindicators and risk-based reference values for PPP residues.

This report is the first part of a two-part report on the methodology for the derivation of Soil Guideline Values for Plant Protection Product residues and intends to review the current state of the methodologies used to derive risk-based reference values for PPPs. The first part will support the second part, which is a proposed methodology to derive reference values for PPP residues in agricultural soils from the Ecotox Centre and EnviBioSoil.

The current report can be divided in four parts. The first part of the report (section 1) intends to give an overview of what are soil reference values, their application and use. The second part (section 2) describes the general steps used for the derivation of soil reference values. The third part (section 3) focuses on the description of some of the most important methodologies used in prospective and retrospective soil risk assessment. Finally, the fourth part (section 4), intends to compare the derivation process of some of the main methodologies by using two case studies.

This extensive review has the focus on methodologies that have been used to derive values for PPPs and, when possible, under agricultural land use. Among all the methodologies reviewed and presented in this report, there are two for prospective and four for retrospective risk assessment that have been selected and described in more detail due to their relevance in the regulatory context. The two prospective methodologies are the one used by the European Food Safety Authority (EFSA) for the PPP authorization and the one used by the European Chemical Agency (ECHA) for the authorization of biocidal products. The four retrospective methodologies have been developed and applied in the following countries: The Netherlands, Canada, the US and Australia; and have been used as reference methodologies by many other countries.

Two active ingredients used as PPPs were selected for the case studies: the herbicide diuron and the fungicide fluazinam. The two substances contrast in terms of datasets (quality and availability of data), mode of action and physico-chemical properties. The two prospective and the four retrospective methodologies previously mentioned were applied to both datasets (diuron and fluazinam). The results showed large differences between the soil protection values, mostly driven by the inclusion or exclusion of the most sensitive group of organisms from the dataset, the approach used for the derivation, the food chain model used (for highly bioaccumulative substances like Fluazinam) and the assessment factors applied to account for uncertainties.

The review and better understanding of the methodologies and their feasibility after being applied to the case studies will be used as the foundation for a proposal of a methodology to derive risk-based reference values for PPP residues in agricultural soils in Switzerland.

Content

1 Introduction

1.1 Background and objectives

Plant Protection Products (PPPs) are widely applied in Swiss agriculture and their impact on environmental and human health is of growing concern. In order to minimize the risk of PPP in the environment and promote their sustainable use, the Swiss Federal Council approved on the 6th of September 2017 the Action Plan for PPP (AP-PPP) (Swiss Federal Council, 2017).

PPP applied to crops can also enter the soil, where they might persist for several days up to several years as active ingredient or as transformation product and might eventually leach into water bodies. To assess their risk for soil organisms, some standard laboratory bioassays on terrestrial organisms are required for PPPs before being placed on the market. New tests may also be required during the authorization renewal process of the active ingredient or when the PPP is being re-assessed on the level of the EU Member states or Switzerland. However, knowledge from post-authorization studies on the exposure and the effects of PPP residues and their transformation products in an everyday use is still limited and not legally required.

The AP-PPP includes measures for better protecting Swiss agricultural soils. The measure 6.3.3.7 in particular aims at developing a long-term monitoring of PPP residues in soil. In order to assess the effects of PPP residues on soil organisms, risk-based reference values for PPP residues should be available by 2025 and bioindicators for the effects of PPP residues on soil fertility should be developed by 2027. A collaboration between the Swiss Soil Monitoring Network (NABO), the Ecotox Centre and EnviBioSoil has been created to implement the required measures (Godbersen et al., 2019a). The NABO is in charge of analyzing PPP residues in soil since 2018 and of developing a monitoring for PPP residues in soils by 2024. The Ecotox Centre and EnviBioSoil were commissioned to develop bioindicators and derive risk-based reference values for PPPs under the AP-PPP Measure 6.3.3.7.

In this report, the term used in the section 6.3.3.7 of the AP-PPP “risk-based reference value” and “soil protection value” are considered synonyms. “Soil protection value” is used to describe the limit concentration of a substance in the soil[1], which is expected to cause no harm to potentially exposed organisms. In Switzerland, soil protection values exist mostly for metals and for some organic persistent contaminants but not for currently used PPPs[2]. In order to avoid misinterpretations with other Swiss soil protection values derived for non-PPPs (Swiss Federal Council, 2020a), it was agreed that the soil protection values developed by the Ecotox Centre and EnviBioSoil in the frame of the AP-PPP would be called Soil Guideline Values (SGV). The SGV will be applied as reference values for PPP residues to protect long-term soil fertility in agricultural soils.

The feasibility of deriving SGV needs to be evaluated through the selection of the appropriate methodology. In order to support this decision making, a literature review was conducted to provide an overview of the state of the art of methodologies for deriving soil protection values. The present document is the first of a two-part report for the derivation of SGV and focuses on compiling and comparing the different existing methodologies worldwide for the derivation of soil protection values (see also Appendix 1 for further information). In addition to the literature review (Sections 2 and 3), the most relevant methodologies were applied as case studies to two PPP (Section 4 and Appendix 2). The information gathered in this literature review and case studies (report – Part 1) will inform the second part of the report, which will detail the recommended

[1] Usually expressed in mg active substance/kg soil dry weight (= mg a.s./kg d.w.).
[2] Copper is the only substance used as PPP which already has a soil protection value in Switzerland (Swiss Federal Council, 2020a). However, this substance was not foreseen for the derivation of soil protection values for agricultural soils, since the presence of this metal in soils cannot be attributed exclusively to its use as PPP (Godbersen et al., 2019b).

methodology for the derivation of soil protection values for Swiss agricultural soils under the specific objectives of the AP-PPP.

1.2 Ecological risk assessment and soil protection values

Depending on the area of application, two different general approaches have evolved in parallel in soil risk assessment. One approach is designed to be applied in authorization and registration of chemical substances such as PPPs or hazardous chemicals (Aqeel et al., 2014; Calow and Forbes, 2003). It is a prospective approach and aims at predicting the impact that a compound might cause, following a planned activity or release. This approach is usually applied before the release of substances in the environment or when a substance needs to be re-evaluated. For PPPs, the effect of active substances, formulated products and mixtures is usually assessed by means of experimental studies, often under laboratory or controlled conditions with specific test organisms that are exposed to the substance of interest. More realistic experiments using mesocosms or field studies can also be performed but are much rarer in the literature and not always required for regulation. There are different methodologies applied in prospective risk assessment, some of which involve the derivation of soil protection values (hazard assessment preceding the risk assessment) and others do not (direct risk assessment) (see section 3.1 for further information about methodologies on prospective risk assessment for soils). Prospective risk assessments use predicted environmental concentrations (PEC) for risk characterization of a substance.

For PPPs (active substances (a.s.) and formulated products), the European Food and Safety Authority (EFSA) has defined the data requirements in Commission Regulation (EU) No 283/2013 (European Commission, 2013a) and Commission Regulation (EU) No 284/2013 (European Commission, 2013b), respectively, in order to show that no adverse effects will occur following the release of the PPPs in the environment. For assessing the hazard for the soil ecosystem, a chronic standard laboratory toxicity test with earthworms is mandatory for all active substances and formulated products that can contaminate the soil. For PPPs applied as soil treatments directly to soil either as a spray or as a solid formulation, testing is required for the collembolan *Folsomia candida* and the soil mite *Hypoaspis aculeifer*. Furthermore, a test on soil microbial activity should be provided with nitrogen transformation as endpoint. Finally, effects of PPPs should be tested for non-target higher plants, at least at a screening level, by using at least six species from six different families covering mono- and dicotyledons. In a similar way, the European Chemical Agency (ECHA) assesses the effects of biocides during the authorization process (ECHA, 2018). As some active substances may be used both as PPP and as biocide, the same active substance might be subject to two different authorization processes. However, the toxicity tests with terrestrial organisms, which are required for product authorization of PPPs and biocides, are generally few and limited to a small number of standard species.

The second approach was developed to assess the soil quality at a given site. This retrospective approach addresses effects that might have already occurred at a site following an exposure to a given substance after its release, in an everyday use. The retrospective risk assessment might provide additional information on the actual risk of some compounds that may not have been sufficiently addressed during the prospective risk assessment (Knacker et al., 2008). The most common approach used in retrospective risk assessment to identify the hazard of a substance is by deriving one or multiple soil protection values for single substances. Those values can also be used to evaluate mixture or matrix-based effects when testing environmental samples. In the retrospective approach, the soil protection values are compared to the substance concentration measured at the site of interest. A risk cannot be excluded when the environmental concentrations are equal or higher than the soil protection value.

Although prospective and retrospective risk assessment may share some of the methodologies to derive soil protection values, the area of application of those protection values is different. For this reason, and in order to adapt the protection values to different regulatory contexts, different interpretations or adaptations of the same methodology may take place.

1.3 Existing soil protection values

As the impact of chemicals is still more frequently studied in aquatic than in terrestrial organisms, protection values are generally more often developed for the aquatic compartment (Chiaia-Hernandez et al., 2017). In Switzerland, Regulatory Acceptable Concentrations (RAC) for freshwater are published by the Food Safety and Veterinary Office (FSVO). RAC are usually derived in order to evaluate the prospective risks of PPPs in water. The German Environmental Agency (UBA) has recently used their RAC in a monitoring campaign designed to evaluate the protectiveness of the prospective risk assessment for the management of small water bodies in Germany. The monitoring was done during the application period and like in the prospective risk assessment, the RAC were compared to peak concentrations. In Switzerland, the retrospective risks are assessed with quality standards laid down in the Swiss Waters Protection Ordinance (Swiss Federal Council, 2020b). In 2021, quality standards for sediments for several contaminants, some PPPs among them, were derived in Switzerland as well[3]. The prospective risk assessment of PPPs also encompasses sediment and soil but RAC have not yet been published for these compartments.

For Swiss soils, retrospective protection values are available only for some metals and a few organic persistent compounds (dioxins, furans, polycyclic aromatic hydrocarbons (PAH) and polychlorinated biphenyls (PCB)). These values are included in the Swiss Ordinance relating to Impacts on the Soil (OIS) (Swiss Federal Council, 2020a). There are currently no values for non-persistent substances. It is assumed that, because of their degradation, they will not have any long-term effects. They may be derived though if deemed necessary (SAEFL, 2001). The existing values were set on a case-by-case basis, based on their effects on the environment, human health and livestock. Values for inorganic pollutants are based on well-founded analytical investigations in Swiss soils, including ecotoxicological effects (SAEFL, 2001, 1997). However, for organic pollutants, soil protection values are based on emission and exposure measurements, and on existing values from other countries (Annex 1 and 2 of SAEFL 2001).

Other countries have derived retrospective soil protection values for several metals and organic compounds, including some PPPs (see Section 3.2 and Appendix 1). Traditionally, the derivation of soil protection values for PPPs has mainly been associated to the fact that most of those substances belong to the category of persistent organic pollutants (POPs). For this reason, most values for PPPs are derived for substances, which are no longer authorized but are considered contaminants that can be found in the soil years after being withdrawn from the market (e.g., dieldrin, dichlorodiphenyltrichloroethane (DDT), lindane). Soil protection values for PPP that are currently on the market are rare. However, some countries, e.g., the Netherlands, and also some recent research have been working in this direction (Pivato et al., 2017; Vašíčková et al., 2019). In addition, existing soil protection values are often focused on protecting human health and only a few of them aim to assess ecological effects as well. One of the major difficulties in developing soil protection values is the paucity of available soil ecotoxicological data, partly due to the complexity and heterogeneity of the soil matrix. Soil properties may influence the retention and consequent toxicity of a compound to organisms and therefore it is difficult to establish a harmonized methodology for ecological risk assessment (Fishwick, 2004). The terminologies and methodologies used by some of the leading countries deriving soil protection values are described in Table 2 (section 1.3.2).

Soil protection values used in retrospective hazard assessment may include different risk levels and implementations (generic or site-specific).

[3] https://www.oekotoxzentrum.ch/expertenservice/qualitaetskriterien/sediment-qualitaetskriterien/

1.3.1 Risk level

The intensity of an expected risk increases with the concentration of the contaminant in the soil and the competent authority will define the specific measures in each case (Carlon, 2007). A common approach in screening risk assessment consists of distinguishing three levels of protection, resulting in three different soil protection values (Figure 1) (Carlon, 2007; Pivato et al., 2017). At level 1, the risk is considered negligible and the related soil concentration is based on conservative assumptions. This is often used for setting long-term quality objectives for a site and no intervention is needed as long as the level 1 soil protection value is not exceeded. Chemicals, which concentrations reach level 2, are expected to be potentially adverse for the organisms and this, commonly, triggers further investigations. Finally, at level 3, the risk is considered unacceptable and an intervention is generally required (e.g., remediation activities). This classical interpretation of three levels and their definition, as well as the measures that must be taken in case of exceedance, can vary depending on the country (Carlon, 2007). The implementation and the goals of the soil protection values may be different between countries and, thus the limits and definitions of the risk levels may differ from the level system presented in Figure 1. However, there is usually a clear separation between soil protection values used for remediation purposes and soil protection values that are not used for remediation purposes. For this reason, in the current report we avoided writing about risk levels but used the distinction remediation/non-remediation instead. Some cases of how protection levels are applied in different countries are shown in Table 2 (section 1.3.2).

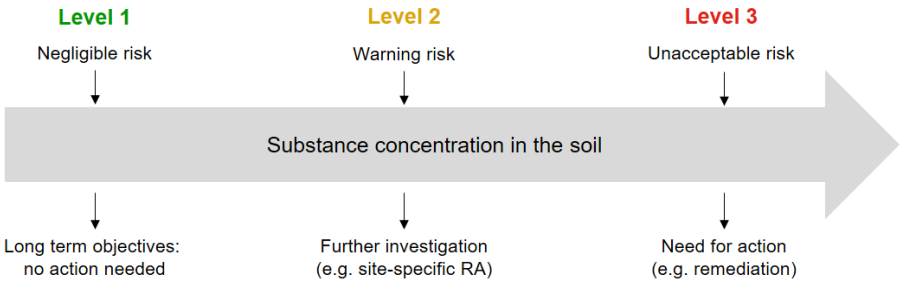

Figure 1: A common approach used in the context of screening risk assessment for the derivation of protection values, according to substance concentration and risk level, adapted from Carlon (2007) and Pivato et al. (2017).

1.3.2 Generic and site-specific values

Generic values indicate the potential for a risk to occur and are generally applicable to all sites, independent of their characteristics. On the other hand, site-specific values are based on site-specific use patterns and characteristics (e.g., soil properties). They also consider environmental and exposure conditions and are thus designed to indicate that the risk may actually be representative only for the specific site (Aqeel et al., 2014; Carlon, 2007). The terms “land use” and “site-specific” should be clearly differentiated. While land use is a concept used in policy referred to different managements of the territory, e.g., agricultural, residential or industrial use, site-specific is used, in this context, to assess the risk of a particular location. Thus, a specific land use could have generic or site-specific soil protection values.

The risk level and its implementation (generic or site-specific values) may vary depending on the decision of the competent authority and influence the derivation of the soil protection value(s) (Table 2). An approach that is commonly adopted by several countries is to derive generic values at a risk level below the remediation level (“warning risk”), which are often called “screening values”, since they allow a first general screening of potentially dangerous substances (Aqeel et al., 2014; Carlon, 2007; Pivato et al., 2017; US EPA, 2001). Contaminants found at lower concentrations are not considered, because they are not expected to cause any harm (Carlon, 2007; Fishwick, 2004; US EPA, 2001) but, if exceeded, usually further investigations are applied. These

investigations are generally associated with a site-specific risk assessment. Many countries derive an additional site-specific clean-up value to account for site-specific land use, environmental conditions, soil type etc. (Carlon, 2007; US EPA, 2003). Some countries might sometimes derive an additional lower screening value, which is most often associated to background concentrations. This lower value was mostly derived in cases of naturally occurring substances that are typical for their geographical region, e.g., metals, but it has also recently been applied to some PPPs (Lamé et al., 2004; Vácha et al., 2014).

Although screening values have similar risk level and application, they can still differ considerably between countries. In order to show the magnitude of this variability, generic screening values for copper are listed in Table 1. In this case, a total of 14 authorities derived a screening value for copper, ranging from 1 to 450 mg/kg soil d.w.

Table 1: Generic soil screening values (at level 2 at the respective countries) for copper from different countries. Some countries may have more than one screening value. In such cases, the range between the minimum and the maximum are listed in the table. Only values including environmental effects were listed (i.e., values considering only human health were not included).

Country	Screening value (mg/kg soil d.w.)
Australia	100
Austria	100
Belgium	40-110
Canada	63-91
Czech Republic	25-450
Denmark	30
Finland	100
Germany	1
Latvia	4-60
Sweden	80-200
Switzerland	150
The Netherlands	40
United Kingdom	35.1
United States	28-100

Differences between existing soil protection values do not only occur due to the different risk levels and/or applications (general or site-specific), but also due to the different methodologies used for the derivation and how they are applied. For the retrospective hazard assessment, the regulatory framework from each authority was established under unique circumstances and thus may have its own level of conservatism, transparency and accuracy. Therefore, even if the same methodology is adopted by several authorities, it might be adapted to cover specific environmental or regulatory needs of a country.

Table 2: Terminology, methodology, risk level and application of retrospective soil protection values used by some of the authorities reviewed in this report.

Country	Name of the value	Methodology	Risk level	Implementation
The Netherlands	Environmental Risk Limit (ERL) and Environmental Quality Standard (EQS) for soil	RIVM 2007 (based on the EC TGD 2003)	Three different risk levels	Generic
Canada	Soil Quality Guideline (SQG)	CCME 2006	Two different risk levels	Generic and site-specific
USA	Ecological Soil Screening Level (Eco-SSL)	US EPA 2005	One risk level	Generic
Australia	Ecological Investigation Level for soil (EIL)	NEPC 2013	One risk level	Generic
Switzerland	Regulatory values (guide, trigger, and clean-up values)	case-by-case (SAEFL 1997, values taken from other countries)	Three different risk levels	Generic

1.3.3 Soil protection values in Switzerland

Switzerland has also applied a similar approach for screening and remediation values in the Swiss soil protection strategy described in the Environmental Protection Act (EPA) (Swiss Federal Council, 2020c) and in the Ordinance relating to Impacts on the Soil (Swiss Federal Council, 2020a) for metals and some organic persistent compounds. Three types of regulatory values for soil are proposed (Figure 2). Guide values are an indication for long-term soil fertility and they consider ecotoxicological effects on soil organisms. Trigger values indicate that negative effects might occur to human health (via food or direct contact) and/or livestock and further investigations must then be conducted. Clean-up values indicate that certain land uses will not be possible without endangering humans, animals or plants and, if exceeded, immediate measures must be taken to avert the danger (i.e., remediation, prohibition of any use and activity of that site). Therefore, different clean-up values are proposed in the Ordinance relating to Impacts on the Soil (Swiss Federal Council, 2020a) for different land uses (agriculture and horticulture, house and family gardens and playgrounds for children) and, depending on the land use, different exposure pathways were considered when deriving the clean-up value. For example, for the agricultural and horticultural land use, the exposure pathways which were considered relevant are: the consumption of contaminated plants by humans or livestock due to soil contamination and the effects on plant growth (direct contact of humans with contaminated soil is not considered relevant in this case) (SAEFL, 1997).

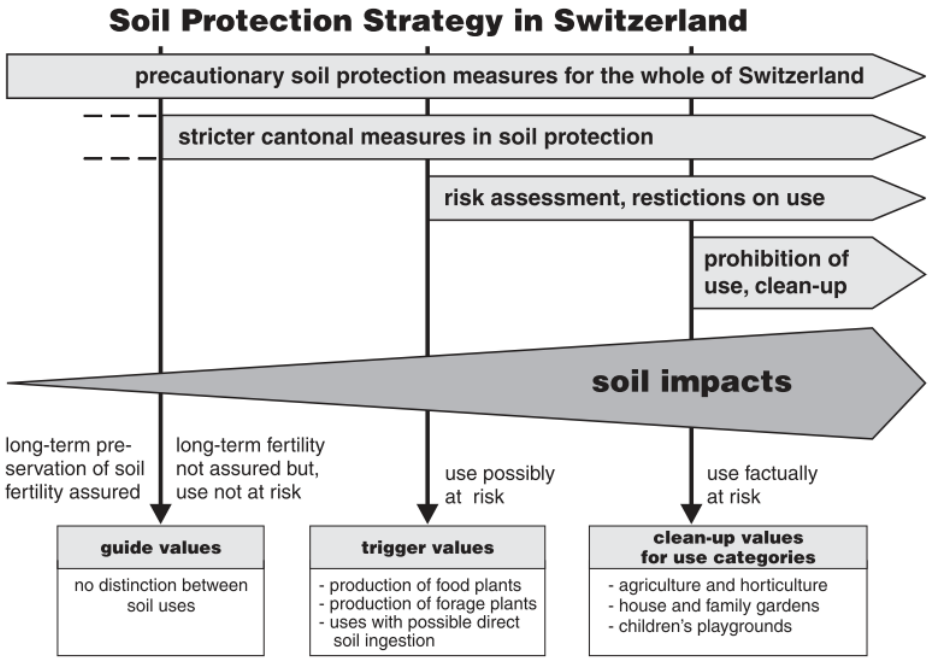

Figure 2: Swiss strategy for soil protection according to the Environmental Protection Act (Swiss Federal Council, 2020c) *and the Ordinance relating to Impacts on the Soil (Swiss Federal Council, 2020a) from the Swiss Agency for the Environment, Forests and Landscape* (SAEFL, 2001).

2 Basic approaches for the derivation of soil protection values

The general principle for deriving soil protection values is similar among authorities. The process is stepwise and includes data collection, data quality assessment, data selection, data extrapolation, and derivation of a final soil protection value (Fishwick, 2004). This chapter briefly illustrates all the four steps (summarized in Figure 3) and the available methodologies that can be used.

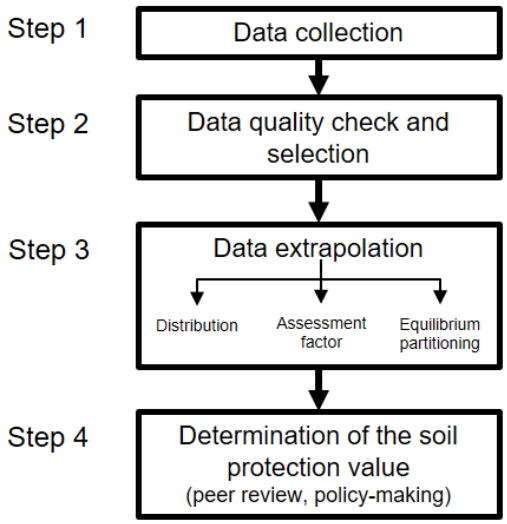

Figure 3: General stepwise procedure for deriving soil protection values, adapted from Fishwick (2004).

2.1 Data collection

The first step is the compilation of the physico-chemical properties and ecotoxicological data for the chemical substance. Such information can be retrieved from peer-reviewed literature, included in the main databases available for various countries, but also information from governments or private agencies, when accessible. Table 3 shows some data often required for PPPs in regulatory frameworks as well as some databases where physico-chemical properties or ecotoxicological data can be extracted.

2.1.1 Physico-chemical properties

The most relevant physico-chemical properties of the substance are gathered in order to evaluate its environmental behavior and fate. The physico-chemical properties give not only general information about the substance, but, some of them, can also be used as an early screening to predict the behavior of the substance in the soil and the environment. Some of those parameters are, for example, the log K_{ow} and the bioconcentration/bioaccumulation factors, which indicate the likelihood for bioaccumulation along the food chain, or the log K_{oc}, which describes the adsorption behavior of the substance to soil organic carbon.

2.1.2 Ecotoxicological data

All available information on ecotoxicological effects is collected for organisms related to the soil ecosystem. The effect of a chemical is commonly assessed by means of ecotoxicological bioassays, where organisms are exposed to a soil with a range of different concentrations of a substance. The effects can be measured by several types of responses (endpoints) that may occur

in the short-term (acute effects, e.g., mortality) or in the long-term (chronic effects, e.g., reproductive output, growth, biomass production). Such tests are most often performed in the laboratory, under controlled conditions for a given period of time, with standard species exposed to a single substance. This is generally the case in the context of authorization of chemical substances. For instance, the authorization of PPPs requires, at least, results of sublethal effects[4] on earthworms. Other tests that might be required are reproduction tests with collembola and mites, tests on microbial activity (e.g., nitrogen transformation) and tests with terrestrial plants (see section 3.1.1 for more details). Bioassays performed by means of mesocosms or field studies may also be available, but although more realistic, they are also more difficult to interpret and compare.

For laboratory studies, the relationship between exposure and effect is described by a dose-response curve, to which statistical models are fitted and from which effect-based concentrations (so-called toxicity parameters) are extrapolated. In this context, toxicity parameters are concentrations[5] of the substance in soil, which cause an effect (expressed as x % of effect) to the test organisms after a specified exposure time. Some of the most common endpoints are related to mortality, growth and/or reproductive output. Effects on mortality are usually expressed as lethal concentrations (LC_x), while for non-lethal effects, toxicity parameters are expressed as effect concentrations or inhibitory concentrations (EC_x or IC_x, respectively). In risk assessment, LC_{50} and EC_{50}/IC_{50} are commonly used to describe results from acute tests (short-term studies), while lower percentages of effect concentrations (e.g., EC_{10}, EC_{25}) are more appropriate to describe results from chronic tests (long-term studies (e.g., inhibition of growth or reduction of reproductive output)). Other frequently used chronic toxicity values are: Lowest Observed Effect Concentrations (LOEC) and No Observed Effect Concentrations (NOEC). The LOEC corresponds to the lowest test concentration that differs significantly from the control. The NOEC is the tested concentration immediately below the LOEC. It is generally assumed that the effects measured in bioassays are negative for the organisms, but, in some cases, especially at lower concentrations of the test substance, the observed effects may be of questionable impact or even beneficial. Therefore, negative effects may be differentiated as adverse and expressed as NOAEC (No Observed Adverse Effect Concentration). For vertebrates (mammals and birds), the toxicity parameters are the same but the concentrations are often expressed as oral daily doses or levels in relation to body weight (kg/kg b.w.), so the toxicity parameters are named LD_x, ED_x, and NO(A)EL/LO(A)EL. The endpoints for terrestrial plants are often expressed in terms of application rates in the field (e.g., kg/ha or lb/ha), so it is common to find the results as Effect Rate (ER_x) and No Observed Effect Rate (NOER).

2.1.3 Quantitative Structure-Activity Relationships (QSARs) and Quantitative Activity-Activity Relationships (QAARs)

Another option to predict the toxicity when no ecotoxicological data for the substance is available is the use of quantitative structure-activity relationships (QSARs) and quantitative activity-activity relationships (QAARs).

QSARs are mathematical relationships, that are empirically derived, between certain physicochemical properties of a given contaminant and the toxicity of such contaminant (EC TGD, 2003; NEPC, 2013). QSAR models first summarize a supposed relationship between chemical structure and biological activity in a data-set of chemicals and then predict the activities of new chemicals.

Similarly, QAARs are used to predict the toxicity of contaminants with the same mode of action to one species using toxicity data of another species (NEPC, 2013).

[4] Sublethal effects: Biological, physiological, demographic or behavioural effects on individuals or populations that survive exposure to a toxicant at lethal of sublethal dose/concentration. A sublethal dose/concentration is defined as inducing no apparent mortality in the experimental population (Desneux et al., 2007)

[5] Units usually expressed as mg active substance per kg of soil dry weight (mg a.s./kg d.w.)

Although several QSARs and QAARs have been well established for the aquatic compartment, much fewer models are available for soil and this strongly limits their use in the derivation of soil protection values (Fishwick, 2004; NEPC, 2013).

Table 3: Common data gathered for the derivation of soil protection values and list of literature, websites and databases, which may contain the information needed.

Data collected	Sources
Physico-chemical properties: Molecular weight [g/mol] Melting point [°C] Boiling point [°C] Vapour pressure [Pa] Henry law's constant [Pa·m^3/mol] Water Solubility [mg/L] Dissociation constant (pK_a) Octanol/water partition coefficient (K_{ow}) Octanol/air partition coefficient (K_{oa}) Carbon/water partition coefficient (K_{oc}) Soil-water partition coefficient (K_p) Soil adsorption coefficient (K_d) Half-life in the soil ($DT_{50,soil}$) **Ecotoxicological data:** Effect concentrations for soil macro- and mesofauna, soil microorganisms, plants and terrestrial vertebrates	**Books:** Tomlin (Tomlin, 2009), Mackay (Mackay et al., 2006) **Databases:** PubChem (NCBI), eChemPortal (OECD), RIVM (the Netherlands), INERIS (France), ECOTOX (US EPA), PPDB (United Kingdom) **Softwares:** EPI Suite™ v. 4.11 (US EPA 2007), IUCLID6 (European Commission 2006) **Other:** Information on registered substances from registration Dossiers (ECHA) and (re-) authorization dossiers (EFSA) Scientific peer-reviewed publications (e.g., Sciencedirect, Web of Science, Scopus)

2.2 Data quality check and selection

Not all toxicity data obtained from ecotoxicological studies is appropriate for deriving soil protection values. The data used for the derivation of soil protection values has to be of good quality, i.e., only relevant and reliable data should be considered. One of the main problems in terrestrial ecotoxicology is the low reproducibility that biotests with soil organisms have shown so far. The introduction of standardized test guidelines for soil organisms helped to reduce multiple interpretations of the same methodology and to provide more complete information about the study (e.g., dose-response graphs or details on statistical methods, etc.). However, even using standardized guidelines, certain ambiguity, which may compromise the reproducibility of a method, can still remain. Therefore, the application of a thorough quality check is important to ensure not only that the test conditions (e.g., test duration, temperature, humidity, etc.) are comparable among different studies, but also that enough information on the bioassay is provided to evaluate the quality of the results.

2.2.1 Quality check

Although each authority defines its own quality criteria for data selection, the main general principles are often similar. For instance, most authorities agree that, if possible, bioassays should follow the currently accepted standard toxicity protocols established by institutions such as the Organisation for Economic Co-operation and Development (OECD), the International Organisation for Standardisation (ISO), the American Society for Testing and Materials (ASTM), or Environment Canada. This guarantees that minimum quality requirements are met (e.g., presence of controls and validity criteria). In addition, sufficient details on the test (i.e., characterization of the tested species and the tested substance – including purity, formulation, etc. –, exposure conditions and duration) and information on the statistical methods (e.g., number of replicates, description of the model, significant differences, etc.) should be provided.

2.2.2 Preferred toxicity parameters

In all cases, the priority is given to chronic data. NOECs, LOECs, EC_{10}, EC_{20}, and/or EC_{25} are usually the most preferred toxicity parameters. Although NOEC and LOEC have been traditionally estimated and applied in risk assessment, in the last decades, their use has been questioned (e.g., Laskowski 1995; OECD 1998, CCME 2006). Those two parameters are highly dependent on the range of concentrations used, the sensitivity of the test controls, replicate number and replicate variability (CCME, 2006). Therefore, if available, the use of statistically meaningful low-level effects (e.g., EC_{10}, EC_{20}, EC_{25}) for the derivation of soil protection values has been recommended in order to reduce the uncertainty in toxicity data (CCME, 2006; EC TGD, 2003; EFSA, 2019).

2.2.3 Selected organisms

Toxicological responses are retrieved for organisms living in direct contact with the soil[6], which are susceptible of being affected by the toxic substance present in the soil. For practical and obvious reasons, the information cannot cover all the species and related exposure pathways of a given soil ecosystem. Thus, the effect is usually evaluated only for a limited number of species, which are divided into taxonomic groups. The most common groups of organisms considered for the derivation of soil protection values are plants, soil invertebrates and microorganisms. While most countries consider effects on plants and soil invertebrates, many of them consider effects on microorganism processes for the derivation of soil protection values as well. As direct comparison of responses at a community level (e.g., microbial processes) with single species tests is not yet possible (RIVM, 2007), results from tests performed with multiple species are often considered separately.

2.2.4 Bioavailability considerations

Soil is a complex matrix and there is a wide diversity of soil types. Physical and chemical properties of a soil have a strong influence on the availability of chemicals to soil organisms and must be considered when evaluating the toxicity of a substance. It is widely accepted that some soil properties, e.g., organic matter and clay content, have a strong influence on the adsorption of chemicals. Recent studies have shown that the persistence of a chemical in soil also has an important influence in its bioavailability (NEPC, 2013; Slomberg et al., 2017; Smolders et al., 2009). Under field conditions, chemicals are submitted to ageing, i.e., the progressive binding to soil particles over time, which consequently reduces their bioavailability, and to leaching, when the chemical is soluble. As most laboratory studies are performed with freshly spiked soils, these two processes are generally not taken into account.

Many authorities consider important to integrate the complexity of processes affecting soil bioavailability (e.g., considering clay content, ageing and leaching factors) for the derivation of soil protection values. However, most of the time, the information about the soil conditions given in toxicity studies is limited (sometimes reduced to only the soil organic matter content). Furthermore, there is still a lack of detailed models that integrate multiple factors and processes involved in soil bioavailability.

Most of the methodologies consider that, for non-ionized organic compounds, bioavailability is driven mainly by organic matter content. Thus, different approaches are followed to account for this soil parameter: the normalization of the toxicity values to some standard soil, giving preference to tests performed under specific organic matter concentrations or even excluding tests performed with conditions that would be unrealistic under specific scenarios. There are other soil properties that may be considered, like clay content, soil texture and soil pH, which can be

[6] Some methodologies consider mandatory the derivation of protection values for other exposure pathways in addition to direct contact with the soil (ex. CCME 2006, US EPA 2005). In other cases, secondary poisoning is triggered if there is potential for bioaccumulation. For all those cases, toxicity data on other organisms like mammals and birds should also be gathered.

considered individually or in combination with other parameters (a typical example would be the classification of the bioavailability of a chemical according to different combinations of pH and organic matter).

2.3 Data extrapolation

Most ecotoxicological data results from laboratory studies performed on organisms expected to be representative of the ecosystem at standard controlled conditions. However, laboratory tests may lead to uncertainties as they do not account for the richness of species diversity and critical ecosystem functions in the real environment (Fishwick, 2004). To deal with such uncertainties, laboratory data needs to be extrapolated in order to reflect the complexity of the ecosystem (Scott-Fordsmand and Jensen, 2002).

There are three main approaches to derive soil protection values extrapolating data from laboratory studies: distribution methods, the deterministic method and the equilibrium partitioning method. The choice of one method over another is generally constrained by the availability of information (i.e., number of toxicity data available). In addition, some authorities can include other considerations, e.g., secondary poisoning or land use in the derivation process. In

Table 4, some advantages and limitations of the different extrapolation methods are described.

2.3.1 Data extrapolation methods

Distribution methods

Most authorities prefer to use distribution methods, since they can be used to plot all toxicity data and have an overall view of the trend of the data. This method can only be used when a large toxicity dataset is available. Generally, toxicity data is ranked from lowest to highest and a percentile of the distribution is selected to derive the soil protection value. There are several approaches proposed by different authorities, which could be assigned to two main groups depending on whether the toxicity data is fitted to a model or not.

- Toxicity data is not fitted to a model:

  It is a simple way to evaluate toxicity values. Usually data are ranked from the lowest to the highest toxicity value and a percentile, which will be the cut-off point, is chosen. This type of distribution is used, for example, by the US Oak Ridge National Laboratory (ORNL, 1998), where the 10^{th} percentile of the LOECs is selected to derive the protection value. Another common approach is to apply the geometric mean (50^{th} percentile) to the toxicity dataset. This is a common procedure adopted, for example, by the United States Environment Protection Agency (US EPA, 2005). However, in some cases, this approach may underestimate the toxicity of some compounds, e.g., when distributions spread over several orders of magnitude (Fishwick, 2004).

- Toxicity data is fitted to a model:

  This is a widely used approach by many authorities. Similar to the other procedure, toxicity data, which is considered to reflect the sensitivities in the ecosystem, is ranked and then fitted to a theoretical model. There are different models that can be used to fit the data. One of the most common is the Species Sensitivity Distribution (SSD), described in the Technical Guidance Document of Risk Assessment from the European Commission (EC TGD, 2003) and also applied by other authorities (e.g., the Netherlands (RIVM, 2007) and Australia (NEPC, 2013)). Toxicity parameters of the same kind (e.g., NOECs/EC_{10}) are fitted, most commonly, to a log-logistic or log-normal model. Usually the concentration value at the 5^{th} percentile is chosen (the hazardous concentration for 5% of species (HC_5)) and used to derive the protection value (Figure 4). This value is expected to protect 95 % of the ecosystem species. Other percentiles can also be chosen. In NEPC (2013), for example, different percentiles are chosen (from the 1st to the 40th percentile) depending

on the land use, assuming that different land uses need different levels of protection. Another example would be the approach used by the Canadian Council of Ministers of the Environment (CCME, 2006), in which toxicity data are fitted to a linear model and then either the 25th or the 50th percentiles are chosen, depending on the land use.

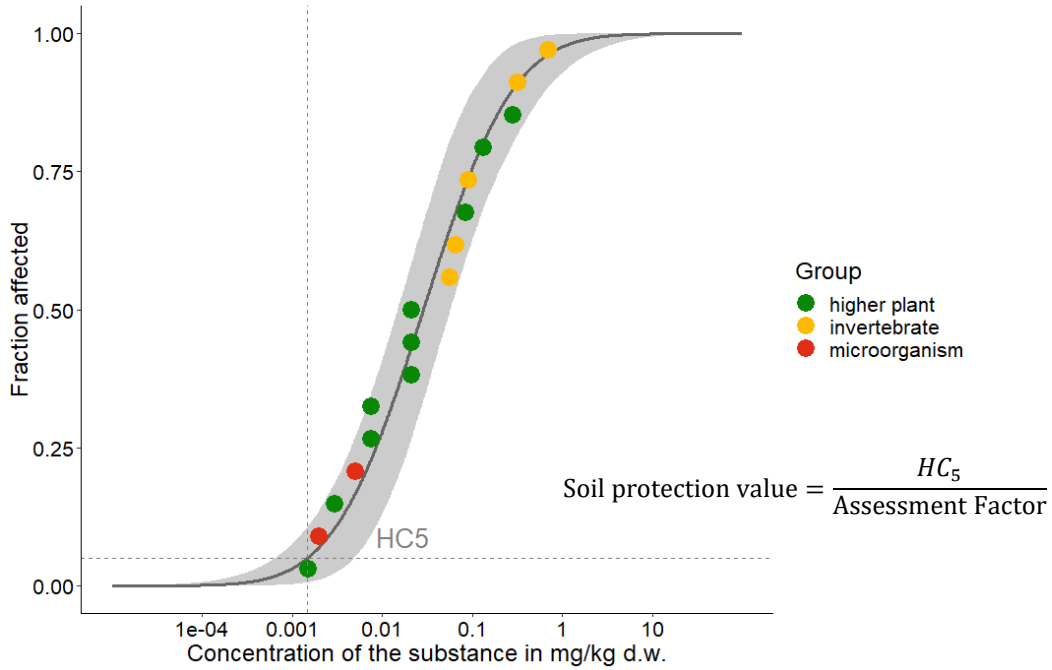

Figure 4: Illustration of the Species Sensitivity Distribution approach, with a cut-off point at the 5th percentile (HC_5).

For any extrapolation method there is always some degree of uncertainty and this is usually accounted for by the use of assessment factors (AFs)[7]. The AF should account for the uncertainties resulting from limited laboratory data, in order to not underestimate the risk for the ecosystem. For large datasets with reliable data, the uncertainty is going to be low and, therefore, the assessment factor can be reduced (or even non-existent). This is the case for the distribution methods, whose assessment factors may range from 1 to 5.

Deterministic method (AF method)

The second method is used mainly when not enough data is available for plotting a distribution. In this case, a toxicity value representing the most sensitive species and endpoint is selected and divided by an assessment factor (AF). The AF for the deterministic method is based on several assumptions, for instance, that differences between acute and chronic values and between laboratory to field conditions are constant (Fishwick, 2004). The size of the AF takes into account the number of species/trophic levels available and the test duration (acute or chronic) and varies amongst the guidelines. Some guidances like, for example, the EC TGD (2003), RIVM (2007) (the Netherlands) and (NEPC, 2013) (Australia), propose a large range of AFs (from 1 up to 1000), while others, such as the CCME (2006) (Canada), use lower AFs (max. 10).

[7] Depending on the methodology assessment factors may have different names, like “safety factor” or “uncertainty factor (UF)”.

Equilibrium partitioning method

The equilibrium partitioning method (EqP) can be used when data on terrestrial organisms is not available. The method was originally developed for sediments and was based on the principle that contaminants were available for sediment dwelling organisms only via the water phase and that their toxicity to such organisms resulted from their concentration in water. The application of this method to the soil compartment is based on the same assumptions (Fishwick, 2004):

- The contaminants in the soil are only available to soil organisms via the water phase
- The toxicity of the contaminants is only due to their concentration in the pore water
- Soil organisms are equally sensitive as water organisms to the same contaminants
- Soil/water partition coefficients can be measured or derived, based on a generic partition method, when the properties of the soil and the contaminant are known

As the method considers solely the contaminant uptake from the water phase and ignores the contamination through the ingestion of particles, the toxicity of compounds, which are adsorbed to the soil may be underestimated. In this case, an AF of 10 is applied for lipophilic compounds (log K_{ow} > 5).

To derive the soil protection value with the EqP approach the following general equation is used:

Equation 1

$$\text{Protection value}_{\text{soil}} = \frac{\text{K}_{\text{soil-water}} \cdot \text{Protection value}_{\text{water}} \cdot 1000}{\text{RHO}_{\text{soil}}}$$

Where:

$\text{Protection value}_{\text{soil}}$	Protection valued for the soil compartment	[mg/kg]
$\text{Protection value}_{\text{water}}$	Protection value for the water compartment	[mg/L]
RHO_{soil}	Bulk density of wet soil	[kg/m^3]
$K_{\text{soil-water}}$	Partition coefficient soil-water	[m^3/m^3]

Table 4: Comparison of the commonly used extrapolation methods to derive soil protection values. List of references used for the table: EC TGD (2003), Fishwick (2004), CCME (2006), RIVM (2007, 2001, 1997), ECHA (2017), EFSA PPR Panel (2017), Environment Agency (2020).

Extrapolation method	Advantages	Limitations
Distribution methods	• All the available data is used for the derivation • Provides an overview of the sensitivity of different species • Some are statistically based (e.g., SSD): confidence intervals to describe uncertainties of the selected percentile can be shown	• Outcome is strictly dependent of the type of regression model • The use of different toxicological endpoints (e.g., reproduction, growth rate) may influence the result • Interactions between species or abiotic factors are not considered • Representability of the selected species may be questioned • Choice of the protection percentile is under discussion • SSD method originally created for the water compartment. Some more validation is needed for soils
Deterministic method	• Simple and easy to use • Applicable to small data sets	• AFs built on precautionary principles and mathematical approaches rather than ecotoxicological experience

Extrapolation method	Advantages	Limitations
	• Choice of the AF is not arbitrary, but there are, generally, transparent rules	• Some AFs taken directly from the aquatic compartment without real validation in the soil compartment (no scientific basis) • Extrapolation based on a single toxicity value (no information on the sensitivity among species)
Equilibrium partitioning method	• It can be applied when no toxicity data for soil organisms is available	• Water toxicity values may not represent the sensitivity of terrestrial organisms or the exposure pathways in the soil • Factors like bioavailability and attainment of the equilibrium between the organisms and the pore water are not considered • Significant over- or underestimations of the soil protection values can occur

2.3.2 Further considerations

Secondary poisoning

Some substances, such as lipophilic organic compounds and some metals, might have the potential to accumulate along the food chain and trigger a risk for higher vertebrates. Toxicity related to bioaccumulation from lower to higher organisms is referred to as secondary poisoning. Bioaccumulation is the result of both bioconcentration and biomagnification of a chemical (OECD, 2010). For the soil ecosystem, OECD (2010) defines bioconcentration as the increase in concentration (of the chemical) in or on the organism, relative to the concentration in the surrounding medium. This is the result of the uptake of a contaminant via body surface and/or ingested soil. On the other hand, biomagnification indicates an increase of the concentration (of the chemical) in or on the organism, relative to the concentration in the food or prey that is ingested by the organism.

The common procedure for assessing secondary poisoning follows four steps:

1- Evaluation of the potential for bioaccumulation

The potential for bioaccumulation can be commonly evaluated through some specific physical properties of the chemical, e.g., its lipophilic character. Among some indications, one of the most common is the octanol/water partition coefficient (log K_{ow}). The trigger value for the log K_{ow} to derive a soil protection value for secondary poisoning varies depending on the different guidances.

2- Estimation of the exposure

The concentration that can be found in higher predators is estimated by means of food chain models, which account for specific exposure pathways. One of the most common pathways is considering that the accumulation occurs from soil to earthworms and from earthworms to worm-eating predators (e.g., birds or mammals). Other exposure pathways that can be considered are the ingestion of food including plants or small soil organisms, but also the incidental ingestion of contaminated soil particles. Once the food chain model is defined, the concentration of the substance that is taken up by a consumer is estimated by means of bioconcentration factors (BCF) and/or bioaccumulation factors (BAF). BCFs and BAFs may be estimated from available literature (preferably field studies) or calculated with models, based on the log K_{ow} of the substance.

3- Estimation of the effect

The hazard of a chemical to vertebrates (mammals and birds) is extrapolated from (eco-) toxicological concentration-response studies usually performed with e.g., rats, mice, dogs and birds. Normally, AFs are applied to the (eco-) toxicological value to extrapolate from laboratory to field

conditions and from acute/subchronic tests to chronic tests and to account for interspecies variation. As experimental toxicity values for mammalian or bird feeding studies are generally expressed as daily dose per body weight (kg substance/kg b.w./day), data needs to be converted into food or soil concentrations.

4- Assessment of the risk

The assessment of secondary poisoning follows the same principle as the common risk assessment, i.e., comparing the estimated exposure to the concentration that is expected not to be of concern. Among the authorities, several methods have been proposed for the derivation of a soil protection value for secondary poisoning. Differences depend mostly on the food chain model/exposure pathway and the wildlife species considered. However, it is generally accepted that the soil protection value for secondary poisoning should be compared with the value derived to protect soil organisms in order to have a unique soil protection value (generally the lowest one of the values) in the end.

Land use

The risk level that is aimed for a soil protection value may depend on the land use and the purpose of the value. For instance, some sites can have a higher ecological value (e.g., parks or protected areas) and, consequently, stricter protective measures should be considered. On the other hand, some sites are already strongly modified by human activity and less protection may be required (e.g., industrial areas). Some countries that have developed different soil values, based on different land use, are Canada (for Agricultural, Residential/Parkland, Commercial and Industrial areas), Australia (for national park/area, urban residential/public open space, commercial/industrial, and agricultural land use) and Switzerland (for agriculture and horticulture, private and family gardens and playgrounds).

Background concentrations

Background concentrations are defined as the concentration of a compound naturally present in the environment, before a significant anthropogenic addition occurred (natural background concentrations), plus the compound levels that have been introduced from diffuse or non-point sources by general anthropogenic activity not attributed to industrial, commercial, or agricultural activities, for example, motor vehicle emissions (Fishwick 2004; NEPC 2013). For the assessment of metals, background concentrations play a crucial role and most methodologies apply some correction or consideration when deriving soil protection values. For synthetic PPPs, the correction of soil protection values due to background concentrations is not expected to be relevant since their introduction in the soil is exclusively due to local anthropogenic practices. However, some authorities may use background concentrations for some persistent PPPs as a pragmatic approach to define the lowest level of protection (e.g., the Netherlands and Czech Republic, see Appendix 1).

Human health

In some cases, soil contamination may cause adverse effects on humans as well and, therefore, soil protection values protecting human health are also commonly derived. Some authorities keep the risk assessment for humans and for the environment separate and others include the exposure to humans in a general terrestrial risk assessment, by selecting the lowest among the derived soil protection values (environment or human health) and keeping a unique soil protection value in the end.

2.4 Determination of soil protection values

The last step following the derivation of a soil protection value is to evaluate its applicability. This includes regulatory and policy considerations and often a peer review (Fishwick, 2004). This is

an important and debated step for policy makers that must ensure that the derived value is sufficiently protective for the ecosystem but at the same time not too conservative, in order to be reasonable in the current political framework. In most countries, soil protection values are established by special laws for contaminated sites and, only in some cases, they are provided by soil and groundwater protection laws (Carlon, 2007). That soil protection values are legally or non-legally binding depends on each authority. For some countries, for example the Netherlands both the scientifically derived soil protection values and soil protection values used in environmental policy are published.

Box 1. Summary of derivation procedure of soil protection values

Step 1: Data collection

- Collection of ecotoxicological and physico-chemical data

Step 2: Data quality check and selection

- Quality check: criteria, scoring
- Preferred toxicity values: chronic or acute, defined percentage of effects
- Selected organisms considered: soil invertebrates, plants, microorganisms (and wildlife)
- Bioavailability: normalization to organic matter content, bioavailability score, soil texture

Step 3: Data extrapolation

- Distribution method: large data set
- Deterministic method: small data set
- Equilibrium partitioning method: no terrestrial data, based on aquatic ecotox data
- Further considerations: secondary poisoning, land use, background concentrations, human health

Step 4: Determination of soil protection value

- Review, policy adjustment

3 Existing methodologies for deriving soil protection values in prospective and retrospective risk assessment

Risk assessment for terrestrial organisms is commonly achieved by deriving soil protection values (hazard assessment) and comparing them with environmental concentrations. Alternative methodologies to the derivation of soil protection values do exist in risk assessment, for example, the methodology used in risk assessment for the authorization of PPPs (section 3.1.1). However, the derivation of soil protection values is, indeed, the most general approach in prospective and retrospective hazard assessment.

The methodologies reviewed in the next sections of this report are well established and have been proposed by some of the leading regulatory authorities worldwide:

- Prospective risk assessment:
    - For the authorization of PPPs, EFSA rely on the Guidance Document on Terrestrial Ecotoxicology (SANCO/10329/2002 (EC SANCO, 2002)), Commission Regulation (EU) No 283/2013 for active substances (European Commission, 2013a) and Commission Regulation (EU) No 284/2013 (European Commission, 2013b) for formulated products
    - The European Chemical Agency (ECHA) uses the methodology proposed in the Technical Guidance Document on Risk Assessment (EC TGD, 2003) for the authorization of new and existing substances (ECHA, 2008) and biocidal products (ECHA, 2017).
- Retrospective risk assessment:
    - The Netherlands: “Guidance for the Derivation of Environmental Risk Limits (within the framework of ‘International and National Environmental Quality Standards for Substances in the Netherlands’ (INS))” (RIVM, 2007)
    - Canada: “A Protocol for the Derivation of Environmental and Human Health Soil Quality Guidelines (for contaminated sites in Canada)” (CCME, 2006)
    - The USA: “US Guidance for Developing Ecological Soil Screening Levels (for contaminants of potential concern at hazardous sites)“ (US EPA, 2005)
    - Australia: “The Australian Guideline on Methodology to Derive Ecological Investigation Levels in Contaminated Soils (in the context of the National Environment Protection (Assessment of Site Contamination) Measure)” (NEPC, 2013)

Some other methodologies (mostly from European authorities) derived soil protection values for PPPs and, in some cases, were applied to agricultural land use. They have also been reviewed and listed in section 3.2.6 and in Appendix 1.

3.1 Prospective risk/hazard assessment for soils

There are two authorities in Europe in charge of the authorization of pesticides: ECHA for biocides and EFSA for PPPs. Both authorities use different approaches. While ECHA performs a hazard assessment via derivation of soil protection values previous to the risk assessment, EFSA uses a direct risk assessment approach (without soil protection values).

3.1.1 European Food Safety Authority (EFSA)

The ecological risk assessment for PPPs in soil is conducted according to the SANCO Guidance Document on Terrestrial Ecotoxicology (SANCO/10329/2002 (EC SANCO, 2002)) that was developed under the Council Directive 91/414/EEC (Council of the European Communities, 1991). This directive was then repealed by the Regulation (EC) No 1107/2009 (European Parliament

and Council of the European Union, 2009), which is the current regulation for the approval of PPPs in the EU. The corresponding regulation for Switzerland is the Ordinance on Plant Protection Products (PSMV/OPPh) (Swiss Federal Council, 2020d), which is, to a large extent, based on the EU regulation 1107/2009. Some of the requirements described in SANCO/10329/2002 have been updated and the current data requirements for active substances under both EU and CH regulation are laid down in Commission Regulation (EU) No 283/2013 (European Commission, 2013a), and in Commission Regulation 284/2013 for the formulated products (European Commission, 2013b). These regulations define the data that need to be provided by the registrants and hence also the bioassays, which must be performed to assess the risk for the soil compartment. Following the new legislative background, SANCO/10329/2002 is currently under revision and several scientific opinions have been written by the EFSA Panel on Plant Protection Products and their Residues (PPR) as precursors to the new guidance document (EFSA PPR Panel, 2017, 2014).

PPPs are developed and released in the environment thereafter with the specific purpose to harm certain target organisms (pests). Thus, the prospective environmental risk assessment (ERA) for PPPs aims to ensure that adverse effects occur to target organisms considered as pests while minimizing the risk to non-target organisms and avoiding long-term repercussions on the environment. For the in-soil assessment, the ERA focuses on specific non-target groups: soil microorganisms, non-target soil meso- and macrofauna (earthworms and other soil invertebrates). For the terrestrial assessment, the consideration is extended to bees, other non-target arthropods, non-target plants and terrestrial vertebrates.

The ERA for PPPs is a tiered approach comparing exposure and effect in order to characterize risk. Different approaches have been developed for prospective risk assessment in the framework of pesticide authorization. While for the authorization of biocides a soil protection value ('predicted no effect concentration' ($PNEC_{soil}$)) is derived first and then compared to a 'predicted exposure concentration' (PEC_{soil}) (see section 3.1.2), no explicit soil protection values are derived using SANCO/10329/2002 for the authorization of PPPs. In this case, the risk for earthworms, mites, collembolans, and non-target plants is assessed based on the toxicity exposure ratio (TER)[8], i.e., the ratio between the toxicity value from the most sensitive of the tested species and the predicted exposure concentration, as defined in the Uniform Principles (Commission Regulation (EU) No 546/2011). The TER is compared to a trigger value and the risk is considered acceptable if the ratio is higher than the defined trigger value (Commission Regulation (EU) No 546/2011 (p. 148); EC SANCO, 2002). The trigger values (generally of five or ten for soil invertebrates) are defined in the Uniform Principles (Commission Regulation (EU) No 546/2011, EC 2011) and play the same role as the assessment factors, i.e., they should take into account uncertainties for the intra- and interspecies variability and the extrapolation of toxicity endpoints from laboratory to field (EFSA PPR Panel, 2017). Even though the approaches may seem very different, computing the TER and comparing it to the trigger value of, e.g., five is equivalent to dividing the TER by an assessment factor (AF) of five and comparing the result to one. In aquatic assessments (EFSA PPR Panel, 2013), the 'regulatory acceptable concentration' (RAC), i.e., toxicity measurement divided by the trigger value, was introduced to make PPP hazard assessment more easily comparable to the PNEC-based risk assessments (EFSA PPR Panel 2017, p. 71). Since 2012, in Switzerland and Germany, RACs for some active substances, using the above-mentioned approach, have been published for surface waters (Knauer and Félix, 2012). Similarly to this approach and supported by additional technical documents, (e.g., European and Mediterranean Plant Protection Organization (EPPO), 2003), the Swiss Federal Office for Agriculture (FOAG) is working on the development of an approach to derive RACs for the soil compartment (personal communication from FOAG experts).

[8] Since the focus of this report is not on all terrestrial organisms but on in-soil organisms (soil invertebrates, microorganisms) and plants, the approach to assess the risk for bees according to SANCO/10329/2002 (EC SANCO, 2002) was considered not relevant for this report and therefore not described.

Methodology

For soil organisms, the TER is derived by dividing the toxicity value (usually a NOEC or EC_x) by the exposure, which is commonly expressed as a predicted environmental concentration (PEC) (Equation 2). If the TER is below a specific trigger value, a risk cannot be excluded and no authorization is granted unless it is clearly established through an appropriate ERA that no unacceptable effects occur under field conditions. This is achieved, for instance, by refining the exposure estimates, or the effect assessment, or by performing higher tier tests.

Equation 2

$$\mathrm{TER} = \frac{\text{toxicity value}}{\mathrm{PEC}}$$

Where:

TER	Toxicity exposure ratio	[-]
toxicity value	Lowest toxicity value (e.g., NOEC or EC_x) for soil organisms and plants	[mg a.s./kg soil d.w.]
PEC	Predicted environmental concentration	[mg a.s./kg soil d.w.]

In the Regulation (EU) No 283/2013 and No 284/2013, for active substances and formulation, respectively, it is described, which bioassays are required for terrestrial organisms. Several criteria, like the type and use of the PPPs, will define which bioassays are required and for which test organisms. In general, when the toxicity of the formulation cannot be predicted on the basis of the data for the active substance, bioassays with the formulation are required (Commission Regulation 284/2013, p. 121). However, in case of certain study types, the use of a representative formulated PPP instead of the active substance may be more appropriate. In those cases, data with the active substance may not be required (further information in Regulation (EU) No 283/2013, Section 8, p. 54).

Data requirements and ERA for each organism group

The bioassays required at the first tier are briefly illustrated in this section. In SANCO/10329/2002 (EC SANCO, 2002), particular attention is also given to substances with a high persistence in soil. Generally, chemicals with a long half-life, require additional and more specific tests (e.g., field tests) (see EC SANCO (2002), p. 28 for further information).

- Non-target soil meso- and macrofauna

  A PPP shall have no unacceptable effects on the environment and therefore its impact on non-target species must be assessed (EU regulation 1107/2009, p. 8). Information provided shall be sufficient to identify, among others, non-target species and population for which hazards arise because of potential exposure, and permit an evaluation of short and long-term risks for non-target species, populations, communities and processes (Commission Regulation 284/2013, p. 4). For non-target soil meso- and macrofauna, studies on earthworms and organisms other than earthworms are performed where required.

  The toxicity of lipophilic organic contaminants to soil organisms usually depends on the organic carbon content of the substrate as this governs adsorption and thus pore water concentration. The artificial substrate commonly used for laboratory tests (OECD artificial soil) has a higher organic carbon content than many natural soils, so it could be expected that the LC_{50} or NOEC would be lower if the tests were conducted in natural soils (van Gestel, 1992). The risk assessment should account for this difference when a test is performed with artificial soil. Therefore, in this case, SANCO/10329/2002 recommends dividing the toxicity data (NOEC, EC_x) by 2, when the log K_{ow} of the tested substance is greater than 2 (EPPO 2003), unless it can be demonstrated by soil sorption data or other evidence that the toxicity is independent of the soil organic carbon.

- Earthworms – sub-lethal effects

  The effect on earthworms must be tested, when the active substance can contaminate the soil, according to the OECD 222 Guideline (OECD, 2016a). Sub-lethal EC_{10}, EC_{20} and/or NOECs are evaluated for growth, reproductive output and behavior.

- Organisms other than earthworms

  When the PPP is applied directly to the soil as a soil treatment (spray or solid formulation), effects on collembola and predatory mites must be evaluated for the active substance and the formulation according to the OECD Guidelines 232 (OECD, 2016b) and 226 (OECD, 2016c), respectively. For PPPs applied as foliar spray, these two tests may also be required by the competent authority or are required if a concern is raised for other non-target arthropods, such as *Aphidius rhopalosiphi* and *Typhlodromus pyri*. The current trigger value for earthworms and other soil meso- and macroinvertebrates is equal to 5.

- Non-target higher plants

  Non-target terrestrial plants (NTTP) are defined as all plants growing outside fields, and those growing within fields that are not the intended pesticide target (EFSA PPR Panel 2014). Data for NTTP are not required, where exposure is negligible (e.g., in the case of rodenticides, substances used for wound protection or seed treatment, or in the case of substances used in stored products or in glasshouses) (EC SANCO, 2002), p. 32; EFSA PPR Panel 2014, p. 13). When bioassays with plants are required, a tiered approach is performed starting with available data and proceeding with further steps if needed. The first tier is an initial screening of the product for herbicidal or plant growth regulatory activity. The data should cover at least six plant species from six different families including both mono- and dicotyledons. A second tier is required for active substances that exhibit herbicidal or plant growth regulator activity (EC SANCO (2002), p. 32; EFSA PPR Panel 2014, p. 12). Specific information on the toxicity of the substance to terrestrial plants through laboratory assays on a selection of plant species is requested (OECD guidelines 208 (OECD, 2006a) and 227 (OECD, 2006b)). There are two options to derive the TER, a deterministic and a probabilistic approach, from which a choice should be made with regard to the data set. The deterministic approach is derived based on the toxicity value for the most sensitive species. If more information is available (from six to ten species), the probabilistic method can be used and the 5^{th} percentile of the SSD is then used to derive the TER.

- Microorganisms

  At least tests with the active substance shall be carried out with soil microorganisms where PPP containing the active substance are applied to the soil or can contaminate soil under practical conditions of use. Unless it can be proven that no exposure occurs to soil microorganisms, the effect of the active substance is assessed through the nitrogen transformation test according to OECD Guideline 216 (OECD, 2000). Tests should be performed with freshly sampled agricultural soils, which have not been treated with any substance that may alter the microbial community for the previous two years (Commission Regulation (EU) No 283/2013) (European Commission, 2013a). The deviation of the microbial activity compared to the untreated control should not exceed 25 % after 100 days.

Bioaccumulation and secondary poisoning

Bioaccumulation of soil organisms is taken into account in order to assess the potential for secondary poisoning in birds and mammals for organic substances with a log $K_{ow} \geq 3$ (EFSA, 2009). The EFSA Guidance on Risk Assessment for Birds and Mammals (EFSA, 2009) illustrates the ERA of PPPs for birds and mammals through evaluation of acute, short term and reproductive

toxicity. Relevant toxicity values are LD_{50}, LC_{50} and NOAEL, which are used to derive the TER. The trigger value is 10 for the acute and short-term and 5 for the long-term toxicity/exposure ratio (EFSA 2009, Regulation EU No 546/2011).

3.1.2 European Chemical Agency (ECHA)

The ERA for most chemicals in Europe follows the methodology that was first presented in the Technical Guidance Document on Risk Assessment, part II (EC TGD, 2003), for assessing the risk of substances to humans and to the environment. Since 2008, this procedure is included in the ECHA Guidance on Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (ECHA, 2008) and later on, in 2015, in the ECHA Guidance on Biocidal Products Regulation (last updated: ECHA, 2017). Although some additional considerations and/or information were added in the ECHA (2017), the methodology used to derive the soil protection value (i.e., $PNEC_{soil}$) remained the same as the one originally described in the EC TGD (2003). Therefore, only in those cases in which the information has been updated from the original guidance (EC TGD 2003), the ECHA (2017) will be cited, otherwise the citations in this report will refer to the original methodology, the EC TGD (2003).

The EC TGD (2003) has also strongly influenced other EU or national hazard assessments, e.g., the "Guidance document to derive environmental quality standards (EQS) under the EU Water Framework directive" (European Commission, 2018, 2011) and thus also the derivation of surface water quality standards implemented in the Swiss water protection ordinance (WPO) (Swiss Federal Council 2020d). For soils, the EC TGD (2003) has also been adopted and adapted, if necessary, by some European countries (e.g., the Netherlands) for the derivation of soil protection values.

The soil protection value derived according to the EC TGD (2003) is called $PNEC_{soil}$ (Predicted No Effect Concentrations for soil organisms). PNECs are defined as concentrations below which unacceptable effects on organisms will most likely not occur. If the environmental concentration reaches the PNEC, then the substance is considered "of concern" and further testing/information or risk management is required.

Data requirements and first considerations

For biocide authorization, standard toxicity tests to assess the effect of biocides on microorganisms, earthworms or other soil-dwelling non-target invertebrates and plants are required, depending on the expected use, for 17 out of 22 product-types[9]. For 16 of them, long-term data with earthworms or other soil-dwelling non-target invertebrates should also be submitted (ECHA 2018, p. 84).

The preservation of the soil community requires protection of all organisms playing a leading role in establishing and maintaining the structure and the functioning of the ecosystem. Therefore, ideally, toxicity data resulting from tests that represent different and significant ecological functions in the soil ecosystem (primary producers (plants), consumers (e.g., invertebrates) and decomposers (comprising microorganisms) should be collected (ECHA, 2017, p. 145).

The collected data is assessed for its quality and completeness. The quality check includes the assessment of adequacy, i.e., data should be reliable (i.e., resulting from a robust test) and relevant (i.e., appropriate for the chosen derivation method). For active biocidal substances, the assessment of the adequacy is illustrated in ECHA (2018) and is carried out by the Member State Competent Authorities (MSCA).

The bioavailability of the test compound in the soil can strongly affect the toxicity of this compound. Soil properties (e.g. organic matter, clay content, soil pH and soil moisture) may affect the

[9] According to ECHA, biocidal products are classified into different types depending on their application (e.g. disinfectants, wood preservatives, etc.). There is a total of 22 product-types that have been described.

bioavailability making the substance more or less biologically available to soil organisms and plants. Toxicity parameters (NOEC, EC_x, LC_x) should ideally be based on studies conducted with soil conditions that favor the bioavailability of the substance to soil organisms. If possible, data should be normalized using relationships that describe the bioavailability of chemicals in soils. For non-ionic organic compounds, bioavailability is assumed to be driven by soil organic matter only. In order to make the results comparable within different soil types, the EC TGD (2003, p.116) recommends for such compounds, a normalization to a standard organic matter content of 3.4 % (Equation 3). Such normalization is only appropriate when the log K_{ow} is expected to be the main driver on the binding behavior of the chemical, and when organisms are expected to be exposed predominantly via pore water.

Equation 3

$$\mathrm{NOEC\ or\ L(E)C_{50[standard]}} = \mathrm{NOEC\ or\ L(E)C_{50\ [exp]}} \times \frac{\mathrm{Fom_{soil(standard)}}}{\mathrm{Fom_{soil(exp)}}}$$

Where:

NOEC or $L(E)C_{50[standard]}$	NOEC or $L(E)C_{50}$ in standard soil	[mg/kg]
NOEC or $L(E)C_{50[exp]}$	NOEC or $L(E)C_{50}$ in experiment	[mg/kg]
$Fom_{soil(standard)}$	Fraction of organic matter in standard soil (0.034)	[kg/kg]
$Fom_{soil(exp)}$	Fraction of organic matter in experimental soil	[kg/kg]

Other general considerations about the mobility, persistence, degradation behavior, endocrine disrupting properties and particular mode of actions of the chemical should also be made previous to the derivation of the soil protection value, although there are not always standard procedures for assessing their relevance.

Data extrapolation

To derive the $PNEC_{soil}$, the distribution (SSD), the deterministic and the equilibrium partitioning approaches (EqP) can be used, depending on the data availability (Figure 5).

- Statistical distribution (SSD)

  The derivation of a $PNEC_{soil}$ using statistical extrapolation techniques can be considered when sufficient data are available. SSDs can only be performed when at least ten NOECs or EC_x (preferably more than 15) from different species covering at least eight taxonomic groups are available. For data on the same endpoint and species, the geometric mean is used as input data. When tests are conducted with different soil types, data should be normalized to 3.4 % organic matter. Test results on microbial mediated processes and single species are considered separately due to fundamental differences between these tests and single species tests (functional vs. structural test, multi-species vs. single species, adapted indigenous microbe community vs. laboratory test species, variability of test design and different endpoints, etc.).

  The data is fitted to a log-logistic or log-normal distribution. The concentration at the 5th percentile and the 50 % confidence interval associated to this concentration is selected for the PNEC derivation. An AF between 1 and 5 is applied to reflect further uncertainties (see Equation 4).

  Equation 4*

$$\mathrm{PNEC_{soil}} = \frac{5\ \%\ \mathrm{SSD}\ (50\ \%\ \mathrm{CI})}{AF}$$

Where:

$PNEC_{soil}$	Predicted no effect concentration in soil	[mg/kg]
5 % SSD	5^{th} percentile of Species Sensitivity Distribution	[mg/kg]
50 % CI	50% confidential interval	[-]
AF	Assessment factor (1 to 5)	[-]

(*) Equation copied from the $PNEC_{water}$ in the EC TGD (2003, p. 105) and adapted for clarity.

The SSD method was originally tested and validated with aquatic organisms. The requirements to perform a SSD for soil organisms have been directly taken from the water compartment. This approach has been under discussion for many years (EC TGD, 2003; RIVM, 2007). In the last update from the ECHA (2017), this discussion has been deleted without further explanation or investigations. Although there are no detailed recommendations for the soil compartment, it is stated for the aquatic compartment that the deterministic method should be applied in parallel to the SSD approach for the sake of comparison (EC TGD 2003, p. 105).

- Deterministic method (AF method)

  Frequently, data is not sufficient to derive a $PNEC_{soil}$ with the SSD approach. When this is the case, the AF method can be used if there is at least one reliable relevant terrestrial test result. The size of the AF depends on the type of data available. Ideally, long-term data from at least one producer, one consumer and one decomposer should be available. When less data is available a higher AF needs to be applied. In general, the lowest available toxicity value is divided by the appropriate AF to derive the $PNEC_{soil}$ (see Table 5). The AFs used for soil are the same as the ones used for the water compartment and not based on comprehensive experience. Further clarifications are given in the guidance document for biocide risk assessment (ECHA, 2017, p. 148-149).

Table 5: Assessment factors for the derivation of the PNECsoil (EC TGD 2003, p. 118).

Information available	**Assessment Factor**
$L(E)C_{50}$ short-term toxicity test(s) (e.g., plants, earthworms, or microorganisms)	1000
NOEC for one long-term toxicity test (e.g., plants)	100
NOEC for additional long-term toxicity tests of two trophic levels	50
NOEC for additional long-term toxicity tests for three species of three trophic levels	10
Species Sensitivity Distribution (SSD) method	5-1, to be fully justified on a case-by-case basis
Field data/data of model ecosystem	case-by-case

In case that only one toxicity test result is available, the $PNEC_{soil}$ should be derived with both the deterministic and the EqP method (see below). The lower of the two derived PNECs is then chosen as final $PNEC_{soil}$.

- Equilibrium partitioning method

  When no data is available for the soil compartment or there are only test results for a single soil dwelling species, the EqP method is applied (see section 2.3.1). This method may not be suitable for lipophilic substances, substances with a specific mode of action or substances with strong adsorption to soil particles. It is important to highlight again that the EqP method cannot replace toxicity data for soil organisms and should consequently only be used as a screening tool for identifying the need of further testing.

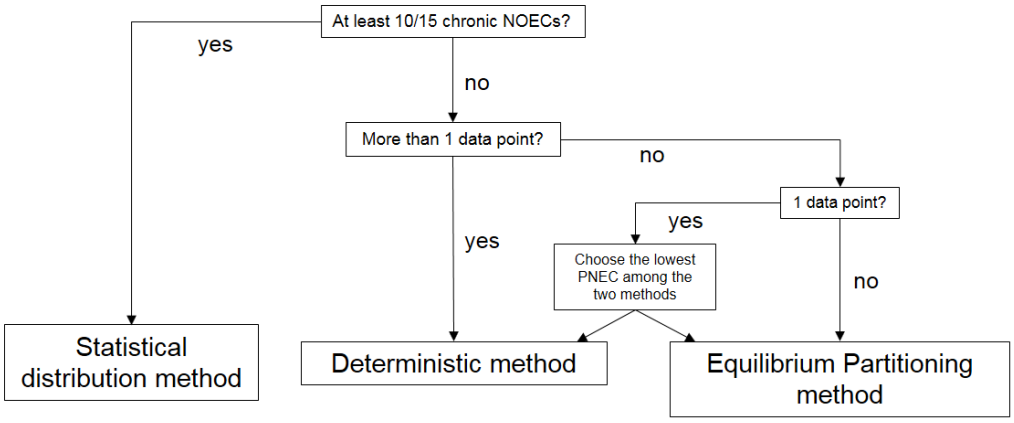

Figure 5: Overview of the extrapolation methods for deriving $PNEC_{soil}$ according to the EC TGD (2003)

Bioaccumulation and secondary poisoning

The bioaccumulation potential is mostly described by a high value of the *n*-octanol/water partition coefficient (log K_{ow}) but there are other cases, where bioaccumulation may occur. According to the EC TGD (2003, p. 123) a substance is potentially bioaccumulative if:

- has a log $K_{ow} \geq 3$; or;
- is highly adsorptive; or;
- belongs to a class of substances known to have a potential to accumulate in living organisms; or;
- there are indications from structural features;
- and there is no mitigating property such as hydrolysis (half-life less than 12 hours)

In the ECHA (2017, p. 155) three trigger values for bioaccumulation have additionally been described:

- Bioconcentration factor (BCF) ≥ 100 L/kg_{ww}; or;
- Bioaccumulation factor (BAF) ≥ 100 L/kg_{ww}; or;
- Biomagnification factor (BMF) > 1

Experimental studies on terrestrial bioaccumulation with earthworms are not always required but could be warranted if information from non-testing methods and/or bioconcentration studies indicate concern (ECHA, 2018, p. 41).

The exposure route considered for secondary poisoning is the bioaccumulation of a chemical from earthworms to worm-eating predators. A PEC for predators ($PEC_{oral,predator}$) is evaluated through the estimation of the contaminant concentration in the earthworm accounting for the concentration of the substance in the worm tissues and the adsorption of the substance to the soil present in the earthworm gut.

For biocides, toxicity studies for mammals are required for all biocide product-types and, for five of them, toxicity data for birds are also mandatory (depending on the expected use) (ECHA 2018, p. 84). Those toxicity values are used as a basis to derive a PNEC for predators through oral exposure ($PNEC_{oral}$). First, test results expressed as daily doses on a body weight basis are converted into concentrations in the food, by multiplying them with test species specific conversion factors (Equation 5). Conversion factors are based on the ratio between body weight (in g) and daily food intake (in g/day) and may be retrieved in the test details. Conversion factors for some standard organisms are provided as well in the EC TGD 2003 (p.129).

Equation 5*

$$\mathrm{NOEC}_{\text{bird or mammal,food,chr}} = \mathrm{NOAEL}_{\text{bird or mammal,oral,chr}} \cdot \mathrm{CONV}_{\text{bird or mammal}}$$

Where:

$NOEC_{bird\ or\ mammal,food,chr}$	NOEC for birds of mammals	[kg/kg_{food}]
$NOAEL_{bird\ or\ mammal,oral,chr}$	5th percentile of Species Sensitivity Distribution	[kg/kg_{bw}/day]
$CONV_{bird\ or\ mammal}$	50% confidential interval	[-]

(*) Equation adapted from the EC TGD (2003, p. 128)

The $PNEC_{oral}$ is finally obtained by dividing the lowest reliable toxicity value (preferably a chronic $NOEC_{food,chr}$, otherwise an acute LC_{50} is also accepted) by an AF, ranging from 30 to 3000 (TGD 2003, p. 130)[10]. Any PNEC based on acute data should be considered tentative. For this reason, in the absence of a chronic study to derive the $PNEC_{oral}$, a high (precautionary) AF of 3000 is applied.

3.2 Retrospective hazard assessment for soils

A large number of approaches have been applied for the derivation of soil protection values for retrospective risk assessment worldwide. However, some regulatory authorities have been leading the development of methods on environmental risk assessment and are used as reference by other countries (Carlon, 2007; Fishwick, 2004). Internationally, there are four main methodologies used that have commonly been adopted and/or adapted by other authorities: the guidance from the Netherlands (RIVM, 2007), the Canadian Guideline (CCME, 2006), the methodology from the U.S. Environmental Protection Agency (US EPA, 2005) and the Australian methodology (NEPC, 2013). These four methodologies have been applied to a broad spectrum of chemicals, mostly for substances that can be commonly found in contaminated soils and may pose a risk to the ecosystem. Nevertheless, they have been used to derive soil protection values for some PPPs as well (see Appendix 1 for details). The mentioned four methodologies are described in detail in the following sections and have been applied in two different case studies (Section 4 and Appendix 2). Other methodologies providing soil protection values for PPPs are also summarized in section 3.2.6.

In total, soil protection values for 103 PPPs, among which 22 still currently authorized in the EU (status as of 7th of June 2021), are available from the countries reported in this review. More information about which soil protection values for PPPs are available and how they were derived is provided in the Appendix 1.

[10] An example of the derivation of the $PNEC_{oral}$ can be found in the Appendix 2, case study Fluazinam

Box 2. Selection criteria for the review of methodologies

Due to the complexity and the heterogeneity of the existing soil protection values for retrospective hazard assessment and in order to accomplish the specific goals set in the AP-PPP (Measure 6.3.3.7), the review of the methodologies in chapter 3.2 "Retrospective Hazard assessment for soils" will focus on describing the derivation of soil protection values with the following characteristics:

- Generic (i.e., not site specific)
- Screening values (values with non-remediation purposes). Other levels may be mentioned if they are part of the same derivation process but it will not be taken into account if countries have specific guidelines for other levels (which is common at the remediation level)
- Protecting in-soil organisms (microorganisms, invertebrates), plants and organisms susceptible to be at risk due to secondary poisoning. Soil protection values to protect human health are not considered in this report.
- Applicable to organic compounds, giving special emphasis to methodologies, which derived soil protection values for PPPs and/or derived specific values for agricultural lands. Measures to correct background concentrations are only applicable for metals and thus, are considered not relevant for PPPs.
- The methodologies described in this report are exclusively scientifically based. Further applications of policy regulations are not discussed in this report

3.2.1 The Netherlands

The National Institute of Public Health and the Environment (RIVM) is in charge of deriving protection values for all environmental compartments, according to the "Guidance for the derivation of environmental risk limits within the framework of 'International and national environmental quality standards for substances in the Netherlands' (INS)" (RIVM, 2007).

The protection values derived according to this Guidance are called Environmental Risk Limits (ERLs). In the Netherlands ERLs for the protection of the ecosystem (water, sediment and soil) and for the protection of human health are derived separately. For the soil compartment ERLs are derived for three levels of protection:

- Negligible Concentration (NC)

- Maximum Permissible Concentration (MPC)

- Serious Risk Concentration (SRC)

MPCs are derived separately for the protection of human health, soil organisms and terrestrial vertebrates, and the lowest of the three is chosen as final MPC. The NC is derived based on the MPC, while the SRC does consider human health and soil organisms, but not terrestrial vertebrates. ERLs are used as scientific advisory values by the Dutch government (Ministry of Housing, Spatial Planning and the Environment, VROM) to set environmental quality standards (EQSs). The main difference between ERLs and EQSs is that the latter have been adopted by the EQS steering committee and may be policy influenced during this adoption process, while ERLs are the primary, purely scientifically derived proposed values. Thus, this chapter will only focus on ERLs derived for the protection of the ecosystem (soil organisms and terrestrial vertebrates), while the corresponding EQSs are only mentioned briefly.

The methodology for the derivation of ERLs for soil follows the EC TGD (2003). The approach proposed by RIVM (2007) is a good exemplification of how the EC TGD (2003) can also be applied to derive soil protection values for retrospective risk assessment.

For the terrestrial compartment, following a similar approach as the one described in Figure 1, three ERLs are derived: NC_{soil}, MPC_{soil} and SRC_{soil}. The methodology used for the derivation of the MPC_{soil} is directly extracted from the $PNEC_{soil}$ derivation from the EC TGD (2003)[11]. The remaining risk limits (NC_{soil} and SRC_{soil}) are subject to separate derivation procedures and are described in the following sections.

Data collection, selection and first considerations

RIVM (2007) provides precise criteria for the evaluation of usefulness and reliability of physico-chemical and toxicological data. The quality of the toxicity values is assessed according to the system developed by Klimisch et al. (1997) (from 1 to 4).

Similar to the EC TGD (2003), toxicity data is also normalized to the organic matter content, but the normalization is applied according to a Dutch standard soil. For non-ionic organic chemicals, the normalization is to an organic matter content of 10 %.

Data extrapolation

The three ERLs (MPC_{soil}, NC_{soil} and SRC_{soil}) are derived according to the procedures described below. A summary of the data extrapolation processes is illustrated in Figure 6.

- Derivation of MPC_{soil}

  The MPC_{soil} is obtained through the calculation of three MPC values that are specific to each receptor group: one MPC to protect in-soil organisms and plants ($MPC_{eco,soil}$), one to protect wildlife ($MPC_{sp,soil}$) and one to protect human health ($MPC_{human,soil}$, not presented in this report). The lowest among the three values is selected as the final MPC_{soil}.

  The $MPC_{eco,soil}$ is derived in the same way as the $PNEC_{soil}$ described in the EC TGD (2003) (see section 3.1.2 and RIVM (2007, p. 92) for further information), i.e., by applying the SSD method, the deterministic and/or the EqP method, depending on the data availability.

- Derivation of NC_{soil}

  The NC_{soil} corresponds to a more protective concentration that would cause only negligible effects to the terrestrial ecosystem. When harmonized to the Dutch policy (as an EQS), this becomes a so called “target value” and should guarantee long-term quality of a site. The NC_{soil} is obtained by dividing the MPC_{soil} by an assessment factor of 100, which is defined as a safety margin allowing for combination toxicity (RIVM 2007).

- Derivation of SRC_{soil}

  The SRC_{soil} is used as a trigger value in the framework of soil remediation. When harmonized as EQS, this becomes the so called “intervention value” and at this level, soil functions are expected to be already seriously affected or threatened. In general, the SRC is based on the geometric mean of the toxicity endpoints.

Bioaccumulation and secondary poisoning

The indications of a potential for bioaccumulation are the same as the ones described in the EC TGD (2003, p. 123). When one or more of the triggers are met, a $MPC_{sp,soil}$ must be derived.

[11] Some extra clarifications have been given in RIVM (2007) due to the interpretation of the EC TGD (2003), but the methodology to derive the soil protection value remains the same.

The $MPC_{sp,soil}$ is derived for worm-eating predators using the same methodology as in the EC TGD (2003). Once the $MPC_{sp,soil}$ is derived, the value is normalized to a Dutch standard soil (i.e., 10 % organic matter).

The MPC obtained to protect wildlife is considered for the derivation process of the final soil protection value by choosing the lowest MPC among the different ones derived ($MPC_{eco,soil}$, $MPC_{sp,soil}$ or $MPC_{human,soil}$). Thus, the protection of wildlife for secondary poisoning is integrated from the final derivation of the MPC_{soil} and, consequently, of the NC_{soil} as well, but not for the derivation of the SRC_{soil}.

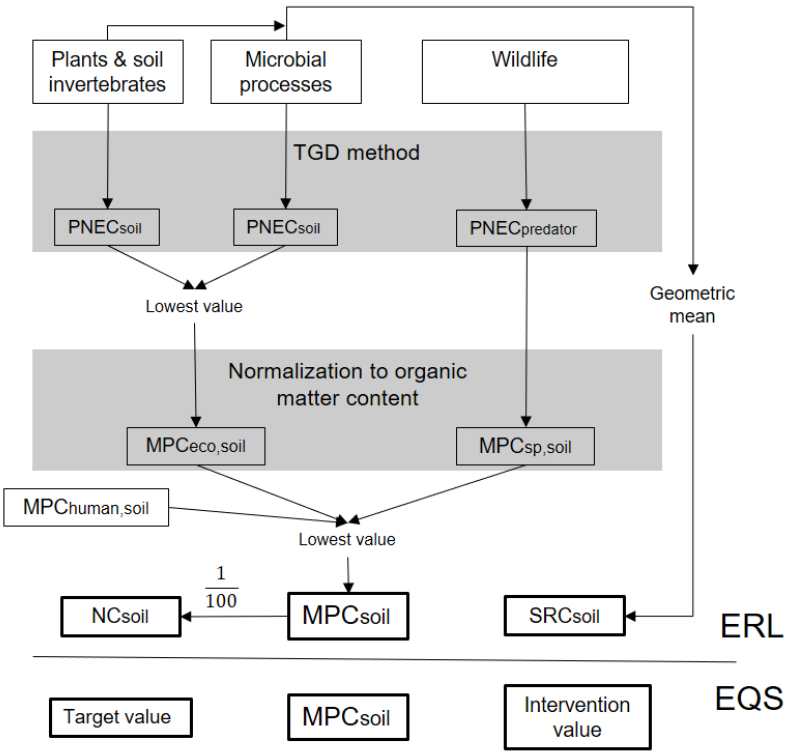

Figure 6: Overview of the Dutch derivation method for deriving ERLs and EQSs for soil, for organic contaminants, according to RIVM (2007).

Further development of soil policy in the Netherlands

The Dutch soil policy has changed considerably in the last two decades. One important change is that target values based on NC are being replaced by background values (Swartjes et al., 2012). In Crommentuijn et al. (2000) it was mentioned that the factor of 100 used to derive the NC was not scientifically based, but rather an empirical security approach, and as such, it could still be under- or overprotective. Many of the derived NC, and even some MPC, were lower than the limits of detection (RIVM, 1997). Therefore, for pragmatic reasons, background values have been used, instead, mainly for naturally occurring substances, but also for many persistent PPP (Lamé et al., 2004). Background concentrations were calculated from soil samples of relatively undisturbed soils in agricultural areas and nature reserves, covering all relevant soil types. The 95th percentile of the measured concentrations was chosen as the background value. In case this value was below the detection limit, the detection limit was used as background value instead (Swartjes et al., 2012). However, for many PPPs, the risk-based NC is still available and applied (see Appendix 1). In 2008, the Dutch contaminated land management has switched to a 'fitness for-use-approach', promoting a sustainable soil management (Swartjes et al., 2012). For this purpose, background concentrations and SRC are used to evaluate the level of contamination and

the adoption of further soil management measures. In case background concentrations are exceeded, the soil material would only be suitable for residential and/or industrial land use but not for agricultural use, for example.

3.2.2 Canada

The methodology to derive soil protection values proposed by the Canadian Council of Ministers of the Environment (CCME) offers a different picture from the European ecological risk assessment. The Canadian soil protection values are described in "A Protocol for the derivation of environmental and human health soil quality guidelines", published in 2006 (CCME, 2006). The soil protection values derived according to CCME (2006) are called "Soil Quality Guidelines" (SQG). Separate SQG are developed for the protection of environmental and human health: soil quality guidelines for the environment (SQG_E) and for human health (SQG_{HH}). The lower SQG (SQG_E or SQG_{HH}) becomes the final soil quality guideline (SQG_F).

The CCME risk assessment approach assumes that different land uses may require different levels of protection, with the agricultural system being the most sensitive land use compared to other land uses like e.g., industrial sites. An important common principle exists for all land use categories defined in the CCME (2006). For each land use, the level of ecological protection provided by the SQG ensures that the land has the potential to support most activities likely to be associated with that land use. SQG are used at a generic screening level and in some cases can be modified to meet remediation goals.

The SQG derived according to CCME (2006) are generic values, based on conservative assumptions, which indicate the potential risk posed by a substance in the soil ecosystem. In some cases, SQGs can be suitable to be applied to a specific contaminated site, either directly or with some modification to the conditions of the site. However, in many cases, generic SQG may not be appropriate and other remediation objectives must be derived[12].

According to the CCME (2006) the following factors are the main drivers of the soil risk assessment and are therefore included in the derivation of SQG:

- Land use: Agricultural, Residential/Parkland, Commercial and Industrial

- Exposure pathways and exposure scenarios (e.g., soil contact, soil and food ingestion)

- Potential receptors (e.g., soil-dependent organisms, mammalian and avian species)

The CCME pays particular attention to the consideration of the adequate ecological receptors that may be affected by the chemical under consideration. Ecological receptors must be here intended in a broad sense for defining all organisms that might be potentially affected (not only soil invertebrates). When identifying the potential receptors, protection should be given particularly to key species that maintain land use primary activities and/or species that are particularly sensitive to the chemical.

The final goal is to identify the adverse effects to the identified receptors that are directly or indirectly exposed to the contaminant present in the soil. To do this, various deriving procedures are used. Each of them reflects a specific category of receptor and exposure pathway, resulting in several types of SQG (Table 6). The lowest among all the derived SQG is chosen as the generic SQG_E.

Data collection, selection and first considerations

According to the CCME (2006) the acceptability of the information should be verified through a data evaluation process. The collected toxicity values are classified as "acceptable" or "unac-

[12] For the derivation of site-specific values, used as clean-up goals or for monitoring remediation efforts, the reference is made to the Guidance Manual for Developing Site-specific Soil Quality Remediation Objectives for Contaminated Sites in Canada (CCME, 1996b).

ceptable" for SQG_E derivation. Ecotoxicological information is collected for the two main categories of receptors: soil-dependent organisms (plants, soil invertebrates, and microorganisms), for which the exposure pathway is via direct contact with the contaminated soil, and mammalian and avian species (wildlife, livestock), for which the exposure is via the ingestion of contaminated food or soil. In general, data from long-term studies are preferred for SQG_E derivation, but as their availability is limited, short-term test results can be used as well.

The CCME (2006) classifies the different exposure pathways into three types. The first type are the **required pathways**, whose evaluation is essential for the derivation of the SQG_E, i.e., if no sufficient data is available, a protection value cannot be derived (e.g., soil contact for soil-dependent organisms). In addition to required pathways, other two types of exposure scenarios and organisms can be considered, although they may not always be mandatory for the derivation of the final SQG_E. The **applicable pathways** are exposure pathways that must be included in the derivation process if sufficient data is available, but if data is insufficient for its evaluation, the final SQG_E can still be calculated (e.g., data on aquatic organisms, when the substance is soluble and there is a potential risk that the water is in contact with contaminated soil). The third type is composed of pathways for which often not enough data is expected to be available or the derivation method is still uncertain (e.g., microorganisms). These are named **check values** and may or may not be included in the derivation process, depending on expert judgement.

Table 6: Ecological receptors considered for each exposure pathway and land use. [a)] pathway required for all substances [b)] required only for substances that biomagnify [c)] check mechanism [d)] required only for soluble organic compounds [e)] only for non-volatile compounds.

Exposure pathway (SQG derived)	**Agricultural**	**Residential/ Parkland**	**Commercial**	**Industrial**
Soil Contact (SQG_{SC})	Plants and soil invertebrates[a]	Plants and soil invertebrates[a]	Plants and soil invertebrates[a]	Plants and soil invertebrates[a]
Soil and Food Ingestion for primary consumers (SQG_{1C})	Primary consumers[a]	Primary consumers[b]	None	None
Soil and Food Ingestion for secondary and tertiary consumers ($SQG_{2C,3C}$)	Secondary and tertiary consumers[b]	Secondary and tertiary consumers[b]	None	None
Nutrient and Energy Cycling (SQG_{NEC})	Microbial processes[c]	Microbial processes[c]	Microbial processes[c]	Microbial processes[c]
Freshwater Life (SQG_{FL})	Freshwater organisms[d]	Freshwater organisms[d]	Freshwater organisms[d]	Freshwater organisms[d]
Livestock Watering and Irrigation ($SQG_{LW,IR}$)	Plants and livestock[d]	None	None	None
Offsite Migration (SQG_{OM-E})	None	None	Variable[c,e]	Variable[c,e]

The lowest among these SQG within the land use is selected as final SQG_E for each land use

Data extrapolation

As shown in Table 6, there are multiple SQG for each exposure pathway and receptor array. The specific procedures for the derivation of the SQG are described in the following points.

- Derivation of SQG for Soil Contact (SQG_{SC})

  SQG_{SC} considers direct exposure of the contaminant to plants and soil invertebrates. If sufficient data is available, a separate SQG_{SC} should be derived for both plants and soil invertebrates. The level of protection that is aimed for depends on the land use category. Based on the land use, the following intermediate values are derived:

- For agricultural and residential/parkland areas, a threshold effect concentration (TEC) is derived. This is defined as the contaminant concentration, at which only minimal effects on ecological function would be observed.
- For commercial and industrial lands, an effect concentration - low (ECL) is derived. This should indicate that only a low level of adverse effects would be expected to occur in less than half of the species in the terrestrial community.

Three methods are available for the SQG_{SC} extrapolation, depending on the number of data available. These are described hereafter in order of decreasing preference and increasing conservatism. In some cases, the methods need the application of an uncertainty factor (UF), chosen based on general guiding criteria and in conjunction with expert judgement. The process is summarized in Figure 7.

1. Weight of Evidence Method

This method requires at least ten data points from three studies and at least two data points on soil invertebrates as well as two data points on plants. The preferred endpoints are IC_{25} and EC_{25} (or IC_x/EC_x with a percentage of effect the closest to 25 %, generally between 20 % to 30 %). If these are insufficient, a combination of effect and no observed effect concentrations is used (i.e., LOECs, NOECs, and LC/EC_x, with $x \leq 50$)). All acceptable ecotoxicological data are ranked and fitted to a linear model. From the ranked distribution, a percentile, named Estimated Species Sensitivity Distribution ($ESSD_x$), is selected to derive either the TEC or the ECL:

- The TEC corresponds to the 25th percentile ($ESSD_{25}$), divided by an UF (from 1 to 5).
- The ECL corresponds directly to the 50th percentile ($ESSD_{50}$).

2. Lowest Observable “Adverse” Effect Concentration

If insufficient data is available for the weight of evidence method, only LOECs are used as input data and if necessary UF are applied. The method requires at least three studies reporting LOEC values and at least one data point on plants and one data point on soil invertebrates:

- The TEC is equal to the lowest available LOEC, divided by an UF (from 1 to 5).
- The ECL is equal to the geometric mean of all acceptable LOECs.

3. Median effective concentration

The last method is only used for agricultural and residential/parkland land use and when only EC_{50} and/or LC_{50} values are available. For this, at least three studies and at least one data point on plants and one data point on soil invertebrates are required.

- The TEC is equal to the lowest EC_{50} or LC_{50}, divided by an UF (from 1 to 10).

Finally, the TEC or the ECL is compared to a check value for nutrient and energy cycling to develop the SQG_{SC}.

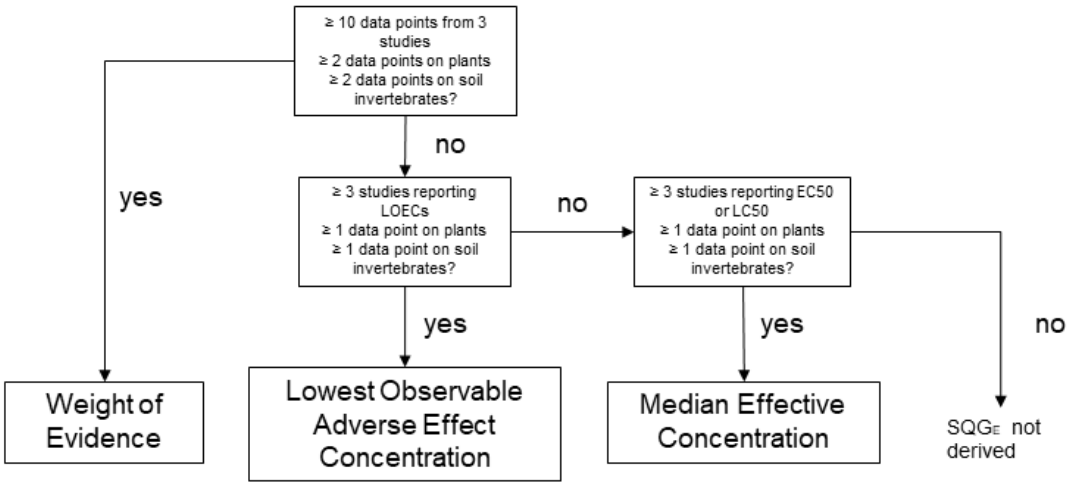

Figure 7: Overview of the Canadian extrapolation methods for deriving SQG for soil contact (SQG_{SC}) according to CCME (2006).

- Derivation of SQG for Soil and Food Ingestion (SQG_I) (Secondary poisoning)

  CCME considers the exposure from ingestion of contaminated soil and food, depending on the land use and the availability of data. As the grazing of herbivores on agricultural land is a well understood mechanism and is considered to be the main route of exposure for these receptors, the impact on wildlife is evaluated only for primary consumers and for agricultural land use. However, if the contaminant has a strong tendency to bioaccumulate (e.g., BAF or BCF > 5000 or log K_{ow} > 5 (CCME 2006, p. 13)), additional SQG_I should be derived for secondary and tertiary consumers and for residential/parkland land uses as well. The final SQG_I is then the lowest among the values derived for each consumer level. The impact on wildlife is evaluated through a stepwise procedure that is equal for primary, secondary and tertiary consumers, but using different BCFs and BAFs that are specific for each trophic level. The application of UF is guided by general criteria and expert judgement.

  Briefly, for each category of consumer, the exposure to a contaminant is estimated through the calculation of soil and food ingestion rates and is expressed as dose per body weight. On the other hand, the toxicity is estimated by dividing lowest available toxicity value by an UF, to obtain the Daily Threshold Effects Dose (DTED). The SQG_I is then extrapolated by posing the exposure equivalent to the effect in a model that takes into account, when possible, the bioavailability of the chemical.

- Derivation of SQG for Nutrient and Energy Cycling (SQG_{NEC})

  This pathway considers the effect of a substance on microorganisms. As data is expected to be limited for this category, this is used as a check value only, i.e., the SQG_{NEC} value is not mandatory to derive the final SQG_E and it is used only when sufficient data is available.

- Derivation of SQG for freshwater life (SQG_{FL})

  The value is derived through an adaptation of a model developed by the British Columbia Contaminated Sites Soil Task Group (CSST). It aims to evaluate the migration of the contaminant from soil to freshwater life. SQG_{FL} is generally only derived for soluble organic compounds and if water surface bodies are present in the vicinity of the site (see the case study for diuron in the Appendix 2 or CCME (2006) Appendix C for further information on the derivation of SQG_{FL}).

- Derivation of SQG for livestock watering (SQG_{LW}) and irrigation water (SQG_{IR})

  As for freshwater life, the substance can migrate and contaminate water sources for livestock or for irrigation. The calculation uses similar procedures than for SQG_{FL}.

- Derivation of SQG for Offsite Migration (SQG_{OM-E})

  The value is derived through the Universal Soil Loss Equation and the Wind Erosion Equation, in order to evaluate the transfer of non-volatile contaminants from less sensitive to more sensitive land uses (e.g., from commercial to agricultural). Given the uncertainties in the derivation method, this is only used as a check value.

- Additional exposure pathways

  If considered to be of particular concern, some additional pathways may need to be considered. One example is dermal contact of wildlife with contaminated water.

The lowest among all derived SQG is chosen as final SQG_E. Besides the SQG for the environment (SQG_E), the protocol describes, as well, all the steps to derive the SQG for human health (SQG_{HH}). The lower of the SQG_E and the SQG_{HH} is selected as final SQG (SQG_F).

The final protection value is ultimately evaluated for considerations other than toxicity (e.g., aesthetic concerns, explosive hazards), or for potentially toxic degradation products. Finally, if the derived SQG_F is lower than the analytical detection limit, it should be mentioned that analytical techniques may not be able to detect such values.

Chemical bioavailability

The bioavailability of organic chemicals is expected to be influenced by several factors, including organic carbon content, pH, ion exchange capacities, clay content and ageing. The CCME (2006, p. 47) recommends that, when possible, values should be derived separately for two soil texture types (coarse and fine). However, this is not often the case, because of limited availability of data. Some jurisdiction may apply soil type considerations only at a site-specific level. In addition, SQG should ideally be derived reflecting the properties of typical Canadian soils. According to the CCME (2006), bioavailability conditions from the toxicity data used for the derivation of SQG should be evaluated (in particular, organic carbon content and pH). The protocol does not recommend to normalize the results to a standard soil. However, if more than 50 % of the data used for the derivation of the soil contact guideline reflect low bioavailability conditions (e.g., organic carbon content equal or greater than 6 % and high pH), consideration should be given to applying an uncertainty factor. If all of the data reflect low bioavailability conditions, the soil contact guideline should be classified as a provisional guideline (CCME 2006, p.48).

3.2.3 United States of America

The US Environmental Protection Agency (US EPA) has derived a set of soil protection values for several frequent contaminants in the soil. The method used is described in the Guidance for Developing Ecological Soil Screening Levels, revised in 2005 (US EPA, 2005) and the protection values derived according to this Guidance are called Ecological Soil Screening Levels (Eco-SSLs). The aim of the Eco-SSLs is to identify the contaminants that are of potential concern to those groups of organisms that are in contact with the soil or that ingest biota that live in or on soil. Eco-SSLs are used to determine whether an additional ecological site study is required, they are purposely conservative and generic, and not adapted to be used as site-specific clean-up standards.

In total, four Eco-SSLs are derived for each of the following groups of organisms: plants, soil invertebrates, birds and mammals. The exposure pathways considered are uptake and direct

contact for plants, ingestion of soil and direct contact exposures for soil invertebrates, and incidental ingestion of soils during feeding, grooming and preening as well as ingestion of food contaminated through uptake of soil contaminants for birds and mammals. An overview of the methodology proposed by US EPA (2005) is summarized in Table 8.

Data collection, selection and first considerations

The US EPA (2005) methodology applies a rigorous selection and quality evaluation of the data. Only data from the acceptable literature are selected for the derivation of the Eco-SSLs (see US EPA (US EPA, 2005), p. 3-2 and 3-3 for further information about the Literature Exclusion Criteria and the Study Acceptance Criteria). For both plants and soil invertebrates, chronic toxicity values are preferred, although acute studies with sublethal effects or plant emergence as an endpoint can also be used.

Effect data is then grouped according to the ecologically relevant endpoints and the toxicity values. The preference for endpoints is given to reproductive output > population (e.g., changes in size and age class structures, changes in sex ratio, intrinsic population growth rate…) > growth for soil invertebrates, and biomass production for plants. Only EC_{10}, EC_{20} and bounded[13] NOAECs and LOAECs are used for the derivation procedure. Another relevant value is the Maximum Acceptable Toxicant Concentration (MATC), which is either provided in the study or calculated as the geometric mean of the NOAEC and the LOAEC. The preference for toxicity parameters is EC_{20} > MATC > EC_{10}. Finally, the studies are scored (from 0 to 18) according to specific Study Evaluation Criteria and only the data with a minimum score of 11 (61 % of the maximum score) are used for the Eco-SSL derivation.

The chemical bioavailability of the substance is one of the important criteria considered among the Study Evaluation Criteria. Differences in the chemical properties (i.e., metal cation, metal anion or organic compounds) may lead to different scenarios of bioavailability (see US EPA 2005, p. 2-10, 2-11 for further details). For non-ionizing organic compounds, the score is based on a combination of different factors: log K_{ow}, soil type (natural versus artificial), pH and OM content (Table 7). The scoring is intended to favor relatively high bioavailability: a score of two is applied to natural soils with relatively high or very high bioavailability, a score of one is applied to natural soil with medium bioavailability and to standard artificial soil[14], and a score of zero is applied for natural soil with low or very low relative bioavailability.

Table 7: Qualitative bioavailability score for non-ionizing organic contaminants in natural soil (US EPA, 2005).

Soil type	**Log K_{ow}**	**Organic matter**		
		Low (< 2 %)	**Medium (2 to 6 %)**	**High (6 to 10 %)**
4 < soil pH ≤ 5.5	Log K_{ow} > 3.5	high	medium	low
	Log K_{ow} < 3.5	very high	high	medium
5.5 < soil pH < 7	Log K_{ow} > 3.5	medium	low	low
	Log K_{ow} < 3.5	high	medium	low
7 ≤ soil pH ≤ 8.5	Log K_{ow} > 3.5	low	low	low
	Log K_{ow} < 3.5	medium	low	low

[13] Values are defined as bounded when both NOAEC and LOAEC are available for the same study. Unbounded NOAEC or LOAEC values in turn do not describe a dose-response curve and are thus not retained for the derivation of Eco-SSL for plants and soil invertebrates.
[14] An organic matter content of 10 % is assumed for standard artificial soil.

For birds and mammals, the data evaluation process is similar. The data evaluation process is specific for toxicological studies and, in this case, only studies scoring a minimum of 66 % are considered valid.

Data extrapolation

Two separate Eco-SSLs, for plants and soil invertebrates, are finally derived. Two wildlife Eco-SSLs for two groups of receptors, mammals and birds, are also derived and further explained in the next section.

For the Eco-SSL derivation, studies that pass the Study Evaluation Criteria are ranked by the bioavailability score. The studies with the highest bioavailability score are then selected. The Eco-SSL is calculated as the geometric mean of all the toxicity values with the highest bioavailability. At least three data values are needed for the Eco-SSL derivation. If data is not sufficient, the study (or studies) related to the next highest available bioavailability level is included into the data set, until at least three data values are available for calculating the geometric mean. If there are less than three acceptable studies an Eco-SSL is not calculated.

Bioaccumulation and secondary poisoning

One Eco-SSLs for birds and one Eco-SSL for mammals are derived, by considering both soil and food ingestion. Three surrogate species reflecting three generic trophic levels (e.g., herbivore, ground insectivore, and carnivore) for both birds and mammals are selected, to best represent the actual wildlife.

The exposure is modelled by using bioaccumulation factors from soil to biota and food and soil ingestion rates. On the other hand, the toxicity is assessed through the calculation of a toxicity reference value (TRV), a value for which no adverse effects to wildlife are expected. The TRV is equal to the geometric mean of the NOEAL values for growth and reproductive output. The Eco-SSL is the soil concentration that results when the TRV and the Exposure Dose are equal (for further information about the model see US EPA 2005, p. 4-1).

Table 8: Overview of the methodology for deriving Eco-SSLs for soil organisms and for wildlife, based on US EPA (2005).

Derivation steps	**Plants and invertebrates**	**Wildlife**
1. Gather data	Chronic values (or acute with sublethal effects)	Chronic and oral values (or biochemical, behavioral, pathology and physiology)
2. Select data		
2.1 Select acceptable data	According to criteria	According to criteria
2.2 Group data	EC_{20}, MATC, EC_{10}	NOAEL, NOAEC
2.3 Score data	Select score ≥ 11 out of 18 (61 %)	Select score ≥ 66 %
3. Derive value	Geometric mean of EC_{20}, MATC or EC_{10} ↓ 1 Eco-SSL for plants and 1 Eco-SSL for soil invertebrates	Geometric mean of NOAEL for growth and reproduction, or Highest bounded NOAEL below lowest bounded LOAEL ↓ 1 TRV for birds and 1 TRV for mammals ↓ Apply to food chain models to derive Eco-SSLs

3.2.4 **Australia**

The National Environment Protection Council (NEPC) has derived several soil protection values, called Ecological Investigation Levels (EILs). The EILs are concentrations of a contaminant above which further appropriate investigation and evaluation is required. The methodology is described in the "Schedule B5b of the Guideline on Methodology to Derive Ecological Investigation Levels in Contaminated Soils" (NEPC, 2013) and is inspired by both, the methods used in other jurisdictions (especially the EC TGD (2003)) and the Australian methodology for deriving water and sediment quality guidelines (ANZECC & ARMCANZ, 2000; Simpson et al., 2005; Simpson and Batley, 2007).

Selecting the level of protection for a site or soil is one of the most important steps in the EIL derivation methodology. The level of protection varies depending on:

- The land use category:
    - national park/area with high ecological value
    - urban residential/public open space
    - commercial/industrial
    - agricultural
- The identification of relevant exposure pathways and consequently the species to be evaluated.

  The exposure pathways that can be considered are direct contact with soil, biomagnification, and/or metabolites. For organic contaminants, the exposure pathways can be assessed by three main parameters: the half-life biodegradation rate, the Henry's law constant and the log K_{ow}.

The preferred method for the derivation of soil protection values is the SSD and the level of protection is defined by choosing different percentiles of the distribution. A summary of the percentages of species and microbial processes to be protected in soil with different land uses is given in Table 9.

Table 9: Percentage of species and soil processes to be protected for different land uses, according to NPEC. [a] for potentially biomagnifying substances, [b] if surface area exceeds 250 m^2, [c] if surface area exceeds 1000 m^2, [d] for agricultural crops, [e] for soil processes and terrestrial fauna.

Land use	Standard % protection	Biomagnification[a] % protection
Urban residential / public open space	80	85[b]
Commercial and industrial	60	65[c]
Agricultural	95[d] and 80[e]	98[c,d] and 85[c,e]
National parks / areas with high ecological value	99	99

The priority for protection in agricultural land is given to crops and grass species (95 % of protection), while other native flora is not considered for the derivation of a soil protection value. Despite the high importance of soil organisms and microbial processes for agricultural sites, conditions such as tillage and treatment with PPPs make a high level of protection unrealistic, which is thus lowered to 80 %. Although the agricultural land use was proposed in the original guidance (NEPC 2013), this consideration was not implemented in the actual EILs, which consider only the other three land uses.

Data collection, selection and first considerations

Once the level of protection and the exposure pathways are clearly defined, the EIL derivation can be performed, starting from the data collection step. In Figure 8, there is an overview of the whole EIL derivation process according to the methodology proposed by NEPC (2013).

Toxicity data on plants, soil microbial processes, soil and terrestrial invertebrates and vertebrates is collected. If no data is available for the soil compartment, toxicity values can be predicted by QSARs, QAARs and/or the EqP models can be used (see section 2.3.1). However, it is mentioned in the NEPC (2013, p. 17) that QSARs and QAARs are limited for terrestrial species and the EqP method has not been validated for Australian soils.

Ecotoxicological data is submitted to a rigorous process of screening, quality assessment and standardization. The screening of the collected (or predicted) data consists of assessing the suitability of the toxicity data, according to acceptance criteria. Successively, toxicity values are scored for quality, and sorted in three classes (≤ 50 % = unacceptable, between 51 % and 79 % = acceptable, ≥ 80 % = high quality). The two highest categories are retained for the derivation process.

Preference is given to chronic toxicity tests performed with endemic species and to the following toxicity parameters: 30 % effect data > LOEC > 10 % or 50 % effect data > NOEC and MATC. Because soil toxicity data is usually scarce, data can be standardized, by using conversion factors (e.g., acute to chronic ratios and/or conversion factors for the toxicity parameters) and by including toxicity data from overseas species.

The last step recommended by NEPC (2013) is the application of ageing and leaching factors (ALF) for chemicals that have been in the soil for more than two years. However, there are currently no AFL for organic chemicals. NEPC (2013) states that it is not possible to derive EILs for aged contamination, when ALF are not available. In such cases, two potential approaches are suggested. First, ALFs should be derived for the substance of concern, through further research. Secondly, direct toxicity assessments should be performed using the soil from the site of investigation and site-specific EILs should be derived. Finally, if ALF are not available, soil protection values for fresh contamination are derived.

Data extrapolation

There are two main extrapolation methods that can be applied depending on the data availability:

- SSD method

  If sufficient data is available, the SSD method must be used. In the NEPC (2013), the SSD method is strongly preferred to the deterministic method because the SSD method is a risk-based approach. However, the minimum data requirements that are commonly set for the SSD (i.e., at least 10/15 NOECs for at least eight taxonomic groups mentioned in the EC TGD (2003)) are rarely met for soil organisms. In order to make the use of the SSD more probable, in the NEPC (2013) the minimum data requirements are reduced to a minimum of five species from at least three taxonomic groups, based on studies by the Danish EPA (Pedersen et al., 1994) and the OECD (OECD, 1995). Nevertheless, they recognize that the SSD is not sufficiently robust when fewer than eight species are used. For this reason, when EILs are derived using only five to eight species, the level of protection that is aimed for should be increased by 5 %, to account for uncertainties in the method.

  According to NEPC (2013), data on the microbial community level can be used for a SSD, together with single species tests. For both data types, the same data requirements are

set, i.e., ≥ five species or functional processes[15] belonging to ≥ three taxonomic or nutrient groups[15]

The chemical bioavailability of a substance may be considered by the normalization of the toxicity data. This normalization should only be performed if the available toxicity data are sufficient to meet the minimum data requirements of the SSD approach. If the toxicity data for a contaminant has been demonstrated to be affected by soil characteristics, toxicity data must be normalized to a standard Australian soil. The values of soil characteristics for normalization to an Australian reference soil are: pH of 6, clay content of 10 %, CEC of 10 mol/kg and organic carbon content of 1 %.

- Deterministic method (AF approach)

  If data is not sufficient for the SSD method, the lowest toxicity value (i.e., NOEC or EC_{10}) is divided by an AF according to Table 10. This approach is considered by the NEPC (2013), a "worst-case scenario" type of approach.

  Table 10: Assessment factors for the AF approach based on NEPC (2013)

Number of species or functional processes available	Number of taxonomic or nutrient groups available	Assessment Factor
< 3	Not applicable	500
≥ 3 and < 5	1	100
	2	50
	3	10
Field data/ data of model ecosystems		10

Bioaccumulation and secondary poisoning

When the contaminant meets the criteria for biomagnification (log K_{ow} > 4) and the contaminated land exceeds a certain minimum surface area, the level of protection is increased in order to extend the protection of terrestrial vertebrates (Table 9).

The Australian approach is based on the principle that values for biomagnifying substances should be more conservative than values derived for soil organisms. For these substances, secondary poisoning is assessed, by using directly the EIL that is derived for soil organisms.

If the EIL for soil organisms was obtained through the SSD method, the level of protection is increased (generally by 5 %) to derive the EIL for wildlife. If the EIL was instead calculated by means of an assessment factor, it is divided by a biomagnification factor (BMF) to obtain the EIL for wildlife. The BMF is retrieved from the literature. If not available, BMF for organic compounds may be predicted based on BMF for compounds that have a similar structure.

[15] For microbial communities, functional processes and nutrient groups are the equivalents to species and taxonomic groups for vertebrates and soil invertebrates, respectively

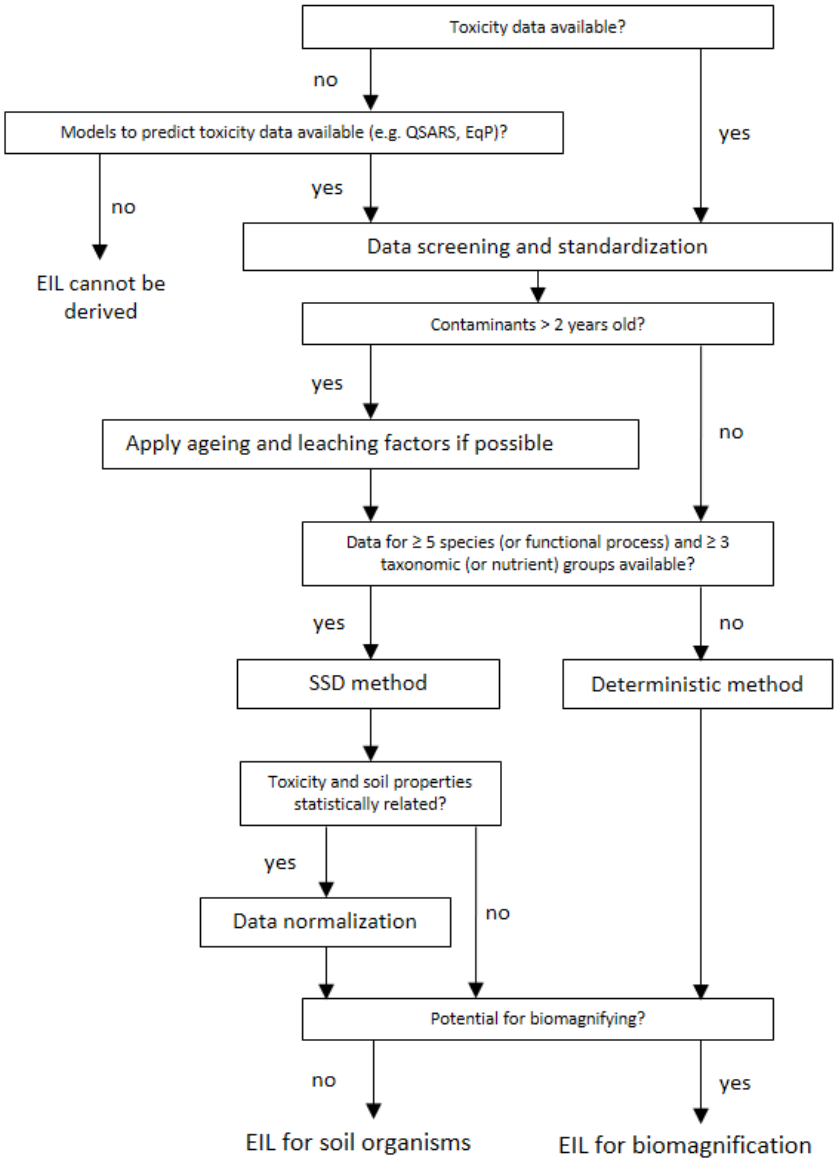

Figure 8: Overview of the Australian methodology for deriving ecological investigation levels (EILs) for organic contaminants. In the end, there is a unique EIL, considering either soil organisms only or both soil organisms and biomagnification (in case biomagnification is triggered). Adapted from NEPC (2013).

3.2.5 Summary of the methodologies

The four methodologies described in sections 3.2.1 to 3.2.4 have been summarized in Table 11.

Table 11 : Description of the main differences among the four methodologies described on the previous chapters (RIVM (2007), CCME (2006), US EPA (2005) and NEPC (2013)) for the derivation of soil protection values in retrospective risk assessment.

	RIVM (2007)	**CCME (2006)**	**US EPA (2005)**	**NEPC (2013)**
Quality assessment of toxicity data	• simple quality check (relevance and reliability is assessed (Klimisch et al. 1997))	• simple quality check (7 selection criteria)	• complex quality check (3 step process: search, screening and quality score)	• complex quality check (3 step process: screening, quality score and standardization)
Derivation methods	• multiple (SSD, AF method, EqP method), depending on data availability	• multiple (weight of evidence, lowest observed adverse effect concentration, median effective concentration), depending on data availability	• single method (geometric mean)	• multiple (SSD, AF method and EqP method), depending on data availability
Land use	• not considered	• 4 different land uses: agricultural, residential/parkland, commercial and industrial • different exposure pathways are considered within each land use	• not considered	• 6 different land uses combined in 4 groups: national parks and areas with high ecological value, urban residential and public open space, commercial and industrial land, agricultural land • different protection levels are considered within each land use
Bioavailability	• only soil organic matter considered • normalization to 10 % organic matter	• organic matter, pH and soil texture considered • no normalization • studies with very high bioavailability conditions discarded and special considerations if low bioavailability	• organic matter, pH and log K_{ow} considered • no normalization • studies with high bioavailability conditions preferred	• organic matter/carbon, pH, CEC and clay content considered only for the SSD method • ageing and leaching factors for aged soils
Organisms considered	• microorganisms, plants and invertebrates	• microorganisms, plants and invertebrates	• plants and invertebrates	• microorganisms, crop plants and invertebrates
Secondary poisoning	• derivation only if trigger values for bioaccumulation are exceeded (e.g., log $K_{ow} \geq 3$) • food chain: earthworms to mammals and/or birds	• derivation depends on the land use and/or if trigger values for bioaccumulation are exceeded (e.g., log $K_{ow} > 5$)	• always derived • food chain: plants, earthworms or small mammals to mammals and birds	• only triggered if log $K_{ow} \geq 4$ • No derivation of extra soil protection value for secondary poisoning but direct adaptation of the value derived

	RIVM (2007)	CCME (2006)	US EPA (2005)	NEPC (2013)
		• food chain: plants to mammals or birds (primary consumer), secondary and tertiary consumer		for direct toxicity, by increasing the level of protection
Number of soil protection values derived[16]	• 3 for direct toxicity with different levels of protection and one for secondary poisoning (if triggered) • Final: 3 soil protection values (different risk levels)	• minimum 4 (1 per land use), maximum 22 • number of protection values depends on: land use, solubility and/or volatility of the substance and bioaccumulation • Final: 4 soil protection values (different land use)	• 4: plants, invertebrates, birds and mammals • Final: 1 soil protection value (the lowest one)	• Final: 1 soil protection value for direct toxicity (which can be lowered to account for secondary poisoning)

[16] The number of soil protection values derived corresponds to the different soil protection values that should be considered according to each methodology. Only ecological soil protection values are considered in the table

3.2.6 Other countries with soil protection values for PPPs

Soil protection values have been derived for most European countries and other countries/regions in the world. However, the review from Carlon (2007) mentioned that most of the soil protection values of European countries used adaptations of the methodologies described in the previous chapters of this report. As mentioned in the introduction of this report, soil protection values to protect in-soil organisms and plants have been mostly derived for metals and other persistent substances, but hardly for PPPs. The four retrospective methodologies described in the previous sections derived soil protection values for certain active substances of organic PPPs but there are also other countries, which derived soil protection values for such active substances. Those countries/regions are listed in Table 12 for further information about the methodologies of the countries mentioned in this table and about the active substances they derived, see the Appendix 1). An extensive research of the methodologies used worldwide would require considerable time and effort, involving sending questionnaires to the different authorities, since the information is not always publicly available and/or in foreign languages. Therefore, the information provided in this table was mostly collected from previous reviews (Carlon, 2007; Fishwick, 2004). When possible, the information has been contrasted and updated, but sometimes it was difficult to find or not even accessible. In those cases, the information refers directly to the data found in those reviews. Although there are some more countries/regions, which derived soil protection values for active substances of PPPs, they were not considered relevant if they are only applied for remediation purposes. This was the case for British Columbia (SABCS, 2009) and Alberta (Alberta Environment and Parks (AEP), 2016), for example.

Apart from the values derived by the different jurisdictions in order to screen levels of chemicals (some of them PPPs) in soils, there have been some scientific publications in which soil protection values for PPPs were derived. Pivato et al. (2017) used the EC TGD (2003) to derive $PNEC_{soil}$ for 13 organic PPPs applied in Italian agricultural soils considering in-soil organisms and plants. Similarly, Vašíčková et al. (2019) performed a retrospective risk assessment using $PNEC_{soil}$ and, also, the SANCO/10329/2002 (EC SANCO, 2002) approach for 68 PPPs (53 parental compounds and 15 transformation products) considering only in-soil organisms.

Due to the time and effort that the case studies require, only the two prospective (sections 3.1.1 and 3.1.2) and the four retrospective approaches extensively explained in this report (sections 3.2.1 to 3.2.4) were considered for the case studies. However, all the other mentioned approaches could be considered for final decisions and recommendations.

Table 12 : List of other countries or regions, which derived soil protection values for PPP.

Country	Name of the soil protection value	Scientific basis	Land use	Generic/ site-specific	Risk level	Organisms considered	Source	Legal basis
Czech Republic	Prevention limits	Percentile of background concentrations	Agricultural	generic	Trigger case-by-case specific risk assessment	-	Vácha et al. (2014)	Decree setting the details of soil quality conservation and about the change of Decree No. 13/1994 Col.
	Indication limits	Human health risk (US EPA, 2002)[17]			Trigger case-by-case specific risk assessment			
Finland	Threshold value	Ecological risk effect-based (EC TGD, 2003, RIVM reports)	-	generic	Negligible risks. Trigger for site-specific risk assessment	Soil organisms and processes	Carlon (2007), Finnish Ministry of Environment (Finnish Ministry of Environment, 2014)	Government Decree on the Assessment of Soil Contamination and Remediation Needs 214/2007
	Lower guideline value	Ecological risk effect-based (RIVM reports) and human health risk	All land uses except industrial	site specific	Risk reduction measures required			
	Upper guideline value		Industrial					
Spain	Generic reference levels	Ecological risk effect-based (EC TGD, 2003)	-	generic	Trigger for specific risk assessment	In-soil organisms and plants; aquatic organisms; terrestrial vertebrates	Tarazona et al. (2005)	Royal Decree 9/2005, which establishes the relationship of potentially polluting activities of the soil and criteria and standards for the declaration of contaminated soils.
		Human health risk (US EPA, 1989)	Three classes: industrial, residential and all land uses			-		
Sweden	Generic guideline values	Human health risk, ecological risk effect-based	Sensitive land use (residential housing and parkland)	generic	Trigger for specific risk assessment	In-soil organisms and plants; terrestrial vertebrates	Carlon (2007), SEPA (2016)	Not legally binding

[17] Indication limits can include limit values of food chain contamination and plant growth inhibition, but according to Vácha et al. 2014, those factors were only used for the derivation of indication limits for risk elements (not for persistent organic pollutants).

Country	Name of the soil protection value	Scientific basis	Land use	Generic/ site-specific	Risk level	Organisms considered	Source	Legal basis
		(RIVM reports) and freshwater risk (CCME, 2006)						
		Human health risk and ecological risk effect-based (RIVM reports)	Less sensitive land use (commercial and industrial) (equivalent to the SRC (RIVM reports))		Trigger for specific risk assessment			
Latvia	Target values	Not reported	-	generic	Indication of sustainable soil quality	Not reported	Latvian Environment, Geology and Meteorology Centre (2017)	Cabinet of Ministers Regulation No 804 "Regulation of the Quality Normatives for Soil and Subsoil" (2005)
	Precaution limit values				Trigger exploration and monitoring			
	Critical limit values				Trigger for remediation			
USA (Oak Ridge National Laboratory)	Ecotoxicological screening benchmarks	Ecological risk effect-based (ORNL, 1998, 1997a, 1997b, 1996)	-	generic	Trigger for further risk assessment	Soil invertebrates (earthworms), soil microbial processes, plants, wildlife	Fishwick (2004), ORNL (1998, 1997a, 1997b, 1996)	Values do not meet particular regulatory policy goals
Ontario	Site Condition Standards	Ecological risk effect-based, human health risk, leaching to groundwater and migration (based partly on CCME (1996a))	Complex selection of land uses related to the groundwater conditions. Agricultural land use considered under some exposure scenarios	Generic	Trigger for specific risk assessment	Soil invertebrates, plants and terrestrial vertebrates	Ontario Ministry of Environment (2007)	Ontario regulation 153/04 (2004)

4 Case studies: Application of the reviewed methodologies

Based on the reviewed methodologies of this report, case studies were conducted and soil protection values for two active substances applied as PPPs were derived: the herbicide diuron and the fungicide fluazinam. The goal of these case studies was to compare the methodologies described in the report. For the derivation of the prospective values, we applied a variation of the EFSA approach used for the derivation of RAC values as well as the ECHA approach using the EC TGD (2003). For the derivation of the retrospective values, we applied the Dutch RIVM (2007), the Canadian Guideline (CCME, 2006) the methodology from the U.S. Environmental Protection Agency (US EPA, 2005) and NEPC (2013) from Australia. The current case studies will highlight the very different strategies and point out the consequences for the derivation of soil protection values. Some general considerations concerning the application of the different methodologies and the results of the case studies are described in the next sections. Further detailed information about the derivation processes can be found in the Appendix 2 of this report.

Disclaimer:

Similar to the procedure used for water and sediment Environmental Quality Standards (EQS) derived by the Ecotox Centre, Soil Guideline Values (SGV) will be based on data from the PPP (re-) authorization dossiers and supplemented by data from publicly available literature. The studies from PPP (re-) authorization dossiers went through to an extensive evaluation process by the Rapporteur Member State (RMS). In contrast, the quality of toxicity studies from scientific publications needs to be evaluated first, before being used for the derivation of soil protection values. Because the main goal of the current case studies is to compare the different methodologies, the use of data from PPP (re-)authorization reports was considered sufficient at this point and thus, only this data was used. However, further exploration of studies from the public literature will be considered for the final SGV derivation.

The soil protection values derived for this report are used exclusively to make a comparison between methodologies. The limited dataset used for the derivation of the soil protection values for the case studies may be different from the dataset used by other authorities. This may lead to differences in the derivation process and/or the final soil protection value. Therefore, direct comparisons between the values derived in this report and values derived by other authorities are strongly disadvised.

4.1 General considerations

4.1.1 Quality assessment of the toxicity studies

PPP authorization is based on data from studies, which had a quality evaluation assessment performed by a Rapporteur Member State (RMS). Therefore, all the studies listed in the (re-)authorization report could be used for the derivation of PNEC and RAC values. RIVM (2007) and the CCME (2006) have a similar quality assessment of the literature. Neither of the two approaches has very rigid quality criteria and are more based on expert judgment. For both methodologies, the quality assessment of the studies by the RMS was considered sufficient for the case studies. On the contrary, the US EPA (2005) and NEPC (2013) are methodologies fundamentally based on an exhaustive search, screening and quality check of toxicity studies. Both approaches have more rigid criteria and clearly defined steps for the assessment of the studies. Because of the differences on the validity criteria applied by the US EPA (2005) and NEPC (2013) compared to RIVM (2007) and CCME (2006), special emphasis has been given to this process for the two former methodologies in the case studies.

For the US EPA (2005), the assessment of reliable literature consists of three steps:

1. Screening of studies appropriate for use in deriving Eco-SSLs (Literature Exclusion Criteria)
2. Identification of publications which included at least the minimum information necessary for deriving an Eco-SSL (Study Acceptance Criteria)
3. Extraction of study data and scoring (Study Evaluation Criteria).

For NEPC (2013), the toxicity data is suitable if the following criteria are fulfilled:

1. Acceptance criteria
2. Quality assessment criteria
3. Standardization (if necessary)

Thus, a complete quality assessment of the toxicity tests from PPP (re-) authorization dossiers presented for the case studies was performed for US EPA (2005) and NEPC (2013).

Diuron is used mainly as an herbicide, but it can also be used as a biocide. The biocide authorization is processed by ECHA. In this latter case, only the information on registered substances was available online (https://echa.europa.eu/registration-dossier/-/registered-dossier/13520). It is mentioned on the website that: "Information on Registered Substances comes from registration dossiers which have been assigned a registration number. The assignment of a registration number does however not guarantee that the information in the dossier is correct or that the dossier is compliant with Regulation (EC) No 1907/2006 (the REACH Regulation). This information has not been reviewed or verified by the Agency or any other authority. The content is subject to change without prior notice." Therefore, because no own quality assessment is performed on the data used for the case studies (see section 1.1.1), a review by an authority was mandatory to assure the quality of the studies. As mentioned above, data from the Information on Registered Substance is not validated and was therefore not used for the case studies.

4.1.2 Preferred endpoints and toxicity parameters

If available, chronic endpoints from long-term studies were chosen. If a test showed several valid endpoints, recommendations from the RMS for the selection of the most relevant endpoints were followed.

The preference for the most relevant toxicity parameters differs depending on the methodology used for the derivation of the soil protection value. Below, a list of the preferred values (from most to least preferred) for each methodology is described:

- TGD (2003, p. 123), RIVM (2007, p. 45) and RAC values: NOEC[18] or EC_{10} > $L(E)C_{50}$

- US EPA (2005, p. 3-5): EC_{20} > MATC[19] > EC_{10}

- CCME (2006, p. 42): EC_{25} > LOEC > NOEC

- NEPC (2013, p. 21): EC_{30} > LOEC > EC_{10} or EC_{50} > NOEC and MATC

In case the preferred toxicity parameter was not reported in the study, the next available value following the preference rank above was taken into consideration.

[18] Some studies reported a NOEL (No Observed Effect Level) instead of a NOEC (No Observed Effect Concentration). Both parameters are considered as synonyms in this report.
[19] The MATC (Maximum Acceptable Toxicant Concentration) is the geometric mean between the NOEC and the LOEC of the same study.

4.1.3 Terrestrial plant studies

The existing non-target terrestrial plant tests are mostly considered short-term tests (Environment Canada, 2004; OECD, 2006a, 2006b). However, it is generally accepted by the scientific community[20], that they can be regarded as long-term studies if the proper endpoints (e.g., growth, reproduction, biomass) and the appropriate toxicity parameters (i.e., EC_{50} and additional EC_x and/or NOEC values) are reported. Tests with plants are considered for all the methodologies described in this report, except for the derivation of RAC (personal communication from FOAG experts).

The studies for non-target terrestrial plants are usually described extensively. To summarize, only the most relevant endpoints and toxicity parameters were listed in the tables containing the ecotoxicological data (in the Appendix 2, Tables 2 and 8 for diuron and fluazinam, respectively).

4.1.4 Selection of the substances

The active substances diuron and fluazinam were chosen for the case studies (Table 13) based on the following considerations:

- They were included in the initial list of candidate substances selected for the derivation of SGVs in Switzerland (Campiche et al., 2020).
- They are active substances representing two different categories of PPPs: herbicide (diuron) and fungicide (fluazinam).
- The intrinsic properties of the substances and their behavior in the environment are very different (e.g., solubility in water and octanol-water partition coefficient (log K_{ow})). Thus, different scenarios could be represented in the derivation of soil protection values.
- The amount and variety of ecotoxicological data available were very different between both substances. Thus, different derivation methods within each methodology could be used.

4.1.5 Data used in the case studies for the derivation of soil protection values

Both substances were authorized as PPP by the European Commission at the time of the first selection of candidate substances for the derivation of SGV (Campiche et al., 2020). Although diuron has been recently banned for its use as PPP in Switzerland (Swiss Federal Council, 2020d), it was still kept as a case study. Indeed, the ecotoxicological effects of diuron are well documented and the large number of soil toxicity values available compared to other substances allows a thorough comparison of the different methodologies. Commonly, bioassays conducted with the active substance and the formulated product are publicly available and described in the (re-)authorization dossiers, together with the evaluation of the RMS. In order to have a complete data set, both, bioassays with the active substance and the formulation, were considered for the derivation of soil protection values for the case studies. Although the toxicity of the metabolites should generally be explored and/or considered for risk assessment, this was not considered for the case studies and only bioassays with the parent material were taken into account.

Higher tier studies like field studies are commonly considered for the derivation of soil protection values as well. The exposure of organisms under field conditions aims to simulate a real case scenario. Thus, field studies may help to perform an appropriate risk assessment in cases were

[20] RIVM (2007, p. 39): "OECD guideline 208: Terrestrial Plants, Growth Test. According to the test guideline, the recorded endpoints should be the LC_{50} for emergence and the EC_{50} for growth. As such, the test is an acute test. However, because exposure is from seed to plant, the test may be interpreted as chronic if NOECs or EC_{10}s are recorded for the above mentioned endpoints, especially if the exposure duration is prolonged to, for example, 28 days."
ECHA Guidance on BPR (2017, Vol IV Part B+C p. 148): "…The study is in principle a short-term study. However, it was decided that it also can be considered a long-term study under certain circumstances, provided that in addition to the EC_{50} also a NOEC/EC_{10} was derived from this test."
CCME (2006): "Long-term plant toxicity tests have also come into use in recent years, based on endpoints including plant growth and life cycle flowering (Environment Canada 2004; ASTM 1996; ASTM 1991)"

potential risk in lower tier risk assessments was identified. However, field studies are highly complex and may lead to differences in the evaluation between different authorities. For this reason, and in order to get comparable results between the different methodologies, field studies were not included in the dataset. Only ecotoxicological studies performed under laboratory conditions were considered for the case studies.

Table 13: Substance selection for the case studies and available ecotoxicological data.

Active substance	Category of PPP	Available regulatory documents	Number of accepted studies (a. s. and formulation studies)
diuron	herbicide	EC RAR (EC RAR, 2018)	2 studies for earthworms 1 study for collembola 1 study for mites 2 studies for microorganism transformation tests 4 studies for non-target plants (15 species)
fluazinam	fungicide	EC DRAR (EC DRAR, 2019), EC DAR (EC DAR, 2006)	4 studies for earthworms 3 studies for collembola 2 studies for mites 1 study for microorganism transformation tests 3 studies for non-target plants (13 species)

4.2 Results and discussion of the case studies

Table 14 shows the results obtained after the application of the two prospective and the four retrospective methodologies previously mentioned in the report (see the Appendix 2 for a full description of the derivation process of the case studies).

For some methodologies, the final soil protection value has to be normalized to account for differences in organic matter content from the test conditions to the defined soil conditions in the respective country/region. This is the case for EC TGD and RIVM. Although EFSA does not account for regional soil conditions, corrections are also made for those tests using artificial soils in case that the substance tends to be adsorbed to the soil (i.e., log K_{ow} > 2). If the main exposure pathway of the substance is the direct toxicity, like for diuron, the results without normalization, i.e., with the organic matter content used in the bioassay, were also shown in Table 14. This allowed a direct comparison with other approaches, which do not normalize the values (e.g., CCME and NEPM). Since fluazinam is a substance with a high bioaccumulation potential, the exposure pathway to protect higher trophic levels from a risk of secondary poisoning had to be explored for most of the methodologies. For some methodologies, (RAC-EFSA, EC TGD and RIVM), the normalization to a defined organic matter/organic carbon content is required in the model used for the derivation process. It is well known that one of the main factors influencing the adsorption of organic chemicals in soil is its organic matter. Therefore, the models used by EFSA, EC TGD and RIVM guidances, require a default value of organic matter and/or organic carbon content to account for the adsorption of the substance to the soil particles. This will determine the amount of substance that can be transferred from the soil to the earthworms and, later, to earthworm-eating predators. In case that the value for secondary poisoning was lower than the one for direct toxicity, the soil protection value to protect secondary poisoning was chosen. This was only the case for the RAC value but not for the soil protection values from the EC TGD or RIVM. For this reason, the final RAC could only be presented as a normalized value.

For the plant studies, different bulk soil densities have been applied in order to convert application rates (e.g., g/ha) to concentrations in soil (mg/kg d.w.) following what was specified in the guidances: 1.5 g/m^3 for the EC TGD (2003) and 1.7 g/m^3 for the CCME (2006). The differences after applying those two soil bulk densities were considered minimal and did not influence the comparison of final soil protection values.

In most cases, it was possible to derive a soil protection value with the available data. For the CCME methodology, only the SQG_{SC} could be derived. However, no final SQG value could be proposed for fluazinam, since data of grazing animals to calculate secondary poisoning (SQG_I) was missing, and, according to that methodology, no final protection value can be proposed for a bioaccumulative substance if the SQG_I is missing.

Table 14 : Summary table with the results obtained after the application of the different methodologies to the case studies diuron and fluazinam. In general, values are shown without any normalization to organic matter content. In case where normalization was required by the methodology, both values, normalized and not normalized, are shown. Abbreviations: norm. = normalized, OM: organic matter.

Region – Methodology	**Soil protection value**	**Diuron mg a.s./kg d.w.**	**Fluazinam mg a.s./kg d.w.**
EFSA	RAC	2.14 (not normalized) 1.1 (normalized)	 0.0027 (norm. 2 % OC)
EC TGD (2003)	$PNEC_{soil}$	0.000075* (not normalized) 0.00015 (norm. to 3.4 % OM)	0.0054 (not normalized) 0.008 (norm. to 3.4 % OM)
The Netherlands – RIVM (2007)	$MPC_{eco,soil}$	0.000075* (not normalized) 0.00044 (norm. to 10 % OM)	0.025 (not normalized) 0.11 (norm. to 10 % OM)
Canada – CCME (2006)	SQG_E	0.0011	not possible
USA – US EPA (2005)	Eco-SSL	73	11
Australia – NEPC (2013)[21]	EIL	0.002 (crop species) 0.011 (soil invertebrates and microbial processes)	0.071 (crop species) 0.25 (soil invertebrates and microbial processes)

**** The method used by RIVM is the same as the one used in the EC TGD. Therefore, the soil protection values are the same when no normalization to organic matter was applied. To simplify, the results of the not normalized values will be mentioned in the text only as EC TGD values.***

4.2.1 Diuron

Large differences were observed between the soil protection values derived by the different methodologies. For diuron, the main route of exposure was direct toxicity according to all methodolo-

[21] According to NEPC two soil protection values were derived for the agricultural land use. When using the SSD method, a level of protection of 95 % for the crop and grass species is used because the aim is to protect the crops. However, it is also mentioned that the use of some agricultural practices (e.g. tillage, pesticides) make it unrealistic to protect in-soil organisms at the same level and, therefore, the protection level is reduced to 80 %.

gies. Since diuron is an herbicide, it was expected that plants would be the most sensitive organisms. Therefore, the main factor that influenced differences between soil protection values was the inclusion or exclusion of data on plants. The methodologies, which did not include plants for the derivation, i.e., US EPA (due to the quality criteria applied to the plant studies) and RAC (by default), showed much higher values than the rest. Still big differences existed between the soil protection values from US EPA and the RAC (34-fold) due to the two very different approaches used for derivation. While the RAC was based on the NOEC of the most sensitive chronic study (i.e., earthworm in this case) and an assessment factor was applied to it, the US EPA value was based on the geometric mean of all the accepted studies (i.e., earthworm, mite and collembolan) and no further assessment factor was applied. As all the accepted studies by US EPA showed low sensitivity to diuron and no assessment factor was used, this resulted in a much less conservative value compared to the RAC.

From the methodologies that included in-soil organisms but also plants in the derivation, the lowest soil protection value resulted from applying the EC TGD methodology, followed by CCME and NEPC. The soil protection values from CCME and NEPC (for crop species) were 15 and 27 times higher than the $PNEC_{soil}$ (EC TGD, 2003), respectively. Two main factors influenced these differences. The first one is the method used for the derivation. Distribution methods could be used for CCME and NEPC, since the data requirements are less strict than for EC TGD. For the EC TGD, only the deterministic approach (AF method) could be applied. The deterministic approach ignores all other data except the lowest and generally applies a higher assessment factor than the distribution methods. For this reason, the deterministic approach is an example of the "worst-case scenario" type of approach (NEPC, 2013) and may lead to more conservative values than by applying a distribution method. The second factor that influenced the soil protection values is the choice of the toxicity parameters. While EC TGD used NOEC for the derivation, CCME and NEPC used LOEC and/or EC_{30}. The use of LOEC-type data leads to less conservative soil protection values than the approaches using NOEC. The use of LOEC-type data could be preferred in case of assessing soil protection values for contaminated sites. This was the case for Australia, where the soil protection values were applied in places where a certain degree of contamination was assumed (personal communication from M. Warne).

One of the main differences between the distribution methods from CCME and NEPC is that the first one uses a linear model to fit the data while the second one uses a sigmoidal model (Burr type III). It could be observed in section 1.6.2.1 of the Appendix 2 that the application of a linear model to the data was probably not the best model for the dataset. For this reason, a refined fitting excluding the less sensitive organisms (in-soil organisms) was proposed for CCME. Another difference between the two approaches is the level of protection used. In CCME, a less conservative level of protection is applied and the soil protection value accounts for the protection of 75 % of the species (25^{th} percentile of the distribution). In NEPC, however, a level of protection of 95 % for the crop and grass species and 80 % for in-soil organisms was applied. Although NEPC selects more protective percentiles, the fact that CCME applies an assessment factor to the percentile and NEPC does not, reduced the differences in the final protection values between both approaches.

Finally, it could be observed that, when methodologies normalize the values to organic matter content, the final soil protection value changed significantly. Although the same derivation method was applied to EC TGD and RIVM, due to the different normalizations (3.4 % and 10 % organic matter for EC TGD and RIVM, respectively), the normalized soil protection values differed 3-fold.

4.2.2 **Fluazinam**

Fluazinam is a highly lipophilic substance (log K_{ow} of 5 (worst case-scenario)). Therefore, it is expected that one of its main exposure routes is bioaccumulation along the food chain and a secondary poisoning assessment was mandatory according to all methodologies. However, for other substances with lower lipophilicity, i.e., log K_{ow} between 3 and 5, bioaccumulation might be

mandatory to assess for some but not for all approaches. This is due to different trigger values, which are used according the different guidances.

Most approaches account for secondary poisoning via the food chain. This is the case for the RAC, EC TGD, RIVM, CCME and US EPA. The approach used according to NEPC, on the other hand, does not consider any food chain model. This methodology accounts for the potential bioaccumulation of a substance by applying an increased protection level to the soil protection value derived for direct toxicity. This biomagnification protection is applied by increasing the percentage of protection up to 98 % and 85 %, for crop species and in-soil organisms, respectively, when using the distribution approach (without biomagnification the values would be 95 % and 80 % for plants and in-soil organisms, respectively, as it was already mentioned in the diuron case study).

The remaining methodologies derived soil protection values for secondary poisoning via the food chain. CCME and US EPA consider complex food chain models of bioaccumulation with different exposure pathways. According to CCME, the exposure from plants to grazing animals is a required pathway for highly bioaccumulative substances (log K_{ow} > 5) and also wildlife (secondary and tertiary consumers) should be included in the derivation. On the other hand, for the US EPA approach, three trophic groups (e.g., herbivore, ground insectivore and carnivore) for both mammals and birds should be considered. For these two approaches, which consider a complex food chain of bioaccumulation (CCME and US EPA), no value could be derived for secondary poisoning due to the lack of studies presented in this report. A soil protection value for secondary poisoning could only be derived for those methodologies which use a more simple exposure route (from earthworm to earthworm eating predator) (EFSA, EC TGD and RIVM). For all methodologies in which both soil protection values, for direct toxicity and secondary poisoning, could be derived (EFSA, EC TGD and RIVM), the value for secondary poisoning was only lower for the EFSA methodology. This low value for secondary poisoning observed by the RAC may be due to the methodology applied, based on dry soil concentrations instead of the pore water mediated approach used by EC TGD (2003), and the use of estimated bioconcentration factors for earthworms instead of experimental bioaccumulation factors. For EC TGD and RIVM, the values derived for direct toxicity were lower than for secondary poisoning. Consequently, regardless of the high bioaccumulation of fluazinam, the risk for higher trophic levels via secondary poisoning was lower than the risk for plants and/or in-soil organisms via direct toxicity. As for diuron, the inclusion/exclusion of studies played an important role in the final value. For example, US EPA does not include microorganisms in the derivation, which in fact showed the lowest values in the dataset. This led to major differences compared to methodologies like ECHA and RIVM, which considered microorganisms as the most sensitive group of organisms. An additional factor influencing the strong difference between the soil protection values was the use of relatively high assessment factors applied in the EC TGD and RIVM (50 in both cases) due to uncertainties in the dataset compared to US EPA, which does not apply any AF. The uncertainties detected in the dataset (for example, the large number of studies reporting unbounded values) were not accounted for by certain methodologies, e.g., EFSA and NEPC, for which those values were included in the derivation.

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6 Abbreviations

AF (or UF)	Assessment Factor (or Uncertainty Factor)
ALF	Ageing and Leaching Factors
AP-PPP	Action Plan for Plant Protection Products
ASTM	American Society for Testing and Materials
BAF	Bioaccumulation Factor
BCF	Bioconcentration Factor
BMF	Biomagnification Factor
BPR	Biocidal Products Regulation
CCME	Canadian Council of Ministers of the Environment
CEC	Cation Exchange Capacity
CI	Confidence Interval
CSST	Contaminated Sites Soil Task Group (British Columbia)
DDT	Dichlorodiphenyltrichloroethane
DTED	Daily Threshold Effects Dose
$DT_{50,soil}$	Half-Life in the Soil
EC TGD	European Technical Guidance Document on Risk Assessment
$EC_{(x)}$	Effect Concentration (causing x % of effect)
ECHA	European Chemicals Agency
ECL	Effect Concentration – Low (CCME)
Eco-SSL	Ecological Soil Screening Level (US EPA)
$ED_{(x)}$	Effect Dose (causing x % of effect)
EFSA	European Food and Safety Authority
EIL	Ecological Investigation Level (NEPC)
EqP	Equilibrium Partitioning method
EQS	Environmental Quality Standards (general term widely used in Europe or RIVM)
$ER_{(x)}$	Effect Rate (causing x % of effect)
ERA	Ecological Risk Assessment
ERL	Environmental Risk Limit (RIVM)
$ESSD_{(x)}$	Estimated Species Sensitivity Distribution (percentile) (CCME)
FOAG	Federal Office for Agriculture
FSVO	Federal Food Safety and Veterinary Office
$HC_{(x)}$	Hazardous Concentration (for x % of species)
HCH	Hexachlorocyclohexane
γ-HCH	Lindane (gamma-hexachlorocyclohexane)

HQ	Hazard Quotient
$IC_{(x)}$	Inhibitory Concentration (causing x % of inhibition)
INERIS	Institut national de l'environnement industriel et des risques
ISO	International Organization for Standardization
K_d	Soil adsorption coefficient
K_{oa}	Octanol/Air partition coefficient
K_{oc}	Octanol/Carbon partition coefficient
K_{ow}	Octanol/Water partition coefficient
K_p	Soil/Water partition coefficient
$LC_{(x)}$	Lethal Concentration (causing x % of effect)
$LD_{(x)}$	Lethal Dose (causing x % of effect)
LO(A)EC	Lowest Observed (Adverse) Effect Concentration
LO(A)EL	Lowest Observed (Adverse) Effect Level
MATC	Maximum Acceptable Toxicant Concentration
MPC	Maximum Permissible Concentration (RIVM)
MSCA	Member State Competent Authorities
M_w	Molecular weight
NABO	Swiss Soil Monitoring Network (Nationale Bodenbeobachtung, Agroscope-NABO)
NC	Negligible Concentration (RIVM)
NCBI	National Center for Biotechnology Information
NEPC	National Environment Protection Council (Australia)
NO(A)EC	No Observed (Adverse) Effect Concentration
NO(A)EL	No Observed (Adverse) Effect Level
NOER	No Observed Effect Rate
OECD	Organization for Economic Co-operation and Development
OM	Organic Matter
ORNL	Oak Ridge National Laboratory
PAH	Polycyclic Aromatic Hydrocarbons
PCB	Polychlorinated Biphenyls
PEC	Predicted Environmental Concentration
pK_a	Dissociation constant
PNEC	Predicted No Effect Concentration (ECHA)
POP	Persistent Organic Pollutant
PPDB	Pesticide Properties Database
PPP	Plant Protection Product
QAARs	Quantitative Activity-Activity Relationships

QSARs	Quantitative Structure-Activity Relationships
RAC	Regulatory Acceptable Concentration
REACH	Registration, Evaluation, Authorization and Restriction of Chemicals
RHO_{soil}	Bulk density of wet soil
RIVM	National Institute for Public Health and the Environment (The Netherlands)
RMS	Rapporteur Member State
SAEFL	Swiss Agency for the Environment, Forests and Landscape
SGV	Soil guideline value (Switzerland)
SQG	Soil Quality Guideline (CCME)
SRC	Serious Risk Concentration (RIVM)
SSD	Species Sensitivity Distribution
TEC	Threshold Effect Concentration (CCME)
TER	Toxicity exposure ratio
TRV	Toxicity Reference Value
UBA	German Environmental Agency (Umweltbundesamt)
US DoE	United States Department of Energy
US EPA	United States Environmental Protection Agency
VROM	Ministry of Housing, Spatial Planning and the Environment (The Netherlands)

7 Glossary

Adverse effect	Change in the morphology, physiology, growth, development, reproductive output or life span of an organism, system, or (sub)population that results in an impairment of functional capacity, an impairment of the capacity to compensate for additional stress, or an increase in susceptibility to other influences.
Assessment	Evaluation or appraisal of an analysis of facts and the inference of possible consequences concerning a particular object or process.
Assessment factor	Numerical adjustment used to extrapolate from experimentally determined (dose-response) relationships to estimate the agent exposure below which an adverse effect is not likely to occur.
Bioaccumulation	Net result of the uptake, distribution and elimination of a substance in an organism due to exposure through all routes, i.e., air, water, soil and food.
Bioaccumulation factor (BAF)	Concentration of a substance that is taken up by a consumer, due to exposure to all routes, i.e., air, water, soil and food.
Bioconcentration	(when referred to soil) Net result of the uptake, distribution and elimination of a substance in an organism due to soil pore water exposure.
Bioconcentration factor (BCF)	(when referred to soil) Concentration of a substance that is taken up by a consumer, due to soil pore water exposure.
Biomagnification	Accumulation and transfer of chemicals via the food chain, resulting in an increase of the internal concentration in organisms at higher levels in the trophic chain.
Clean-up value	Generic limit concentration of a substance in the soil that, if exceeded, is expected to cause an unacceptable risk to potentially exposed organisms. It commonly triggers the need for remediation activities.
Dose–response assessment	Analysis of the relationship between the total amount of an agent administered to, taken up by, or absorbed by an organism, system, or (sub)population and the changes developed in that organism, system, or (sub)population in reaction to that agent, and inferences derived from such an analysis with respect to the entire population.
Effect	Change in the state or dynamics of an organism, system, or (sub)population caused by the exposure to an agent.
Effect assessment	Combination of analysis and inference of possible consequences of the exposure to a particular agent based on knowledge of the dose-effect relationship associated with that agent in a specific target organism, system, or (sub)population.
Endpoint	Measurable (ecological) characteristic that is related to the valued characteristic chosen as an assessment point.

Expert judgement	Opinion of a person with extensive expertise in a particular subject.
Exposure	Concentration or amount of a particular agent that reaches a target organism, system, or (sub)population in a specific frequency for a defined duration.
Hazard	Inherent property of an agent or situation having the potential to cause adverse effects when an organism, system, or (sub)population is exposed to that agent.
Hazard assessment	A process designed to determine the possible adverse effects of an agent or situation to which an organism, system, or (sub)population could be exposed. The process includes hazard identification and hazard characterization. The process focuses on the hazard, in contrast to risk assessment, where exposure assessment is a distinct additional step.
In-soil organisms	Species that dwell primarily in the soil and soil litter (including soil invertebrates and microorganisms) (EFSA 2017).
Intermediate risk	Situation, defined by a specific contaminant concentration, where potentially adverse effects to exposed organisms cannot be excluded. This concentration commonly triggers further investigations and is often defined as trigger or screening value.
Long-term exposure	Duration of exposure to a contaminant that usually last from several weeks to years. Common long-term effects influence reproductive output, growth or other endpoints observable during the life cycle of the test organism. Often referred to as chronic exposure. Although a clear definition varies from study to study, these tests usually produce NOEC, LOEC or EC/ICx values.
Negligible risk	Situation, defined by a specific contaminant concentration, where adverse effects to exposed organisms cannot be excluded on the long- term. This concentration commonly triggers no or limited action and is often defined as target value.
Prospective risk assessment	Risk assessment approach aiming at predicting the impact that a compound might cause, following a planned activity or release. It is applied in the context of authorization and registration of chemical substances. In this approach, effect concentrations are compared to predicted environmental concentrations.
Retrospective risk assessment	Risk assessment approach aiming at assessing the quality of a given site. It addresses effects that might have already occurred at a site following an exposure to a given substance after its release. In this approach, effect concentrations are compared to measured environmental concentrations.
Risk	The probability of an adverse effect in an organism, system, or (sub)population caused under specified circumstances by exposure to an agent.
Risk assessment	A process intended to calculate or estimate the risk to a given target organism, system, or (sub)population, including the identification of attendant uncertainties, following exposure to a particular agent, taking into account the inherent characteristics of the

	agent of concern as well as the characteristics of the specific target system. The risk assessment process includes four steps: hazard identification, hazard characterization (related term: Dose– response assessment), exposure assessment, and risk characterization. It is the first component in a risk analysis process.
Risk level	Intensity of the risk expected to occur, due to a specific concentration of a contaminant in the medium. Risk levels can be commonly classified as negligible (1), intermediate (2), and unacceptable (3).
Screening value	In this report, this is intended as a generic limit concentration of a substance in the soil which, if exceeded, is expected to cause an intermediate risk to potentially exposed organisms and which generally triggers further investigations.
Short-term exposure/effect	Duration of exposure to a contaminant that usually rapidly induce an effect. A common short-term effect is mortality. Often referred to as an acute exposure. Although a clear definition varies from study to study, these tests usually produce EC50/LC50 values.
Soil Guideline Values	Soil protection values that must be derived for PPPs in the context of the Swiss AP-PPP.
Soil protection value	Generic term describing any limit concentration of a substance in the soil, which is expected to cause no or little harm to potentially exposed organisms. Usually expressed in mg active substance/kg soil dry weight (= mg/kg a.s. d.w.).
Soil quality	The capacity of a soil to function within ecosystem and land-use boundaries to sustain biological productivity, maintain environmental quality, and promote plant and animal health.
Target value	Generic limit concentration of a substance in the soil which, if exceeded, is expected to cause a negligible risk to potentially exposed organisms. Below this value, no adverse effects on the long-term are expected to occur.
Toxicity	Inherent property of an agent to cause an adverse biological effect.
Trigger value	See screening value.
Unacceptable risk	Situation, defined by a specific contaminant concentration, where effects to exposed organisms are high. This concentration commonly triggers the need for actions, such as remediation activities and is often defined as clean-up value.
Uncertainty	Imperfect knowledge concerning the present or future state of an organism, system, or (sub)population under consideration.
Validation	Process by which the reliability and relevance of a particular approach, method, process or assessment is established for a defined purpose. Different parties define “Reliability” as establishing the reproducibility of the outcome of the approach, method, process, or assessment over time. “Relevance” is defined as establishing the meaningfulness and usefulness of the approach, method, process, or assessment for the defined purpose.

8 Indices

8.1 List of Figures

8.2 List of Tables

Appendix 1 Additional information about the reviewed methodologies

Disclaimer:

The last update of the information provided in this Appendix was in June 2021

1 Introduction

This appendix provides a summary of how soil protection values have been derived for PPPs by the methodologies reviewed in the main report[22]. In general, the countries classify the derived substances with the broader term “pesticide”, rather than “PPPs”, or use no classification at all. For this reason, for this appendix, a substance was considered as PPP if it met the two following criteria:

The substance was present in at least one of the following three databases for pesticides: European pesticide database[23] (EU PDB), Pesticide Properties database[24] (PPDB), and Tomlin (2009).

The current or past use of the substance for crop protection was identified. E.g. pesticides used only as biocides (e.g., wood/paint preservatives, insect repellents for human use only, etc.) were not retained.

In addition, metabolites were also considered if the parent material was a PPP (e.g., DDD/DDE = metabolite of DDT).

The same criteria used for the review report (chapter 3.2, Box 2) were used, i.e., only generic screening values (i.e., values with non-remediation purposes) and considering effects on the environment (i.e., not on human health) are included. A list of the 103 PPPs (including sums and metabolites), for which soil protection values are available is provided in Table A1.1.

In case the methodology is not already described in the report, a short description is provided in this appendix. When possible, additional relevant information about which kind of studies were used by each methodology is mentioned (e.g., if studies using formulations were used for the derivation of soil protection values).

Most methodologies reviewed in the report have derived soil protection values for contaminants that can frequently be found in contaminated soils. These include most commonly metals and organic contaminants, such as industrial chemicals (e.g., solvents, flame retardants, intermediates or derivatives from manufacturing processes, etc.) and some pesticides. Most countries do not have a specific term for them and the guidances use simply general terms like “substances/contaminants at contaminated sites” (e.g. CCME, 2006; Finnish Ministry of the Environment, 2007; Ministerio de la Presidencia, 2005; NEPC, 2013). In the USA, the substances for which soil protection values are derived, are contaminants that are “frequently of ecological concern at hazardous waste sites”, which are commonly known as Contaminants of Potential (Ecological) Concern (COP(E)C) (ORNL, 1997a, 1997b).

[22] Main report in this Appendix 1 refers to “Methodology proposal for the derivation of Soil Guidance Values for Plant Protection Product residues (Part 1)”
[23] https://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/active-substances/?event=search.as, status at 12.2020
[24] http://sitem.herts.ac.uk/aeru/ppdb/en/atoz.htm, status at 12.2020

Most PPPs considered by the reviewed methodologies, are not authorized under the European Regulation[25] for several years and are well-known soil contaminants (e.g., Persistent Organic Pollutants[26]) (see Table A1.1). Most of these PPPs were probably also not authorized at the point in time when their respective soil protection values were derived. It seems thus clear, that at the time of their derivation, soil protection values were produced mostly for PPPs which were considered more as “recognized soil contaminants” (i.e., old and banned PPPs known to be toxic but still present in soil), rather than for PPPs that were currently applied to agricultural fields. RIVM is the only exception, which has values for several currently authorized PPP.

[25] Regulation (EC) No 1107/2009, status: February, 2021
[26] http://www.pops.int/TheConvention/ThePOPs/tabid/673/Default.aspx

Table A1.1: List of PPPs (including sums and metabolites of PPPs), for which soil protection values have been retrieved. Information about the authorization status in Europe, according to Reg. (EC) No 1107/2009 (European Parliament and Council of the European Union, 2009) and Switzerland (CH) according to OPPP = Swiss Ordinance on PPPs (Swiss Federal Council, 2021) and to OFAG = PPP index [27] has been added (For metabolites and sums the symbol "-" signalizes that the authorization status is not applicable). Also, information whether the PPP is planned to be monitored in Swiss agricultural soils by NABO [28]; and countries that derived soil protection values for the respective PPPs is included in the table. For countries having more than one soil protection value, the name of the value is added in brackets: The Netherlands (BC = background concentrations, NC = negligible concentrations), USA (ER-L = effects range-low, Eco-SSL = ecological screening level). Bold PPPs are Persistent Organic Pollutants (Status: June 2021).

Substance	**Authorization status in Europe (in brackets if status differs in CH)**	**Planned for NABO monitoring**	**Countries that derived soil protection values**
1,2-dibromoethane	not approved	no	Sweden
1,2-dichloropropane	not approved	no	Ontario, Spain, USA (ER-L)
1,3-dichloropropene	pending (not approved)	no	Spain
2,4-D	approved	no	The Netherlands (NC), Spain
2,4,5-T (2,4,5-trichlorophenoxyacetic acid)	not approved	no	The Netherlands (NC)
2,4,5-trichlorophenol	not approved	no	Finland, Latvia, The Netherlands (NC), Ontario, Spain, USA (ER-L)
2,6-dichloro-4-nitroaniline (dichloran)	not approved	no	The Netherlands (NC)
4-chloro-3-methylphenols	not approved	yes	The Netherlands (BC)
4,6-dinitro-o-cresol (DNOC)	not approved	no	The Netherlands (target value[a])
Aldicarb	not approved	no	The Netherlands (NC)
Anilazine	not approved	no	The Netherlands (NC)
Atrazine	not approved	yes	Finland, Latvia, The Netherlands (BC)
Azinphos ethyl	not approved	no	The Netherlands (NC)
Azinphos-methyl	not approved	no	The Netherlands (BC)
Benomyl	not approved	no	The Netherlands (NC)
Bifenthrin	not approved (approved by OFAG until 07.22)	no	The Netherlands (NC)
Biphenyl	not approved	no	USA (ORNL)
Captafol	not approved	no	The Netherlands (NC)
Captan	approved	no	The Netherlands (NC)
Carbaryl	not approved	yes	Latvia, The Netherlands (BC)
Carbofuran	not approved	no	Latvia, The Netherlands (BC)

[27] https://www.psm.admin.ch/de/produkte" \o "https://www.psm.admin.ch/de/produkte, status as of February 2021.
[28] The PPP planned to be monitored by NABO are listed in table 6 of the attachment 6.1 of the Annual Report of soil monitoring for the Measure 6.3.3.7 of the Action plan for PPP (Godbersen et al., 2019).

Chlordane (sum)	not approved	no	The Netherlands (BC), Ontario, Spain, USA (ER-L)
Chlorfenvinfos	not approved	no	The Netherlands (NC)
Chloridazon	not approved (approved by OFAG)	no	The Netherlands (NC)
Chlorpyrifos	not approved (approved by OPPP, and by OFAG until 05.2021)	yes	The Netherlands (NC)
Chlordecone	not approved	no	USA (ER-L)
Chlorothalonil	not approved (approved by OPPP)	no	The Netherlands (NC)
Cyanazine	not approved	no	The Netherlands (NC)
Cypermethrin	approved	no	The Netherlands (NC)
Daminozide	approved	no	The Netherlands (NC)
DDT	not approved	no	Australia, The Netherlands (BC, NC), Ontario, USA (Eco-SSL and ER-L)
DDD (DDT metabolite)	-	yes	Latvia, The Netherlands (BC, NC), Ontario
DDE (DDT metabolite)	-	no	Latvia, The Netherlands (BC, NC), Ontario, Spain
DDT/DDD/DDE sum	not approved	DDD only	Canada, Czech Republic, Finland, Latvia, The Netherlands (BC), Sweden
Desmetryn	not approved	no	The Netherlands (NC)
Diazinon	not approved	no	The Netherlands (NC)
Dinoseb	not approved	no	The Netherlands (NC)
Dinoterb	not approved	no	The Netherlands (NC)
Disulfoton	not approved	no	The Netherlands (NC)
Diuron	not approved (approved)	yes	The Netherlands (NC), Sweden
Drins sum	not approved	no	Latvia, The Netherlands (BC)
Aldrin	not approved	no	The Netherlands (BC), Ontario, Spain, Sweden (together with dieldrin), USA (ER-L)
Dieldrin	not approved	no	Finland, The Netherlands (BC), Ontario, Spain, Sweden (together with aldrin), USA (Eco-SSL and ER-L)
Endrin	not approved	no	The Netherlands (BC), Ontario, Spain, USA (ER-L)
Isodrin	not approved	no	The Netherlands (BC)
Endosulfan	not approved	metabolite endosulfan sulfat only	Finland, The Netherlands (NC), Ontario, Spain, USA (ER-L)
α-endosulfan	not approved	metabolite endosulfan sulfat only	The Netherlands (BC)

Ethoprophos	not approved	no	The Netherlands (NC)
Fenitrothion	not approved	no	The Netherlands (NC)
Fenthion	not approved	no	The Netherlands (NC)
Fentinhydroxide[b]	not approved	no	The Netherlands (BC)
Flutolanil	approved	yes	The Netherlands (NC)
Folpet	approved	no	The Netherlands (NC)
Heptachlor	not approved	no	Finland, The Netherlands (BC), Ontario, USA (ER-L)
Heptachlor Epoxide (heptachlor metabolite)	-	no	The Netherlands (BC)
Heptenophos	not approved	no	The Netherlands (NC)
Hexachlorobenzene	not approved	no	Ontario, Spain, USA (ER-L)
Hexachlorocyclohexane (HCH) sum	not approved	no	Czech Republic, Latvia, The Netherlands (BC)
α-HCH	not approved	no	The Netherlands (BC), Spain
β-HCH	not approved	no	The Netherlands (BC), Spain
γ-HCH (lindane)	not approved	no	Finland, The Netherlands (BC), Ontario, Spain, USA (ER-L)
Isoproturon	not approved	no	The Netherlands (NC)
Linuron	not approved	yes	The Netherlands (NC)
Malathion	approved (not approved)	no	The Netherlands (NC)
Maneb	not approved	no	The Netherlands (NC)
MCPA	approved	no	Latvia, The Netherlands (BC)
Metam-sodium	approved (not approved)	no	The Netherlands (NC)
Metamitron	approved	no	The Netherlands (NC)
Metazachlor	approved	no	The Netherlands (NC)
Methabenzthiazuron	not approved	no	The Netherlands (NC)
Methomyl	not approved (approved by OFAG until 07.22)	no	The Netherlands (NC)
Methoxychlor	not approved	no	Ontario, USA (ER-L)
Metobromuron	approved	no	The Netherlands (NC)
Metolachlor	not approved (S-metholachlor approved)	yes (S-metolachlor)	The Netherlands (NC)
Mevinphos	not approved	no	The Netherlands (NC)
Myclobutanil	approved	yes	The Netherlands (NC)
Oxamyl	approved (not approved)	no	The Netherlands (NC)
Oxydemeton-methyl	not approved	no	The Netherlands (NC)
Parathion-ethyl	not approved	no	The Netherlands (NC)
Parathion-methyl	not approved	no	The Netherlands (NC)
Penconazole	approved	yes	The Netherlands (NC)

Pentachloroaniline (quintozene metabolite)	-	no	Sweden (together with quintozene), USA (ER-L)
Pentachlorophenol	not approved	no	Canada, Finland, The Netherlands (BC), Ontario, Spain, USA (ER-L)
Permethrin	not approved	no	The Netherlands (NC)
Phoxim	not approved	no	The Netherlands (NC)
Pirimicarb	approved	yes	The Netherlands (NC)
Propachlor	not approved	no	The Netherlands (NC)
Propoxur	not approved	no	The Netherlands (NC)
Pyrazophos	not approved	no	The Netherlands (NC)
Quintozene	not approved	no	Sweden (together with pentachloroaniline)
SDS-3701 (chlorotalonil metabolite)	-	no	The Netherlands (NC)
Simazine	not approved	no	The Netherlands (NC)
Tebuconazole	approved	yes	The Netherlands (NC)
Telodrin	not Approved	no	The Netherlands (BC)
Thiabendazole	approved	yes	The Netherlands (NC)
Thiocyanates sum	not approved	no	The Netherlands (BC)
Thiram	not approved (approved)	no	The Netherlands (NC)
Trichlorfon	not approved	no	The Netherlands (NC)
Tri-allate	approved (not approved)	yes	The Netherlands (NC)
Trifluralin	not approved	no	The Netherlands (NC)
Zineb	not approved	no	The Netherlands (NC)
Non-chlorinated pesticides sum	-	-	The Netherlands (BC)
Organo-nitrogen and organophosphorus pesticides sum	-	-	The Netherlands (BC)

[a] Target value is the EQS-equivalent (policy adopted) to the Negligible Concentration (RIVM 2007)
[b] Sum of triphenyltin acetate, triphenyltin chloride and fentin hydroxide: only the latter of the three is a PPP

2 RIVM

The RIVM database[29] provides several types of soil protection values. Among them, the ones that are relevant for this review are the Negligible Concentrations (NC), which are based on the Maximum Permissible Concentrations (MPC, divided by 100). In total, the RIVM database currently lists soil protection values for 94[30] PPP (see Table A1.1).

[29] https://rvszoeksysteem.rivm.nl/. Soil protection values are named in the database as follows: Negligible Concentrations = “Grond verwaarloosbaar risiconiveau (Grond VR)”, Background Concentrations = “Achtergrondwaarde”.
[30] The exact number of PPPs is slightly lower because some categories, such as sums/groups of substances and metabolites, are counted as one.

After 2000, many of the scientifically derived NC that were available (especially for metals) in the Netherlands, were not practical because they were too low and were therefore replaced by background values (Swartjes et al., 2012). This has also been the case for 29 persistent PPPs (Lamé et al., 2004).

For most of the other PPPs available in the RIVM database (i.e., for which the NC is still available and has not been replaced by the background value), the information about the derivation process of MPC and NC is provided. Reference is made, for the majority of those PPPs, at the RIVM report: "Maximum Permissible Concentrations and Negligible Concentrations for pesticides" (RIVM, 1997). Few other PPPs are described in other two reports: "Towards integrated environmental quality objectives for several compounds with a potential for secondary poisoning" (RIVM, 1994) and "Maximum Permissible Concentrations and Negligible Concentrations for aniline derivatives" (RIVM, 1998). These three reports are based on an older RIVM methodology than the current one described in the main report, i.e., RIVM (2007). This former methodology was in principle similar to RIVM (2007). However, some differences from the current guidance could be observed, e.g., minimum data requirements for performing a SSD with only four data points (instead of the current 10/15), and slight changes in the numeric values of the AF (the AF from the EPA-modified method were applied instead of the current ones (RIVM, 1997, p. 55)).

In the report of RIVM (1997), pesticides were considered a particular type of substance with two main characteristics: they usually have a specific mode of action and they are addressed to cause an effect on target organisms. Thus, it is mentioned that important differences in species sensitivity can exist for pesticides, depending on (their group of) mode of action. It is also mentioned that pesticides can strongly affect not only target species, but also some groups of species that, often have similar characteristics to the targets (e.g., non-target soil dwelling insects/arthropods may be as sensitive to insecticides as the target insects). When there are reasons to expect that the data available is representative of the most sensitive species, the extrapolation method may be adjusted. For instance, if the deterministic method was used for an herbicide, and only acute data for plants, but not for other species was available, the AF could still be reduced.

For pesticides, the available toxicity data for soil organisms was always scarce and all MPC (and thus NC) derived by RIVM (1997) were obtained by either the deterministic or the EqP method (when sufficient data for soil was not available). In general, the paucity of data available for the derivation of soil MPC often led to the derivation of low and conservative values. By dividing the MPC by 100 to obtain the NC, this observation was even more evident, leading often to values below the analytical detection limits (Crommentuijn et al., 2000).

Additional information about the studies used by RIVM for the derivation of soil protection values:

- The ecotoxicological studies on plants used for the derivation of the MPC and NC for the available PPPs were performed as soil treatment (i.e., no foliar application)[31].
- Only studies performed in agreement with the natural route of exposure are considered (RIVM, 1997).
- The use of formulation as the test substance for bioassays was accepted and equally considered as the data with the active substance, if containing at least 80 % active substance (RIVM, 1997).

[31] Due to the large number of PPPs derived by RIVM, only plant studies from herbicides were reviewed. However, it is not expected that a different approach is carried out for other types of PPPs.

3 CCME

The CCME database[32] provides two Soil Quality Guidelines (SQG) for PPPs (DDT and metabolites, and pentachlorophenol[33]). The methodology used is the Protocol from 1996 for the derivation of environmental and human health soil quality guidelines (CCME, 1996), which is a former version of the CCME methodology of 2006 (CCME, 2006), reviewed in the main report. The main difference is that the former methodology does not include consideration of two soil texture classes. Details on the derivation procedure for DDT could not be found, but some information on the studies and the exposure pathways that were considered for the two substances can be found in their respective factsheets (CCME, 1999, 1997). The final SQG for DDT was based on the value protective of the environment, considering soil contact, microorganisms, and consumers (secondary poisoning), while the final SQG for pentachlorophenol was based on the value protective of human health.
The studies on plants used to derive the SQG for DDT and for pentachlorophenol were all performed with soil application, testing both the technical/formulation and purified/active substance.

4 US EPA

The US EPA methodology (2005, also described in the main report) has been used to derive Eco-SSL for three PPPs (DDT and metabolites, dieldrin, and pentachlorophenol). The values can be found in their database[34] and the detailed derivation process is illustrated in the three respective (US EPA, 2007a, 2007b, 2007c). For DDT and dieldrin, the derivation of Eco-SSL for plants and for soil invertebrates was not possible, because most studies were invalidated at the quality check step. For instance, for DDT, of 195 studies initially available for plants, only one study passed all the quality criteria. As a result, for both insecticides, Eco-SSL could only be derived for birds and mammals. The Eco-SSL for pentachlorophenol was the geometric mean of the accepted studies, having the highest bioavailability score, for both plants and soil invertebrates.

Additional information about the studies used by the US EPA for the derivation of soil protection values:

- If concentrations in the soil were not correctly reported, the study was invalidated. Therefore, tests where the substance was applied via spray application (e.g., foliar application in plants tests) and the corresponding concentrations in the soil were not reported, were not accepted (US EPA, 2007a, 2007b, 2007c). Studies on plants[35] used to derive Eco-SSL were performed with soil application (US EPA, 2007a, 2007c).
- Studies performed with test medium other than artificial or natural soil were not accepted (US EPA, 2005).
- The use of formulation as the test substance for bioassays was accepted (US EPA, 2005).

5 NEPC

The NEPC methodology (2013, also described in the main report) has been used to derive the Ecological Investigation Level (EIL) for the insecticide DDT. The detailed description of the derivation process is illustrated in the Schedule B5c of the National Environment Protection (Assessment of Site Contamination) Measure of April 2011 (NEPC, 2011). The value for DDT was derived through the SSD method, using data for two plant species (germination and growth, according to

[32] http://st-ts.ccme.ca/en/index.html
[33] Although the major use of pentachlorophenol is not agricultural, this substance had a minor use in the past as herbicide for crops (US EPA, 2007c). For this reason, and because several countries have derived a value for it, pentachlorophenol is considered as a PPP in this appendix.
[34] https://www.epa.gov/chemical-research/interim-ecological-soil-screening-level-documents
https://www.epa.gov/chemical-research/interim-ecological-soil-screening-level-documents
[35] One of those studies could not be retrieved

the ISO test guideline no. 11269-2 (ISO 11269-2, 2012), i.e., soil application), earthworms and collembolans (reproduction), six microbial processes and six bird species.

6 Czech Republic

The Czech law includes soil protection values for two PPPs (sum of DDT/DDD/DDE and sum of α-/β-/γ- HCH) in the Decree Ministry of Environment of Czech Republic No. 153/2016. Col. (Czech Decree 152, 2016). These are called prevention limits and are used as trigger for site-specific risk assessments. Prevention limits are derived from the background concentrations, which are based on the measure of 560 samples of Czech agricultural soils (Vácha et al., 2014). Ecotoxicological data from soil organisms was not taken into account.

7 Spain

The Spanish legislation includes three separate generic soil protection values (generic reference levels, NGR) for the following three groups of organisms: soil organisms (invertebrates, plants and microorganisms), aquatic organisms and terrestrial vertebrates. There is no distinction between land uses, but regional authorities may decide which site-specific considerations should be taken to protect organisms in that area. The values for soil organisms and terrestrial vertebrates are derived according to the EC TGD (2003) (Tarazona et al., 2005). The NGR derived for the protection of the ecosystem are provided in the Royal Decree 9/2005, BOE-A-2005-895 (Ministerio de la Presidencia, 2005) and include nine PPPs (aldrin, chlordane, DDE, dieldrin, endosulfan, endrin, 2,4-D, lindane, and pentachlorophenol). In parallel to the development of soil protection values, the Spanish legislation includes as well direct toxicity testing of soil samples and leachates taken from the site of interest, by means of acute bioassays (Tarazona et al., 2005). Thus, Spain has two ways to investigate whether a site is contaminated: 1) if soil protection values are exceeded and 2) if soil samples and/or leachates pose acute adverse effects.

8 Latvia

The Latvian law includes, in the Regulation No 804 “Regulation of the Quality Normatives for Soil and Subsoil”[36], target values for seven PPPs (sum of DDT/DDE/DDD, sum of drins = aldrin + dieldrin + endrin, sum of HCHs, atrazine, carbaryl, carbofuran and MCPA). The guidance for deriving Latvian target values has not been found. However, those values are the same than the Dutch target values[37], that were provided in the Dutch Circular on target and intervention values (VROM, 2000).

9 Finland

The Finnish law includes a generic type of soil protection value, called threshold value. This value is derived like a PNEC, according to the EC TGD (2003) or RIVM (2007) methodologies, and integrated some socio-economic considerations (Carlon, 2007). The values, are provided in the Government Decree on the Assessment of Soil Contamination and Remediation Needs 214/2007 (Ministry of the Environment, 2007). Threshold values are available for six PPPs (atrazine, sum of DDT/DDD/DDE, dieldrin, endosulfan, lindane, heptachlor, and pentachlorophenol). No dossiers describing in detail how these values were derived, were found.

[36] https://likumi.lv/ta/en/en/id/120072
[37] Dutch Target Values are the EQS-equivalent (i.e., policy adopted) to the Dutch Negligible Concentrations

10 Sweden

Sweden proposes Generic Guideline Values, not legally binding. A separate value is derived for the protection of each of the following categories: soil environment, human health, ground- and surface water and the final soil protection value is the lowest between them (SEPA, 2009). For the protection of soil environment, organisms considered are in-soil organisms, plants and terrestrial vertebrates (SEPA, 2016a). Swedish values for soil are largely based on data compilations from other authorities, especially RIVM, but also CCME, US EPA, ORNL, and (re)-authorization dossiers for PPPs. The Swedish approach follows the RIVM methodology but slightly adapted in order to consider two land use types: sensitive land use is defined as "where land quality does not limit the choice of land use […]38. Most soil ecosystems as well as groundwater and surface water are protected". Less sensitive land uses is defined as: "where land quality limits the choice of land use to e.g., offices, industries or roads […]38 The soil quality provides conditions for soil functions that are important in less sensitive land use, for example, vegetation can be established and animals temporarily stay in the area. Groundwater at a distance of about 200 meters and surface water are protected" (SEPA 2009, p. 22). If soil protection values were taken from other international authorities (e.g., RIVM), reevaluations of the data and/or the derivation process were performed by the Swedish authorities.

Sweden has derived general guideline values for the protection of all compartments for five PPPs (1,2 dibromoethane, aldrin-dieldrin, sum of DDT/DDD/DDE, diuron, and quintozene-pentachloroaniline). The derivation process of values for the soil environment only is described in individual dossiers available on the website[39] (SEPA, 2016b, 2016c, 2016d, 2016e, in Swedish).

For the Swedish approach, the same criteria about acceptance of studies for the derivation of soil protection values were applied as the ones described in the chapter for RIVM above.

11 ORNL

The Oak Ridge National Laboratory (ORNL) in the USA, has derived several screening values (Effects Range Low, ER-L) for organic contaminants, each value considering one specific group of organisms, i.e., earthworms, microorganisms, plants, wildlife. For the first three, the soil protection value was in principle derived by ranking the effect data and selecting subsequently the 10th percentile of the distribution (ORNL, 1997a, 1997b). For wildlife, the method was inspired by the US EPA methodology for deriving human toxicity values from animal data (ORNL, 1996).

For earthworms, four values for three PPPs (1,2-dichloropropane, 2,4,5-trichlorophenol, pentachlorophenol), and for one metabolite (penthachloroaniline, metabolite of quintozene) are available (ORNL, 1997a), while for microorganisms, two values for PPPs (hexachlorobenzene and pentachlorophenol) are available (ORNL, 1997a). For plants, there are values for three PPPs (2,4,5-trichlorophenol, biphenyl, pentachlorophenol) (ORNL, 1997b). For wildlife, ER-L were separately derived for ten PPPs (aldrin, chlordane, chlordecone, DDT, dieldrin, endosulfan, endrin, heptachlor, lindane, pentachlorophenol) (ORNL, 1996).

Additional information about the studies used by ORNL for the derivation of soil protection values:

- For plants, the studies used for the derivation of values for PPPs were performed through soil application. However, the methodology can also accept studies that used nutrient/mineral solution as test medium (i.e., not soil) (ORNL, 1997b).
- Tests with filter papers are not accepted (ORNL, 1997a).
- All checked studies used to derive soil protection values for PPPs were performed with the active substance.

[38] Additional considerations with regard to the protection for human health are also provided.
[39] https://www.naturvardsverket.se/Stod-i-miljoarbetet/Vagledningar/Fororenade-omraden/Riktvarden-for-fororenad-mark/Berakningsverktyg-och-nya-riktvarden/

12 Ontario

The Regulation of the Canadian Province of Ontario 153/04 (2004)40 includes generic standards for 13 PPPs. Those standards consider four different receptors/exposure pathways (1. human health, 2. terrestrial ecological receptors, i.e., plants, soil invertebrates, birds and mammals, 3. leaching, and 4. vapour migration) and scenarios, defined by land use, potability of groundwater, soil depth and soil texture. The lowest from all values describing the receptor/exposure pathways, which is the most relevant to the considered scenario is adopted as final soil standard. The methodology is described in detail in the Rationale for the *development of generic soil and groundwater standards for use at contaminated sites in Ontario* (MOE, 2007). The derivation of values for plants and soil invertebrates is based on the CCME methodology (1996) or if not possible, existing values from CCME and RIVM methodologies were adopted. For birds and mammals, the general CCME methodology is followed. The Rationale describes how the two separate types of values, one for soil invertebrates and plants and one for birds and mammals, are derived for the 14 PPPs (aldrin, chlordane, DDD, DDE, DDT, dieldrin, endosulfan, endrin, heptachlor, hexachlorobenzene, lindane, methoxychlor, and pentachlorophenol).

Additional information about the studies used by Ontario for the derivation of soil protection values:

- Studies performed with filter paper are not accepted (MOE, 2007).
- All checked studies[41] on plants that were used to derive the existing standards were laboratory
  assays on seedling emergence, i.e., soil application, except for one field study with spray application of a formulation (Perfect et al., 1979).
- Studies using formulations were used equally to studies with active substance (MOE, 2007).

[40] https://www.ontario.ca/laws/regulation/r04153
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VROM, 2000. Circular on target values and intervention values for soil remediation. Netherlands Gov. Gaz. 2000, 1–12.

Appendix 2 Case studies

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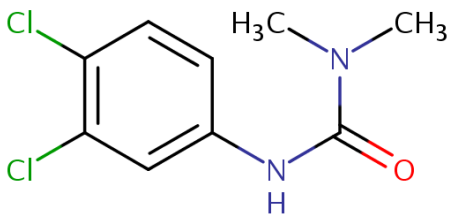
1 Case study for the herbicide diuron

1.1 General data

Diuron is a systemic herbicide and is absorbed via the roots into the plant. It is strongly inhibiting the photosynthesis, by blocking the electron flow in photosystem II (Metz et al., 1986). Among the properties of concern according to ECHA, diuron is under assessment as endocrine disrupting substance[42].

Table A2.1: General information for diuron

IUPAC Name	N'-(3,4-Dichlorophenyl)-N,N-dimethylurea	
CAS registry number	330-54-1	
EU Number	206-354-4	
Molecular formula	$C_9H_{10}Cl_2N_2O$	
Code SMILES	CN(C)C(=O)NC1=CC(Cl)=C(Cl)C=C1	
Pesticide Category	Herbicide, phenylurea	
Molecular weight	233.09 g/mol	
Log K_{ow}	2.78 (Wildi et al., 2019)	
K_{oc}	339 (log K_{oc} = 2.53) (Wildi et al., 2019)	
Water solubility	37.4 mg/L (25°C); 35.6 mg/L (35°C) (RAR 2018, Vol.3 B2 p. 5)	
Henry's law constant	1.97e-11 atm m^3/mol (20°C) (2e-06 Pa m^3/mol in RAR 2018 Vol. 3 B2 p.4) K_H dimentionless[43] = 8.19e-10	
$DT_{50,soil}$ ($t_{1/2s}$ in eq. 7)	4-8 months (average: 0.5 years) (Tomlin, 2009)	
EU Classification	Acute Tox.4 – H302; Carc. Cat. 2 – H351; Aquatic Chronic 1 – H410; STOT RE 2 – H373; Aquatic Acute 1 – H400[44] (EU Pesticides database. Status: July 2020)	

1.2 Ecotoxicological data

Ecotoxicological values available for diuron are presented in Table A2.2. The ecotoxicological data was collected from the Renewal Assessment Report for the reauthorization of Diuron as a PPP (EC RAR, 2018).

Due to the large amount of data reported in the EC RAR (EC RAR, 2018), only the most relevant endpoints and toxicity parameters for each one of the methodologies were listed in Table A2.2. The most relevant endpoints were selected according to the Rapporteur Member State (RMS) recommendation (EC RAR 2018 Vol.3 B9 p. 134). The most relevant toxicity parameters were

[42] ECHA Endocrine Disruptor (ED) list: https://echa.europa.eu/ed-assessment?p_p_id=disslists_WAR_disslistsportlet&p_p_lifecycle=1&p_p_state=normal&p_p_mode=view&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_disslists_WAR_disslistsportlet_javax.portlet.action=searchDissLists

[43] Henry's law constant dimensionless calculated with EPA On-line Tools for Site Assessment Calculation (https://www3.epa.gov/ceampubl/learn2model/part-two/onsite/henryslaw.html)

[44] H302: Harmful if swallowed; H351: Suspected of causing cancer; H410: Very toxic to aquatic life with long lasting effects; H373: May cause damage to organs through prolonged or repeated exposure; H400: Very toxic to aquatic life

listed according to the preferred value of each methodology (see section 4.1 “General considerations” of the main report[45] for further information), i.e., NOEC for the EC TGD (EC TGD, 2003), EC_{20} and MATC for the US EPA (US EPA, 2005), EC_{25} and LOEC for the CCME (CCME, 2006) and EC_{30} and LOEC for the NEPC (2013). The NOEC, LOEC and EC_x were extracted directly from the EC RAR (2018) and the MATC was calculated for this report.

The studies shown in Table A2.2 were performed either with the active substance, i.e., diuron technical grade with purities ranging from 96.8 % to 98.2 %, or with the representative formulations (trade names: Diuron 80 % SC, Diuron 80 SC, Diuron 800 SC and Karmex 80 WG). The following studies/endpoints from the EC RAR, 2018, Vol. 3 CP B9 have not been considered valid, and thus not shown in the table, due to the following reasons:

- Luna (2013): EC_{10} for collembolan reproduction considered not reliable by the RMS.
- Stojanowitsch (2014): not considered valid since it is unclear if the reported concentrations are expressed as active substance or formulation.
- Gimeno (2013a): Study considered “not acceptable” by the RMS.

[45] Main report in this Appendix 2 refers to “Methodology proposal for the derivation of Soil Guidance Values for Plant Protection Product residues (Part 1)”.

Table A2.2: Soil ecotoxicological data for diuron from EC RAR (2018)*. Values resulting from calculations are rounded to two significant figures. Some unit conversion and/or calculations are specific for certain methodologies. In order to improve the clarity of which data was used for each methodology, the methodology (EC TGD, 2003; NEPC, 2013; RIVM, 2006; US EPA, 2005; RAC-EFSA and CCME, 2006) is specified in parenthesis. Abbreviations: Conc.=concentration, OC=organic carbon, OM=organic matter, CEC=cation exchange capacity, Appl. = application, a.s.=active substance, lb/ac=pounds/acre.*

Species & Taxonomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parameter**	**Appl. rates** (original units for plant studies in lb or g a.s.)	**Conc. mg a.s./kg d.w.**[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	**Corrected values**[47] (RAC-EFSA)	**Normalized conc. mg a.s./kg d.w., 3.4 % OM**[48] (EC TGD, 2003)	**Normalized conc. mg a.s/kg d.w., 10 % OM**[49] (RIVM, 2007)	**Conc. mg a.s./kg d.w.** (CCME, 2006)[50]	**Soil type**	**Source**
Eisenia fetida/andrei (earthworm)	Karmex 80 WG (81.2 % a.s.)	Reproduction	56 days	NOEC	-	10.7	5.35	3.6	10.7	10.7	OECD soil: 10 % sphagnum peat, 20 % kaolin clay, 69 % industrial sand and approx. 1 % $CaCO_3$, pH 6.2-6.3	Stäbler, 2001 cited in EC RAR, 2018, Vol. 3 CP B9, p.103
				LOEC	-	26.7	13	9.1	26.7	26.7		
				MATC	-	17	8.5	5.7	17	17		
Eisenia fetida (earthworm)	Diuron 80 % SC (63.45 % a.s.)	Survival, weight and reproduction	56 days	NOEC, LOEC and MATC	-	> 31.678	> 16	> 10.8	> 31.678	> 31.678	Artificial soil: 10 % sphagnum peat, 20 % kaolinite clay, 70 % industrial	Ansaloni, 2013 cited in EC RAR, 2018, Vol. 3 CP B9, p.104

[46] The final results of the non-target terrestrial plant tests were given originally in lb/acre. To derive a PNEC according to the EC TGD (2003), values were converted to mg/kg d.w. following the recommendations from the ECHA (2017, p. 149): "If no information can be derived from the test, a default soil depth of 10 cm and soil density of 1500 kg/m³ dry soil should be used." No default values in NEPC (2013) were defined. In order to be able to derive the soil protection values according to this methodology, the same default values as for the EC TGD (2003) were applied.

[47] According to SANCO/10329/2002, tests performed with artificial soils, which usually contain higher organic carbon content than many natural soils, should be corrected if the log K_{ow} of the substance is greater than 2. This correction was applied to earthworm, mite and collembolan tests, but not to microorganism transformation tests. Plants are not included in the RAC derivation, therefore, no value was shown in the table.

[48] Normalization according to the EC TGD (2003). Conversion to a standard soil, defined as a soil with an organic matter content of 3.4 % (corresponding to 2 % organic carbon (EC TGD, 2003 p. 43)).

[49] Normalization according to the RIVM (2007). Conversion to a standard soil, defined as a soil with an organic matter content of 10 % (corresponding to 5.88 % organic carbon (RIVM 2007, p. 50).

[50] In order to derive the SQG according to CCME (2006), values were converted from lb/acre to mg/kg d.w. using a bulk soil density for coarse-grained soils of 1.7 g/cm³ (CCME 2006 p. 182). A default value for the depth is not specified in the protocol. In order to make the different methodologies as comparable as possible, the same depth as for the EC TGD (2003) methodology (10 cm) has been assumed for the conversion.

Species & Taxonomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parameter**	**Appl. rates** (original units for plant studies in lb or g a.s.)	**Conc. mg a.s./kg d.w.**[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	**Corrected values**[47] (RAC-EFSA)	**Normalized conc. mg a.s./kg d.w., 3.4 % OM**[48] (EC TGD, 2003)	**Normalized conc. mg a.s/kg d.w., 10 % OM**[49] (RIVM, 2007)	**Conc. mg a.s./kg d.w.** (CCME, 2006)[50]	**Soil type**	**Source**
											quartz sand and 0.14 % $CaCO_3$	
Folsomia candida (collembolan)	Diuron 80 % SC (63.45 % a.s.)	Reproduction	28 days	NOEC	-	76.0	38	52	152	76.0	Artificial soil: 5 % sphagnum peat, 20 % kaolinite clay, 74.93 % quartz sand and 0.07 % $CaCO_3$, pH 6.33-6.83	Luna, 2013 cited in EC RAR, 2018, Vol. 3 CP B9, p.108
				LOEC	-	129.1	65	88	258	129.1		
				EC_{20}	-	49.65	25	34	99	49.65		
Hypoaspis aculeifer (mite)	Diuron 80 % SC (63.45 % a.s.)	Reproduction	14 day	NOEC	-	345	172	235	691	345	Artificial soil: 5 % sphagnum peat, 20 % kaolin clay, 74.93 % quartz sand and 0.07 % $CaCO_3$, pH 6.38-6.43	Ansaloni, 2013 cited in EC RAR, 2018, Vol. 3 CP B9, p.111
				LOEC	-	621	310	423	1243	621		
				MATC		463	231	315	927	463		
micro-organisms	a.s. (98.2 % purity)	Nitrogen transformation (nitrification)	91 days	10 % inhibition	-	10.7	10.7	26	76	10.7	loamy sand, pH 5.3 (KCl), carbon 0.83 % (soil collected at Laacherhod, Germany)	Blumenstock, 1989 cited in EC RAR, 2018, Vol. 3 CA B9, p.120
				25 % inhibition	-	53.3	53.3	128	378	53.3		
				3 % stimulation	-	10.7	10.7	17	51	10.7	loamy silt, pH 4.8 (KCl), carbon 1.23 %, nitrogen 0.17 (soil collected at Höfchen, Germany)	
				29 % inhibition	-	53.3	53.3	87	255	53.3		

Species & Taxonomic group	Substance tested	Test type & Endpoint	Duration	Parameter	Appl. rates (original units for plant studies in lb or g a.s.)	Conc. mg a.s./kg d.w.[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	Corrected values[47] (RAC-EFSA)	Normalized conc. mg a.s./kg d.w., 3.4 % OM[48] (EC TGD, 2003)	Normalized conc. mg a.s/kg d.w., 10 % OM[49] (RIVM, 2007)	Conc. mg a.s./kg d.w. (CCME, 2006)[50]	Soil type	Source
		Carbon transformation (induced soil respiration)	91 days	2 % inhibition	-	10.7	10.7	26	76	10.7	loamy sand, pH 5.3 (KCl), carbon 0.83 % (soil collected at Laacherhod, Germany)	Anderson, 1989 cited in EC RAR, 2018, Vol. 3 CA B9, p.119
				16 % inhibition	-	53.3	53.3	128	378	53.3		
				7 % inhibition	-	10.7	10.7	17	51	10.7	loamy silt, pH 4.8 (KCl), carbon 1.23 %, nitrogen 0.17 (soil collected at Höfchen, Germany)	
				36 % inhibition	-	53.3	53.3	87	255	53.3		
Allium cepa (terrestrial plant)	a.s. (97.3 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.375 lb/ac	0.28	-	0.68	2.0	0.25	sandy loam, pH 6.7, 1.4 % OM, CEC=6.5 meq/100g	Heldreth & McKelvey, 1996 cited in EC RAR, 2018, Vol. 3 CA B9, p.130[51]
				LOEL	0.75 lb/ac	0.56	-	1.4	4.0	0.49		
				MATC	0.53 lb/ac	0.40	-	1.0	2.8	0.35		
				EC_{25}	0.187 lb/ac	0.14	-	0.34	1.0	0.12		
		Seedling emergence (shoot dry weight)	14 days	NOEL	0.0889 lb/ac	0.066	-	0.13	0.39	0.059	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	
				LOEL	0.133 lb/ac	0.099	-	0.20	0.58	0.088		
				MATC	0.109 lb/ac	0.081	-	0.16	0.48	0.072		
				EC_{25}	0.0859 lb/ac	0.064	-	0.13	0.38	0.057		
	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (biomass)	21 days	NOER	17.52 g/ha	0.012	-	0.024	0.070	0.010	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay),	Gimeno, 2013b cited in EC RAR,
				LOER	36.72 g/ha	0.024	-	0.050	0.15	0.022		
				MATC	25.36 g/ha	0.017	-	0.035	0.10	0.015		

[51] A study with non-target terrestrial plants from McKelvey & Kuratle (1992) was reported in the EC RAR (2018, Vol. 3 B9 P.126). Due to the use of standard greenhouse fumigants with some of the species tested that could influence the results, US EPA requested a re-test for those species. A new study from Heldreth & McKelvey (1996) was provided with the re-test. The Rapporteur Member State (RMS) concluded in the EC RAR (2018), that the second study supersedes the original data only for the species were fumigants were used or where a more reliable endpoint could be derived (EC RAR, 2018 Vol.3 B9 p. 130).

Species & Taxonomic group	Substance tested	Test type & Endpoint	Duration	Parameter	Appl. rates (original units for plant studies in lb or g a.s.)	Conc. mg a.s./kg d.w.[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	Corrected values[47] (RAC-EFSA)	Normalized conc. mg a.s./kg d.w., 3.4 % OM[48] (EC TGD, 2003)	Normalized conc. mg a.s/kg d.w., 10 % OM[49] (RIVM, 2007)	Conc. mg a.s./kg d.w. (CCME, 2006)[50]	Soil type	Source
		Seedling emergence (biomass)		EC_{25}	64.16 g/ha	0.043	-	0.087	0.26	0.038	0.98 % organic carbon, pH 8.26	2018, Vol. 3 CP B9, p.123
Zea mays (terrestrial plant)	a.s. (96.8 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.19 lb/ac	0.14	-	0.28	0.83	0.13	sandy loam, pH 6.3, 1.7 % OM	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 CA B9, p.126
				LOEL	0.75 lb/ac	0.56	-	1.1	3.3	0.49		
				MATC	0.38 lb/ac	0.28	-	0.56	1.66	0.25		
				EC_{25}	0.39 lb/ac	0.29	-	0.58	1.7	0.26		
		Seedling emergence (shoot height)	14 days	NOEL	0.75 lb/ac	0.56	-	1.1	3.3	0.49	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	
				LOEL	1.5 lb/ac	1.1	-	2.2	6.6	0.99		
				MATC	1.06 lb/ac	0.79	-	1.6	4.7	0.70		
				EC_{25}	5.7 lb/ac	4.3	-	8.5	25	3.76		
	Diuron 80 % SC (63.45 % a.s.)	seedling emergence (height)	21 days	NOER	17.52 g/ha	0.012	-	0.024	0.070	0.010	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay), 0.98 % organic carbon, pH 8.26	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	36.72 g/ha	0.024	-	0.050	0.15	0.022		
				MATC	25.36 g/ha	0.017	-	0.035	0.10	0.015		
		Seedling emergence (biomass)		EC_{25}	145.52 g/ha	0.10	-	0.20	0.58	0.086		
Triticum aestivum (terrestrial plant)	a.s. (97.3 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.0117 lb/ac	0.0087	-	0.021	0.062	0.0077	sandy loam, pH 6.7, 1.4 % OM, CEC=6.5 meq/100g	Heldreth & McKelvey, 1996 cited in EC RAR, 2018, Vol. 3 CA B9, p.130
				LOEL	0.0234 lb/ac	0.018	-	0.042	0.12	0.015		
				MATC	0.017 lb/ac	0.012	-	0.030	0.088	0.011		
				EC_{25}	0.0294 lb/ac	0.022	-	0.053	0.16	0.019		
		Seedling emergence (shoot dry weight)	14 days	NOEL	1.5 lb/ac	1.1	-	2.2	6.6	0.99	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	
				LOEL	3 lb/ac	2.2	-	4.5	13	2.0		
				MATC	2.1 lb/ac	1.6	-	3.2	9.3	1.4		
				EC_{25}	0.722 lb/ac	0.54	-	1.1	3.2	0.48		
Sorghum vulgare	a.s. (97.3 % purity)		21 days	NOEL	0.0117 lb/ac	0.0087	-	0.021	0.062	0.0077		Heldreth & McKelvey, 1996

Species & Taxonomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parameter**	**Appl. rates** (original units for plant studies in lb or g a.s.)	**Conc. mg a.s./kg d.w.**[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	**Corrected values**[47] (RAC-EFSA)	**Normalized conc. mg a.s./kg d.w., 3.4 % OM**[48] (EC TGD, 2003)	**Normalized conc. mg a.s/kg d.w., 10 % OM**[49] (RIVM, 2007)	**Conc. mg a.s./kg d.w.** (CCME, 2006)[50]	**Soil type**	**Source**
(terrestrial plant)		Vegetative vigor (shoot dry weight)		LOEL	0.0234 lb/ac	0.018	-	0.042	0.12	0.015	sandy loam, pH 6.7, 1.4 % OM, CEC=6.5 meq/100g	cited in EC RAR, 2018, Vol. 3 CA B9, p.130
				MATC	0.017 lb/ac	0.012	-	0.030	0.088	0.011		
				EC_{25}	0.0555 lb/ac	0.041	-	0.1	0.30	0.037		
	a.s. (96.8 % purity)	Seedling emergence (shoot height)	14 days	NOEL	0.75 lb/ac	0.56	-	1.1	3.3	0.49	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 CA B9, p.126
				LOEL	1.5 lb/ac	1.1	-	2.2	6.6	0.99		
				MATC	1.1 lb/ac	0.79	-	1.6	4.7	0.70		
				EC_{25}	0.81 lb/ac	0.61	-	1.2	3.6	0.53		
Beta vulgaris (terrestrial plant)	a.s. (96.8 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.005 lb/ac	0.0037	-	0.0075	0.022	0.0033	sandy loam, pH 6.3, 1.7 % OM	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 CA B9, p.126
				LOEL	0.023 lb/ac	0.017	-	0.034	0.10	0.015		
				MATC	0.011 lb/ac	0.0080	-	0.016	0.047	0.0071		
				EC_{25}	0.0087 lb/ac	0.0065	-	0.013	0.038	0.0057		
	a.s. (97.3 % purity)	Seedling emergence (shoot dry weight)	14 days	NOEL	0.188 lb/ac	0.14	-	0.28	0.83	0.12	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	Heldreth & McKelvey, 1996 cited in EC RAR, 2018, Vol. 3 CA B9, p.130
				LOEL	0.375 lb/ac	0.28	-	0.56	1.7	0.25		
				MATC	0.27 lb/ac	0.20	-	0.40	1.2	0.18		
				EC_{25}	0.128 lb/ac	0.096	-	0.19	0.56	0.084		
Glycine max (terrestrial plant)	a.s. (96.8 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.002 lb/ac	0.0015	-	0.0030	0.0088	0.0013	sandy loam, pH 6.3, 1.7 % OM	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 CA B9, p.126
				LOEL	0.011 lb/ac	0.0082	-	0.016	0.048	0.0073		
				MATC	0.0047 lb/ac	0.0035	-	0.0070	0.021	0.0031		
				EC_{25}	0.012 lb/ac	0.0090	-	0.018	0.053	0.0079		
		Seedling emergence (multiple endpoints)	14 days	NOEL and LOEL	>12 lb/ac	>9.0	-	>18	>53	>7.9	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	

Species & Taxonomic group	Substance tested	Test type & Endpoint	Duration	Parameter	Appl. rates (original units for plant studies in lb or g a.s.)	Conc. mg a.s./kg d.w.[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	Corrected values[47] (RAC-EFSA)	Normalized conc. mg a.s./kg d.w., 3.4 % OM[48] (EC TGD, 2003)	Normalized conc. mg a.s/kg d.w., 10 % OM[49] (RIVM, 2007)	Conc. mg a.s./kg d.w. (CCME, 2006)[50]	Soil type	Source
Brassica napus (terrestrial plant)	a.s. (97.3 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.0469 lb/ac	0.035	-	0.085	0.25	0.031	sandy loam, pH 6.7, 1.4 % OM, CEC=6.5 meq/100g	Heldreth & McKelvey, 1996 cited in EC RAR, 2018, Vol. 3 CA B9, p.130
				LOEL	0.0938 lb/ac	0.070	-	0.17	0.50	0.062		
				MATC	0.066 lb/ac	0.050	-	0.12	0.35	0.044		
				EC_{25}	0.036 lb/ac	0.027	-	0.065	0.19	0.024		
		Seedling emergence (shoot dry weight)	14 days	NOEL	0.188 lb/ac	0.14	-	0.28	0.83	0.12	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	
				LOEL	0.375 lb/ac	0.28	-	0.56	1.65	0.25		
				MATC	0.27 lb/ac	0.20	-	0.40	1.2	0.18		
				EC_{25}	0.0913 lb/ac	0.068	-	0.14	0.40	0.060		
Pisum sativum (terrestrial plant)	a.s. (97.3 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.0117 lb/ac	0.0087	-	0.021	0.062	0.0077	sandy loam, pH 6.7, 1.4 % OM, CEC=6.5 meq/100g	Heldreth & McKelvey, 1996 cited in EC RAR, 2018, Vol. 3 CA B9, p.130
				LOEL	0.0234 lb/ac	0.018	-	0.042	0.12	0.015		
				MATC	0.017 lb/ac	0.012	-	0.030	0.088	0.011		
				EC_{25}	0.0124 lb/ac	0.0093	-	0.022	0.066	0.0082		
	a.s. (96.8 % purity)	Seedling emergence (multiple endpoints)	14 days	NOEL and LOEL	>12 lb/ac	>9.0	-	>18	>53	>7.9	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 CA B9, p.126
	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (mortality)	21 days	NOER	162 g/ha	0.11	-	0.22	0.65	0.10	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay),	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	340.16 g/ha	0.23	-	0.46	1.4	0.20		
				MATC	235 g/ha	0.16	-	0.32	0.94	0.14		

Species & Taxonomic group	Substance tested	Test type & Endpoint	Duration	Parameter	Appl. rates (original units for plant studies in lb or g a.s.)	Conc. mg a.s./kg d.w.[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	Corrected values[47] (RAC-EFSA)	Normalized conc. mg a.s./kg d.w., 3.4 % OM[48] (EC TGD, 2003)	Normalized conc. mg a.s/kg d.w., 10 % OM[49] (RIVM, 2007)	Conc. mg a.s./kg d.w. (CCME, 2006)[50]	Soil type	Source
		Seedling emergence (biomass)		ER_{25}	> 1500 g/ha	> 1.0	-	> 2.0	> 6.0	> 0.88	0.98 % organic carbon, pH 8.26	
Lycopersicon esculentum (Solanum lycopersicon) (terrestrial plant)	a.s. (96.8 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.001 lb/ac	0.00075	-	0.0015	0.0044	0.00066	sandy loam, pH 6.3, 1.7 % OM	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 CA B9, p.126
				LOEL	0.005 lb/ac	0.0037	-	0.0075	0.022	0.0033		
				MATC	0.0022 lb/ac	0.0017	-	0.0033	0.0098	0.0015		
				EC_{25}	0.0017 lb/ac	0.0013	-	0.0025	0.0075	0.0011		
	a.s. (97.3 % purity)	Seedling emergence (shoot dry weight)	14 days	NOEL	0.0938 lb/ac	0.070	-	0.14	0.41	0.062	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	Heldreth & McKelvey, 1996 cited in EC RAR, 2018, Vol. 3 CA B9, p.130
				LOEL	0.188 lb/ac	0.14	-	0.28	0.83	0.12		
				MATC	0.13 lb/ac	0.099	-	0.20	0.58	0.088		
				EC_{25}	0.0848 lb/ac	0.063	-	0.13	0.37	0.056		
	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (biomass)	21 days	NOER	17.52 g/ha	0.012	-	0.024	0.070	0.010	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay), 0.98 % organic carbon, pH 8.26	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	36.72 g/ha	0.024	-	0.050	0.15	0.022		
				MATC	25.36 g/ha	0.017	-	0.035	0.10	0.015		
				ER_{25}	72.96 g/ha	0.049	-	0.099	0.29	0.043		
Cucumis sativus (terrestrial plant)	a.s. (96.8 % purity)	Vegetative vigor (shoot dry weight)	21 days	NOEL	0.005 lb/ac	0.0037	-	0.0075	0.022	0.0033	sandy loam, pH 6.3, 1.7 % OM	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 CA B9, p.126
				LOEL	0.011 lb/ac	0.0082	-	0.016	0.048	0.0073		
				MATC	0.0074 lb/ac	0.0055	-	0.011	0.033	0.0049		
				EC_{25}	0.0053 lb/ac	0.0040	-	0.0079	0.023	0.0035		
		Seedling emergence (shoot height)	14 days	NOEL	0.19 lb/ac	0.14	-	0.28	0.83	0.13	sandy loam, pH 6.3, 1.7 % OM, CEC=4.82 meq/100g	
				LOEL	0.38 lb/ac	0.28	-	0.57	1.7	0.25		
				MATC	0.27 lb/ac	0.20	-	0.40	1.2	0.18		

Species & Taxonomic group	Substance tested	Test type & Endpoint	Duration	Parameter	Appl. rates (original units for plant studies in lb or g a.s.)	Conc. mg a.s./kg d.w.[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	Corrected values[47] (RAC-EFSA)	Normalized conc. mg a.s./kg d.w., 3.4 % OM[48] (EC TGD, 2003)	Normalized conc. mg a.s/kg d.w., 10 % OM[49] (RIVM, 2007)	Conc. mg a.s./kg d.w. (CCME, 2006)[50]	Soil type	Source
				EC_{25}	0.34 lb/ac	0.25	-	0.51	1.5	0.22		
	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (biomass)	21 days	NOER	162 g/ha	0.11	-	0.22	0.65	0.10	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay), 0.98 % organic carbon, pH 8.26	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	340.16 g/ha	0.23	-	0.46	1.4	0.20		
				MATC	235 g/ha	0.16	-	0.32	0.94	0.14		
				ER_{25}	714 g/ha	0.48	-	0.97	2.9	0.42		
Lactuca sativa (terrestrial plant)	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (height)	21 days	NOER	36.72 g/ha	0.024	-	0.050	0.15	0.022	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay), 0.98 % organic carbon, pH 8.26	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	77.12 g/ha	0.051	-	0.10	0.31	0.045		
				MATC	53.22 g/ha	0.035	-	0.072	0.21	0.031		
		Seedling emergence (biomass)		ER_{25}	153.2 g/ha	0.10	-	0.21	0.61	0.090		
Brassica oleracea (terrestrial plant)	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (biomass, height)	21 days	NOER	77.12 g/ha	0.051	-	0.10	0.31	0.045	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay), 0.98 % organic carbon, pH 8.26	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	162 g/ha	0.11	-	0.22	0.65	0.10		
				MATC	111.77 g/ha	0.075	-	0.15	0.45	0.066		
		Seedling emergence (biomass)		ER_{25}	102.32 g/ha	0.068	-	0.14	0.41	0.060		
Daucus carota (terrestrial plant)	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (biomass, height)	21 days	NOER	340.16 g/ha	0.23	-	0.46	1.4	0.20	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay), 0.98 % organic carbon, pH 8.26	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	714.32 g/ha	0.48	-	0.97	2.9	0.42		
				MATC	492.93 g/ha	0.33	-	0.67	2.0	0.29		
		Seedling emergence (biomass)		ER_{25}	596.72 g/ha	0.40	-	0.81	2.4	0.35		
Hordeum vulgare	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (biomass)	21 days	NOER	36.72 g/ha	0.024	-	0.050	0.15	0.022	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay),	Gimeno, 2013b cited in EC RAR,
				LOER	77.12 g/ha	0.051	-	0.10	0.31	0.045		
				MATC	53.22 g/ha	0.035	-	0.072	0.21	0.031		

Species & Taxonomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parameter**	**Appl. rates** (original units for plant studies in lb or g a.s.)	**Conc. mg a.s./kg d.w.**[46] (EC TGD, 2003; RIVM, 2007; NEPC, 2013; US EPA, 2005)	**Corrected values**[47] (RAC-EFSA)	**Normalized conc. mg a.s./kg d.w., 3.4 % OM**[48] (EC TGD, 2003)	**Normalized conc. mg a.s/kg d.w., 10 % OM**[49] (RIVM, 2007)	**Conc. mg a.s./kg d.w.** (CCME, 2006)[50]	**Soil type**	**Source**
(terrestrial plant)				ER_{25}	262.88 g/ha	0.18	-	0.36	1.1	0.15	0.98 % organic carbon, pH 8.26	2018, Vol. 3 CP B9, p.123
Lolium perenne (terrestrial plant)	Diuron 80 % SC (63.45 % a.s.)	Seedling emergence (height)	21 days	NOER	17.52 g/ha	0.012	-	0.024	0.070	0.010	loamy sand soil (75.28 % sand, 16 % silt, 8.27 % clay), 0.98 % organic carbon, pH 8.26	Gimeno, 2013b cited in EC RAR, 2018, Vol. 3 CP B9, p.123
				LOER	36.72 g/ha	0.024	-	0.050	0.15	0.022		
				MATC	25.36 g/ha	0.017	-	0.035	0.10	0.015		
		Seedling emergence (biomass)		ER_{25}	51.6 g/ha	0.034	-	0.070	0.21	0.030		

1.3 RAC values - EFSA

Data evaluation

The quality assessment from the studies was based on the evaluation performed by the RMS and no further assessment was needed for the acceptance of the studies.

1.3.1 Derivation of soil protection value

Direct toxicity

For diuron, valid toxicity data for earthworms, collembolans, mites, microorganisms and terrestrial plants was available in the EC RAR (2018) and listed in Table A2.2. As mentioned in the main report, one of the approaches to perform risk assessment under the PPP authorization legislation is to calculate the regulatory acceptable concentration (RAC). Although there is not yet a definitive guidance available for the derivation of RAC values for soil in Switzerland (nor in EU), the information for decision-taking for diuron and fluazinam has been provided by consulting experts from Agroscope and FOAG. The RAC is calculated by dividing the lowest toxicity measurement by the trigger value described in the Uniform Principles (EFSA PPR Panel, 2017; European Parliament and Council of the European Union, 2011). In Switzerland, the organisms considered for the derivation of RAC values for soils are: earthworms, collembolans, mites and microorganisms (N-mineralization). The most sensitive groups of organisms were microorganisms (N-mineralization) and earthworms. The N-mineralization tests in Table A2.2 are performed with two concentrations of the active substance: 10.7 mg/kg d.w. and 53.3 mg/kg d.w., corresponding to the maximum field application rate (8 kg active substance/ha) and five times the maximum field application rate (40 kg active substance/ha), respectively (EC RAR, 2018, vol.3 B9 p. 121). The effect at the field application rate in sandy soils was always below 25 %, therefore the risk for soil microflora can be categorized as negligible (European and Mediterranean Plant Protection Organization (EPPO), 2003). Thus, the lowest chronic test result selected for the RAC derivation corresponds to a NOEC of 10.7 mg a.s./kg d.w. for an earthworm test with the formulation Karmex 80 WG (study from Stäbler (2001)). According to SANCO Guidance (EC SANCO, 2002), since the toxicity of lipophilic substances is driven by the soil organic carbon content, for substances with a log K_{ow} greater than 2, a correction for artificial soils by dividing the toxicity data by 2 should be performed for laboratory tests. Diuron has a log K_{ow} of 2.78 (Table A2.1), thus the corrected NOEC ($NOEC_{corr}$) for the earthworm study is 5.35 mg a.s./kg d.w. This value should then be divided by the trigger value for long-term exposure described in the Uniform Principles (Commission Regulation (EU) No 546/2011, EC 2011), which is 5 in this case. This results in a RAC of:

$$\boldsymbol{RAC} = \frac{NOEC}{trigger\ value} = \frac{5.35}{5} = \mathbf{1.07\ mg\ a.s./kg\ d.w.}$$

Although the final RAC should be corrected as proposed when using artificial soil for substances that may strongly bind to organic carbon, in order to compare the results with other methodologies, which do not apply this kind of correction/normalization, a RAC with the toxicity value of the same organism and endpoint, but not corrected, is also suggested:

$$\boldsymbol{RAC_{not-corrected}} = \frac{NOEC_{not-corrected}}{trigger\ value} = \frac{10.7}{5} = \mathbf{2.14\ mg\ a.s./kg\ d.w.}$$

Secondary poisoning

According to the EFSA (2009, p. 71), a log Kow ≥ 3 indicates a potential for bioaccumulation of a substance. As shown in Table A2.1, diuron has a log K_{ow} of 2.78 and, therefore, no further evaluation of secondary poisoning is necessary.

1.3.2 Final soil protection value

Since the exposure route via secondary poisoning was not relevant for diuron, a final RAC due to direct toxicity of 1.1 mg a.s./kg d.w. was suggested.

1.4 European Chemical Agency (ECHA)

1.4.1 Data evaluation

The quality assessment from the studies was based on the evaluation performed by the RMS and no further assessment was needed for the acceptance of the studies.

1.4.2 Derivation of soil protection value

Direct toxicity

As mentioned in the EC TGD (2003, p. 116), the ecotoxicological data was normalized to a standard OM content of 3.4 % (see A2.2). Therefore, effect concentrations mentioned in this section will always refer to the normalized concentrations.

According to the ECHA (2017, p. 149), tests on microorganisms using two test concentrations with a control can be used for the environmental risk assessment of biocides. It is mentioned in the guidance that if at least one concentration shows no statistical difference from the control and has an effect value ≤ 15 %, that concentration is the NOEC. There are two studies with microorganisms cited in EC RAR (2018) from Blumenstock (1989) and Anderson (1989), which tested nitrogen and carbon mineralization, respectively (Table A2.2). In both studies, two concentrations were tested and the lowest tested concentrations showed effects lower than 15 %. No significant differences between the lowest concentration and the control were found at the end of the experiment for the loamy silt soil in Blumenstock (1989) and, thus, that concentration was considered the NOEC. In the study from Anderson (1989), the statistical analysis was not reported and, consequently, it was not possible to know if the final values differed from the control or not. For this reason, the lowest concentration (after the normalization) corresponding to the loamy silt soil for N-mineralization was chosen as the most sensitive endpoint. Therefore, the proposed NOEC for microorganisms is 17 mg a.s./kg d.w.

The selection of the derivation method depends on the data availability. Calculation of a $PNEC_{soil}$ using statistical extrapolation techniques can be considered when sufficient data is available. SSDs can only be performed when at least 10 NOECs (and preferably 15 NOECs) are available from at least eight taxonomic groups (EC TGD, 2003, p. 103). Data on microbial mediated processes and single species tests should be considered separately due to fundamental differences between these tests (EC TGD 2003, p. 118). For the case study with diuron, there is data from earthworms, collembolans, mites and plants as single species tests (i.e., four taxonomic groups). Consequently, the minimum requirements to derive a $PNEC_{soil}$ using the SSD approach are not fulfilled.

When toxicity data is available for a producer, a consumer and/or a decomposer the $PNEC_{soil}$ is calculated using assessment factors (AF) (EC TGD, 2003, p. 116). It is generally accepted that the protection of the most sensitive species should protect the structure, and hence the community function (EC TGD, 2003, p. 99). According to this assumption, in case that multiple valid species and endpoints are available, the most sensitive ones should be selected for the $PNEC_{soil}$ derivation. Thus, the critical toxicity data for each trophic level for diuron is listed in Table A2.3.

Table A2.3: Critical toxicological data of the terrestrial organisms for diuron.

Group	Species & Endpoint	Parame-ter	Conc. in mg a.s./kg	Literature
Primary producer	*Lycopersicon esculen-tum* (vegetative vigor: shoot dry weight)	NOEL	0.0015	McKelvey & Kuratle, 1992 cited in EC RAR, 2018, Vol. 3 B9, p.126
Decomposer (nutrient transformer)	Microorganisms (Nitrogen mineraliza-tion)	NOEC	17	Blumenstock, 1989 cited in EC RAR, 2018, Vol. 3 B9 CA, p.120
Decomposer (litter transformer)/ Primary consumer	*Eisenia fetida/andrei*	NOEC	3.6	Stäbler, 2001 cited in EC RAR, 2018 Vol. 3 B9 CP, p.103
	Folsomia candida	NOEC	52	Ansaloni, 2013 cited in EC RAR, 2018, Vol. 3 B9 CP, p.104
Consumer (Secondary consumer)	*Hypoaspis aculeifer*	NOEC	235	Ansaloni, 2013 cited in EC RAR, 2018, Vol. 3 B9, p.111

**Concentrations normalized to 3.4 % organic matter*

In the EC TGD (2003), the role of the earthworms in the ecosystem is not clearly described. It is mentioned in the Appendix IV (p. 287) that the group annelida belongs to the primary consumers, i.e., "organisms that live mainly on living or dead autotrophic organisms or on microorganisms". Other authorities, like RIVM, discussed the role of the earthworms in the trophic chain and mentioned that "the food of these organisms is organic matter in various forms, or plant material, rather than other organisms (predation)" (RIVM, 2007, p. 119). For this reason, earthworms are differentiated from other invertebrates (consumers) and placed within the group of decomposers in RIVM (2007). According to EFSA PPR Panel (EFSA PPR Panel, 2017) earthworms have an important role as a decomposers but also as pest and disease control, by feeding of phytopathogenic fungi. So even if *E. fetida/andrei* can be considered as a decomposer (litter transformer) or a primary consumer, it is in any case from a lower trophic level than *H. aculeifer*, a predatory mite, which feeds on other soil invertebrates, i.e., it is a secondary consumer. Thus, *E. fetida/andrei* and *H. aculeifer* belong to distinct trophic levels. Similar to earthworms, collembolans have been considered as part of the mesofauna in charge of organic matter breakdown but also contributing to control the fungal biomass (EFSA PPR Panel, 2017). Therefore, *Folsomia candida* should be also included in the same trophic level as the earthworms.

According to the EC TGD (2003, p. 118), if there are NOECs for long-term toxicity tests for three species (from different groups of organisms) an AF of 10 can be used. For diuron, there is a NOEC for plants, microorganisms, earthworms, collembolans and mites belonging to four different trophic levels, therefore an AF of 10 can be applied to the concentration derived from the most sensitive organism (*Lycopersicon esculentum* (tomato)). According to the deterministic method (or AF method), this results in a $PNEC_{soil}$ of:

$$\boldsymbol{PNEC_{soil}} = \frac{NOEC_{norm.}}{AF} = \frac{0.0015}{10} = 0.00015\ mg\ a.s./kg\ d.w. = \mathbf{0.15\ \mu g\ a.s./kg\ d.w.}$$

According to the EC TGD (2003) normalization to 3.4 % OM should be applied to all studies prior the $PNEC_{soil}$ derivation, as it was done in the previous equation. However, in order to compare the results with other methodologies, which do not apply this kind of normalizations, a $PNEC_{soil}$ with the toxicity value of the same organism and endpoint, but not normalized, and with the same AF is also shown:

$$\boldsymbol{PNEC_{soil-not\ normalized}} = \frac{NOEC_{not-norm.}}{AF} = \frac{0.00075}{10}$$
$$= 0.000075\ mg\ a.s./kg\ d.w. = \mathbf{0.075\ \mu g\ a.s./kg\ d.w.}$$

Secondary poisoning

According to the EC TGD (2003, p. 123) a substance is potentially bioaccumulative if it has a log K_{ow} > 3. As shown in Table A2.1, diuron has a log K_{ow} of 2.78. The log K_{ow} for diuron is lower than the trigger value proposed in the EC TGD (2003) and there are no other evidences that may indicate that the substance is potentially bioaccumulative. A further evaluation of secondary poisoning is therefore not necessary.

1.4.3 Final soil protection value

Since the exposure route via secondary poisoning was not relevant for diuron, a final $PNEC_{soil}$ due to direct toxicity of 0.15 µg a.s./kg d.w. was suggested.

1.5 The Netherlands – RIVM (2007)

1.5.1 Data evaluation

In general, the quality assessment from the studies follows the system developed by Klimisch et al. (1997). However, since there has been already an evaluation from RMS and the quality assessment would bring to similar results, no re-evaluation has been performed and the validity from RMS regarded as face value.

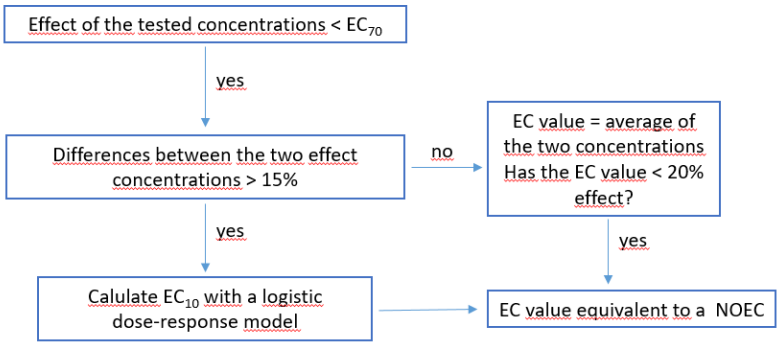
1.5.2 Derivation of soil protection value

Direct toxicity

Similarly to the EC TGD (2003), the ecotoxicological values should also be normalized but to a Dutch standard OM content of 10 % (see Table A2.2). Therefore, effect concentrations mentioned in this section will always refer to the Dutch normalized concentrations.

RIVM (2007) considers three different levels of protection: Negligible Concentration (NC_{soil}), Maximum Permissible Concentration ($MPC_{eco,soil}$) and Serious Risk Concentration (SRC_{soil}).

It is mentioned in RIVM (2007) that the $MPC_{eco,soil}$ is derived in the same way as the $PNEC_{soil}$ described in the EC TGD (2003). However, there is a slight variation on how to calculate the ECx data in case of tests with microorganisms in which two concentrations are tested (RIVM 2007, p. 50). The following should be applied:



For any of the microbial tests, none of the concentrations tested had an effect higher than 70 %. Table A2.4 shows the differences between the effect concentrations. In two cases, for the N- and C- transformation of the loamy silt soils the difference between the effect concentrations where higher than 15 % (32 % and 29 %, respectively). In those cases, a dose-response model was applied (Figure A2.1 B and C). When the difference between the effect concentrations was lower than 15 %, e.g., for the C-transformation test with loamy sand soil, the average of the concentrations was calculated instead. There is one case, for N-transformation in loamy sand soils, in which the effect is 15 %. There is no clear guidance on how to proceed if the difference between the effect concentrations is exactly 15 %. In this case, both methods were tested and expert knowledge was applied to choose the best approach (Table A2.4 and Figure A2.1 A).

Table A2.4. Summary table with the microbial tests described in Table A2.2, in which differences between the effect concentrations are shown. Negative values represent inhibition effects and positive values stimulation effects in the test.

Test	Type of soil	Conc. tested* (mg a.s./kg d.w.)	Effect concentrations (%)	Method used to calculate EC_x	Calcultated EC_x
N-transformation (Blumenstock, 1989)	Loamy sand	76	-10	Average of concentrations	ECx = 227 mg a.s./kg d.w. (average between 76 and 378) (-17.5 % effect) (average between -10 % and -25 % effect)
		378	-25		
	Difference		**-15**		
	Loamy silt	51	+3	Logistic dose-response model	EC_{10} = 217 mg a.s./kg d.w.
		255	-29		
	Difference		**-32**		
C-transformation (Anderson, 2018)	Loamy sand	76	-2	Average of concentrations	ECx= 227 mg a.s./kg d.w. (average between 76 and 378) (-9 % effect) (average between -2 % and -16 % effect)
		378	-16		
	Difference		**-14**		
	Loamy silt	51	-7	Logistic dose-response model	EC_{10} = 211 mg a.s./kg d.w.
		255	-36		
	Difference		**-29**		

**Concentrations normalized to 10 % organic matter*

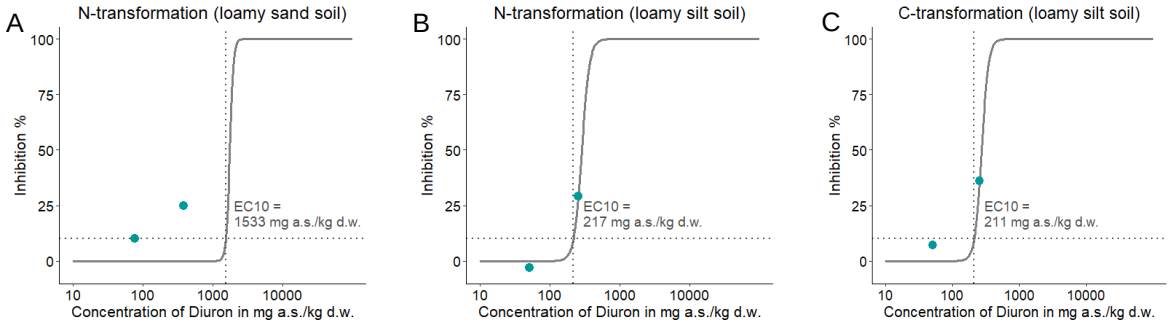


Figure A2.1. Dose-response curves using a two-parameter log-logistic model (maximum fixed to 100 % and minimum fixed to 0 % effect) for the N-transformation tests with loamy sand and loamy silt soils (A and B) and with the C-transformation test with loamy silt soil (C).

For most of the cases, either a dose-response model or an average approach could be applied for the microbial transformation tests and an EC value equivalent to a NOEC could be predicted. When the effects of the tested concentrations differed exactly by 15 % (N-transformation in loamy sand soil) both methods were tested. By applying the dose-response approach, due to the small difference between the effects, only an unrealistically high EC_{10} resulting of an extrapolation rather than an interpolation, could be predicted by the model (Figure A2.1 A). Thus, the average approach, was used (Table A2.4) and a NOEC = 227 mg a.s./kg d.w. was determined.

Although there is this slight variation of the RIVM guidance for the microbial transformation tests compared to the EC TGD (2003), the NOEC values predicted for the microbial processes were still high compared to the sensitivity of plants towards the herbicide diuron. Therefore, the same endpoint (i.e., NOEC for *Lycopersicon esculentum* (tomato)) and AF (10) were applied for the $MPC_{eco,soil}$ as for the $PNEC_{soil}$, which gives the following result:

$$\boldsymbol{MPC_{eco,soil}} = \frac{NOEC_{norm.}}{AF} = \frac{0.0044}{10} = 0.00044\ mg\ a.s./kg\ d.w. = \mathbf{0.44\ \mu g\ a.s./kg\ d.w.}$$

It should also be noted that the $PNEC_{soil\text{-}not\ normalized}$ derived in the previous section would be the same as a not normalized $MPC_{eco\ soil}$ ($MPC_{eco\ soil\text{-}not\ normalized}$).

Secondary poisoning

The assessment of secondary poisoning follows the EC TGD (2003). Therefore, as described in Appendix 1 section 1.4.2, no further evaluation is required for diuron.

1.5.3 Final soil protection value

Since the exposure route via secondary poisoning was not relevant for diuron, a final $MPC_{eco,soil}$ due to direct toxicity of 0.44 µg a.s./kg d.w. was suggested.

1.6 Canada – CCME (2006)

The CCME (2006) methodology differs from other methodologies because it takes into account a wide range of land uses and exposure pathways (see section 3.2.2 in the main report for further information). Because the current work in this report is mainly focused on agricultural land use, only the soil protection value under agricultural land use will be derived in this report.

Data evaluation

Studies should be screened according to whether they should be considered “acceptable” or “unacceptable” for the derivation of the soil protection values. The exhaustive assessment performed by the RMS was considered sufficient and comparable and no further re-assessment was considered necessary.

Derivation of soil protection value

For agricultural soils, several soil protection values should be derived to account for the different exposure pathways: soil contact (SQG_{SC}), nutrient and energy cycling check (SQG_{NEC}) and soil and food ingestion procedure (SQG_{I}). In case the substance is soluble in water, some additional SQG for the agricultural land use should be derived as well: soil to groundwater (freshwater live (SQG_{FL}), livestock watering (SQG_{LW}) and irrigation water (SQG_{IR})).

Soil Quality Guideline for Soil contact (SQG_{SC})

Data selection according to soil type and bioavailability considerations

According to CCME (2006, p. 45), if possible, coarse-grained and fine-grained soils should be considered separately, and soil protection values for the soil contact exposure pathway (Soil Quality Guidelines for Soil Contact (SQG_{SC})) developed for each soil type. The terrestrial tests listed in Table A2.2 were performed with different soil textures, which correspond to different soil types according to CCME (2006). While the earthworm, collembolan, mite and terrestrial plant tests were carried out only with coarse-grained soils, for the microbial transformation tests, two types of soil were used: fine-grained (loamy silt) and coarse-grained (loamy sand). According to CCME (2006, p. 47), the data set should be evaluated on a case-by-case basis and expert judgement applied. The methodology describes several solutions to account for differences in the soil type, based on expert knowledge. In this case, the most appropriate solution is to derive a SQG_{SC} for the soil type for which sufficient data is available. Then, this protection value can be applied to the other soil type as a provisional guideline. For diuron, most studies were performed with coarse-grained soils. Therefore, the SQG_{SC} in this section will be derived using only studies with coarse-grained soils. However, selecting only the coarse-grained soil tests does not compromise the total number of studies because the microbial transformation tests are performed in duplicate with the two different soil textures.

The guideline does not recommend data normalization to account for bioavailability. However, the bioavailability conditions for toxicity studies used to develop the SQG should be evaluated. It is mentioned, that studies conducted under conditions of very high bioavailability (i.e., very low pH and low organic carbon content) may not be relevant when deriving SQG for agricultural land uses, in particular. It is also mentioned that tests performed under conditions of low bioavailability (organic carbon content > 6 % and pH > 7 or pH < 5.5) would need also further considerations (CCME, 2006, p. 47). The selected studies for the derivation of the SQG for diuron in this report (only tests with coarse-grained soils) were not performed under conditions of very high or low bioavailability. Thus, all the studies considered until this point, will be used for the derivation of the SQG.

Derivation of the Soil Quality Guideline for Soil Contact (SQG_{SC})

The soil contact exposure pathway for agricultural land use distinguishes two different groups of organisms. Data on plants and invertebrates are considered separately from data from microbial transformation tests. According to CCME (2006, p. 45), there are two values that can be derived for plants and invertebrates depending on the land use (i.e., the level of protection): the Threshold Effects Concentration (TEC) for agricultural or residential/parkland uses, and the Effects Concentration – Low (ECL) for commercial and industrial guidelines (CCME, 2006, p. 45). Because this report is mainly focused on the

agricultural land use, only the TEC was calculated for diuron. In the end the TEC is compared to a check value for nutrient and energy cycling (SQG_{NEC}) for microbial processes to derive the SQG_{SC}.

Derivation of the Threshold Effects Concentration (TEC)

The minimum data requirements are met to apply the method "weight of evidence" described in CCME (2006, p. 52-54) (i.e., at least ten data points from three studies). If possible, the plant and soil invertebrate data should be evaluated separately. This requires that the data requirements for the method are met by each of the plant and invertebrate data sets. For the plant studies the requirements were met but not for the invertebrates. In this case, data may be combined if there is at least two invertebrate and two plant/crop data. Preferably, IC_{25} or EC_{25} data should be used for the distribution. As EC_{25}/IC_{25} were insufficient, alternatively, effect and no-effect data can be used instead. LOEC values were preferred over NOEC or EC_{50} and only exact values were selected. In case there were two studies for the same species, endpoint, toxicity parameter and exposure conditions, but the exposure duration was different, the data for the longer exposure period was preferred (CCME, 2006, p.49). This was the case for some species of terrestrial plants, which had more than one study for the seedling emergence test, where the longest exposure duration was selected. Both, data for vegetative vigor and seedling emergence tests, were represented in the rank distribution since it better describes the overall plant sensitivity.

For the "Weight of evidence" distribution approach, the data is ranked, and rank percentiles determined for each data point using the following equation (CCME, 2006, p.49):

$$j = \frac{i}{(n+1)} \text{x} 100$$

where,
j = rank percentile
i = rank of the data point in the data set
n = total number of data points in the data set

The graph of the rank percentile against the concentration of the chemical in the soil is shown in Figure A2.2Figure . According to the guidance, the data should be evaluated for anomalies, to ensure that this method is appropriate. The data showed a good fit with a p-value < 0.001 and r^2 of 0.81. However, some influential points were detected and skewed the model to the point that the 25th percentile of the distribution could only be calculated by extrapolation rather than interpolation. Two major influential data points could be detected by the Cooks distance plot (Figure A2.2 B), which correspond to the LOEC of the two least sensitive organisms: mite and collembola. Also, the data point for the earthworm test, although it was not immediately detected on a first data screening for influential data points due to the "closer" proximity to the plant data points, showed a sensitivity 14 times lower than any other data point for plants. This much lower sensitivity of the earthworm, mite and collembola was likely due to the specific mode of action of diuron. Thus, although no specific guidance is given when different sensitivities in the data set are detected and a good fit of the model is compromised, expert knowledge was applied. The final "estimated species sensitivity distribution – 25th percentile" ($ESSD_{25}$), which is the basis for the calculation of the TEC, was calculated only with the data on terrestrial plants (Figure A2.2 C).

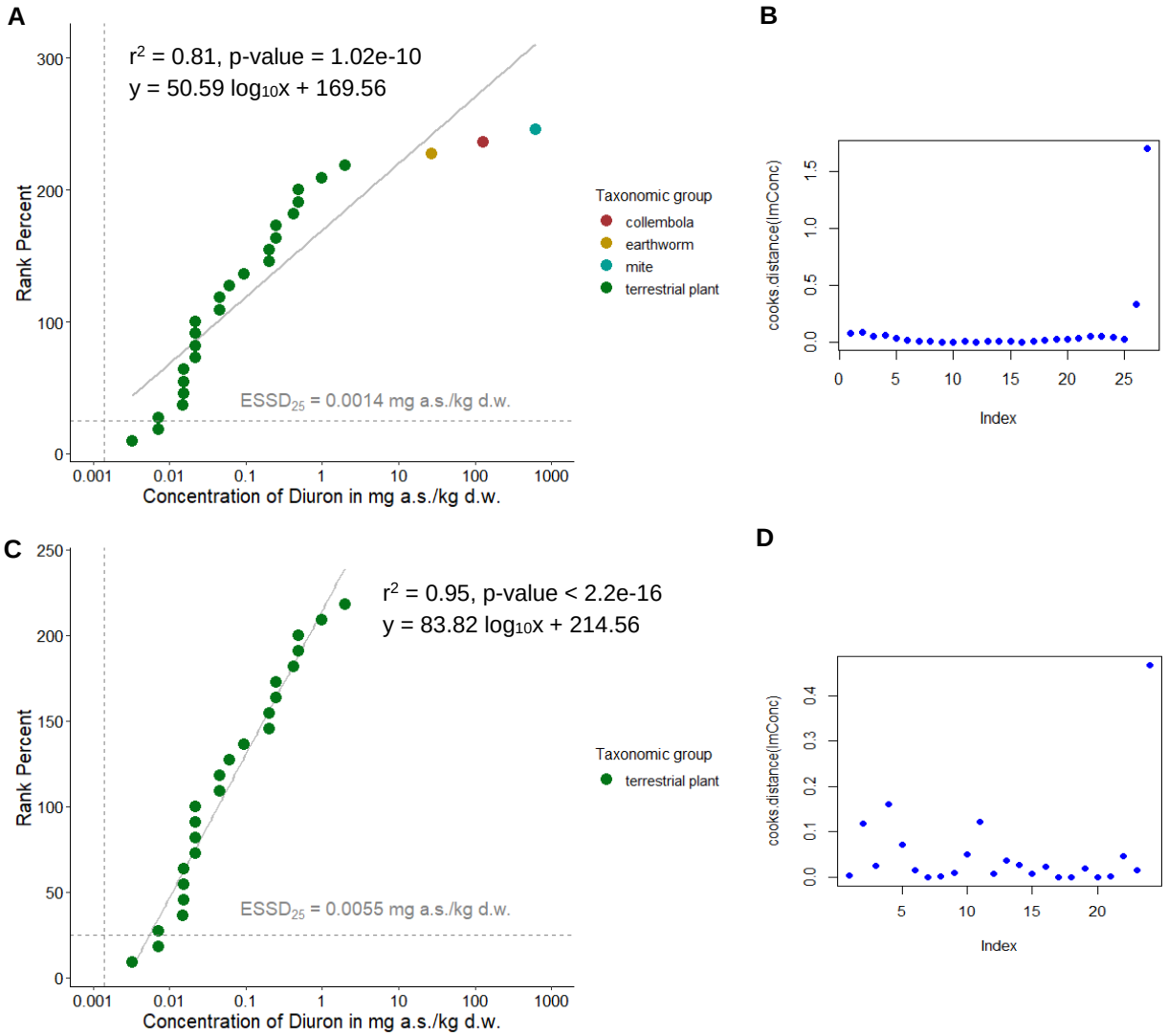


Figure A2.2: Rank probability plot of data including all organisms (A) and only plant studies (C). Figures B and D represent the Cooks distance plots for the respective plots on the left. While in Figure B the influential data points can be observed (on the right), since they are not following the pattern established by the rest of the data, in Figure C there is a more randomized distribution of the data points, showing no specific trends among the data.

Thus, the TEC was calculated from the Rank Probability distribution using the following equation:

$$TEC = \frac{ESSD_{25}}{UF}$$

where,
TEC = threshold effects concentration (mg/kg)
$ESSD_{25}$ = estimated species sensitivity distribution – 25th percentile (25th percentile of the distribution) (mg/kg)
UF = uncertainty factor

The use of an uncertainty factor is not mandatory but it can be used after examining the data. In the CCME (2006, p.52), it is suggested to use an UF between 1 and 5. For diuron, given that the final $ESSD_{25}$ was calculated only with data of one taxonomic group, an UF of 5 was applied to an $ESSD_{25}$ of 0.0055 mg a.s./kg d.w. for the derivation of the TEC:

$$\boldsymbol{TEC} = \frac{0.0055}{5} = 0.0011\, mg/kg\ d.w. = \boldsymbol{1.1\ \mu g/kg\ d.w.}$$

Derivation of the Soil Quality Guideline for Nutrient and Energy Cycling (SQG_{NEC})

In the CCME (2006, p.135), there are several methods described to calculate the SQG_{NEC}. Data on nitrogen-fixation and nitrification is preferred but data on nitrogen mineralization and carbon cycling may be used as well. For diuron, there are two reliable studies, one on carbon cycling (Anderson, 1989) and one on nitrogen mineralization (Blumenstock, 1989). However, a minimum of three studies is required to derive a SQG_{NEC} using any of the methods mentioned in the guideline. Due to insufficient data, no SQG_{NEC} could be derived for diuron.

Derivation of the SQG_{SC}

A comparison between the TEC and the SQG_{NEC} was not possible, since no value for the SQG_{NEC} could be derived for diuron. For this reason, the SQG_{SC} is equal to the TEC:

SQG_{SC} = 1.1 µg/kg d.w.

Soil Quality Guideline for Soil and Food Ingestion (SQG_I)

For most of the land uses described in the guideline, the SQG_I should only be derived if the substance has a strong tendency to bioaccumulate (Bioconcentration factor > 5000 or K_{ow}>10^5). However, for agricultural soils the derivation of a SQG_I is mandatory in order to protect herbivores grazing on agricultural lands (CCME, 2006, p. 56). Additionally, if the substance bioaccumulates, the SQG_I should include effects on the wildlife as well. Diuron has a log K_{ow} of 2.78 (equivalent to a K_{ow} of 602, i.e., < 10^5) (Table A2.1), therefore, only a SQG_I to protect the livestock was considered for diuron.

Oral toxicological data from grazing and foraging species is used to determine which species are potentially at threat from the ingestion of contaminants. According to the CCME (2006, p.57), the minimum data requirements are:

- A minimum of three studies
- At least two of the studies must be oral mammalian studies and one oral avian study
- A maximum of one laboratory rodent study can be used
- A grazing herbivore (e.g., ungulates) with a high ingestion rate to body weight ratio

For diuron, no feeding studies with ruminants were submitted in the re-authorization report (EC RAR, 2018, Vol. 1, p. 59). In the report it is mentioned that, based on the intended uses and the available residue data, the calculated burden for ruminants was found to be below the trigger value and, therefore, no feeding studies were required.

By lacking a grazing herbivore study, the minimum data requirements to determine the Daily Threshold Effects Dose (DTED) could not be met and therefore the derivation of a SQG_I for diuron was not possible.

Soil Quality Guidelines for the protection of Freshwater Life (SQG_{FL})

A substance present in soil can migrate to groundwater and, consequently, may affect the surface water bodies nearby. The SQG_{FL} is derived to evaluate the possible harm that the migration of a substance from the soil compartment to the water bodies nearby can cause. The SQG_{FL} is independent of the land use classification, and may be excluded on a site-specific basis if there are no surface water bodies in the vicinity of the site (CCME, 2006, p. 75). The SQG_{FL} is only required for soluble organic compounds.

Diuron is readily soluble in water (35.6-37.4 mg/L (Table A2.1)) (FAO, 2000) and it could be detected in the water and sediment compartments of several small water bodies in Switzerland from areas strongly influenced by agricultural practices (Spycher et al., 2019; Wildi et al., 2019). The concentration of diuron in water even exceeded repetitively the chronic quality criteria (chronisches Qualitätskriterium (CQK)) for water during the sampling campaign (Spycher et al., 2019). Thus, there is sufficient evidence showing that diuron can leach to the water bodies from areas of agricultural land use and even cause an effect in water and sediment organisms in Switzerland.

The model to calculate SQG_{FL} includes four components, which can be reduced to three for the derivation of generic protection values[52] (CCME, 2006, Appendix C, p. 143):

1. Partitioning of contamination from soil to pore water (leachate)

$$SQG_{FL} = C_L \left\{ K_d + \left(\frac{\theta_w + H'\theta_a}{\rho_b} \right) \right\}$$ *Equation 6*

where,
SQG_{FL} = soil quality guideline for the protection of freshwater life (mg/kg)
C_L = allowable leachate concentration at source (mg/L). For generic guidelines it is assumed that C_L is equal to the concentration of the chemical in leachate at the water table (C_Z)
K_d = distribution coefficient (cm^3/g)
θ_w = water-filled porosity (unitless)
H' = dimensionless Henry's law constant =H x 42.32
H = Henry's law constant ($atm\text{-}m^3/mol$)
θ_a = air-filled porosity (unitless)
ρ_b = soil bulk density in contaminant partitioning zone (g/cm^3)

2. Dilution and mixing of the contamination in the groundwater aquifer

$$C_z = C_{gw} \left\{ 1 + \left(\frac{Z_d K_H i}{IX} \right) \right\}$$ *Equation 7*

where,
C_Z = allowable chemical concentration in leachate at the water table[53] (mg/L)
C_{gw} = allowable chemical concentration in groundwater at the source (mg/L)
Z_d = average thickness of mixing zone (m)
K_H = hydraulic conductivity in the saturated zone (m/y)
i = hydraulic gradient (unitless)
I = infiltration rate (m/y) = precipitation minus runoff and evapotranspiration
X = length of source parallel to groundwater

Z_d described in eq. 2 can be calculated with the following equation:

$$Z_d = r + s$$ *Equation 8*

where,
r = mixing depth available due to dispersion and diffusion (m)
s = mixing depth available due to infiltration rate and groundwater flow rate (m)

r can be calculated using the following equation:

$$r = 0.01X$$ *Equation 9*

where,
X = length of source parallel to groundwater flow (m)

[52] For generic protection values it is assumed that the contamination is in contact with groundwater. Other assumptions for the model are also summarized in the CCME (2006, p.142).
[53] Water table is the upper level of an underground surface in which the soil or rocks are permanently saturated with water

And *s* can be calculated using the following equation:

$$s = d_a\left\{1 - e^{-\frac{2.178\,XI}{K_H i d_a}}\right\}$$ *Equation 10*

where,
d_a = depth of unconfined aquifer (m)
X = length of source parallel to groundwater flow (m)
I = infiltration rate (m/y) = precipitation minus runoff and evapotranspiration
K_H = hydraulic conductivity in the saturated zone (m/y)
i = hydraulic gradient (unitless)

3. Transport of the contamination through the saturated zone to the receptor

$$C_w(x,y,z,t) = \left(\frac{C_{gw}}{4}\right) exp\left\{\left(\frac{x}{2\partial_x}\right)\left[1 - \left(1 + \frac{4L_s\partial_x}{v}\right)^{1/2}\right]\right\} erfc\left[\frac{x - vt\left(1 + \frac{4L_s\partial_x}{v}\right)^{1/2}}{2(\partial_x vt)^{1/2}}\right]\left\{erf\left[\frac{(y + Y/2)}{2(\partial_y x)^{1/2}}\right] - erf\left[\frac{y - Y/2}{2(\partial_y x)^{1/2}}\right]\right\}$$ *Equation 11*

where,
C_w = allowable chemical concentration in water at receptor (mg/L)
x = distance from source to receptor (m)
x,y,z = Cartesian coordinates relating source to receptor (m); y,z assumed to be 0
t = time since contaminant release (years)
C_{gw} = allowable chemical concentration in groundwater at source (mg/L)
δ_x = longitudinal dispersivity tensor = 0.1x
δ_y = lateral dispersivity tensor = 0.1δ_x
L_s = decay constant (y^{-1}) in saturated zone
v = velocity of contaminant (m/y)
Y = source width (m) perpendicular to groundwater flow

L_s can be calculated using the following equation:

$$L_s = \frac{0.693}{t_{1/2s}}(e^{-0.07d})$$ *Equation 12*

where,
$t_{1/2s}$ = biodegradation half-life (y)
d = depth from surface to groundwater surface (m)

v can be calculated using the following equation:

$$v = \frac{K_H i}{n_e R_f}$$ *Equation 13*

where,

K_H = hydraulic conductivity in the saturated zone (m/y)
i = hydraulic gradient (unitless)
n_e = effective soil porosity (unitless). Assumed to be equal as the total porosity of soil (n)
R_f = retardation factor (unitless)

Rf can be calculated using the following equation:

$$R_f = 1 + \frac{\rho_b}{n} K_d \qquad \textit{Equation 14}$$

where,
ρ_b = soil bulk density in saturated zone (g/cm^3)
n = total porosity of soil (unitless)
K_d = distribution coefficient (cm^3/g)

n can be calculated using the following equation:

$$n = 1 - \frac{\rho_b}{2.65} \qquad \textit{Equation 15}$$

K_d can be calculated using the following equation (CCME, 2006, Appendix A, p. 132):

$$K_d = K_{oc} f_{oc} \qquad \textit{Equation 16}$$

where,
K_{oc} = organic carbon partitioning coefficient (L/kg)
f_{oc} = organic carbon fraction of soil (g/g)

In order to calculate the SQG_{FL}, a back calculation was performed. Some default parameters used in the equations have been described in the CCME (2006). In case that a parameter had two different values in the CCME (2006, Appendix I, p. 182), for coarse and fine-grained soils, the value for coarse grained soils was chosen, yet it represents a more conservative option. If this methodology was finally applied to Swiss soils, parameters should be adapted to the Swiss soil conditions. For this case study, only one parameter was used according to Swiss standards: as the chronic Quality Standard for diuron has been established in Switzerland for surface water (Swiss Federal Council, 2020), this value was used in the eq. 7 (C_w) instead of the Canadian Freshwater Life Guideline proposed in the CCME (2006, p. 146).

To calculate the distribution coefficient (K_d) (eq. 11), the following parameters are assumed:

$K_{oc,\ diuron}$ = 339 L/kg (Table A2.1)
f_{oc} = 0.005 g/g (CCME, 2006, Appendix I, p. 182)

$$K_{d,diuron} = 339 * 0.005 = 1.7\ cm^3/g$$

To calculate the total porosity of soil (*n*) (eq. 10), a ρ_b of 1.7 g/cm^3 (coarse-grained soils, CCME, 2006, Appendix I, p. 183) is assumed:

$$n = 1 - \frac{1.7}{2.65} = 0.36$$

To calculate the retardation factor (R_f) (eq. 9), the following parameters are assumed:

ρ_b = 1.7 g/cm^3 (coarse-grained soils, CCME, 2006, Appendix I, p. 182)
n = 0.36 (from eq. 10)
K_d = 1.7 cm^3/g (from eq. 11)

$$R_f = 1 + \frac{1.7}{0.36} 1.7 = 9.04$$

To calculate the velocity of a contaminant (*v*) (eq. 8), the following parameters are assumed:

K_H = 320 m/y (coarse-grained soils, CCME, 2006, Appendix I, p. 182)
i = 0.028 (CCME, 2006, Appendix I, p. 182)
n_e = n = 0.36
R_f = 9.04

$$v = \frac{320 * 0.028}{0.36 * 9.04} = 2.77\ m/y$$

To calculate the decay constant in saturated zone (L_s) (eq. 7), the following parameters are assumed:

$t_{1/2s,diuron}$ = 0.5 y (Table A2.1)
d = 3 m (CCME, 2006, Appendix I, p. 183)

$$L_s = \frac{0.693}{0.5} (e^{-0.07*3}) = 1.12\ y^{-1}$$

To calculate the allowable chemical concentration in groundwater at source (C_{gw})(eq. 6), the following parameters are assumed:

$C_{w,\ diuron}$ = 0.00007 mg/L (Swiss Federal Council, 2020)
x = 10 m (CCME, 2006, Appendix I, p. 183)
y,z = 0 (CCME, 2006, Appendix C, p. 146)
t = 5 y (This parameter was obtained from using the model from eq. 6. Five years is the time that the substance needs to reach a steady state concentration at the receptor)
δ_x = 0.1x = 0.1*10 = 1
δ_y = 0.1δ_x =0.1*1 = 0.1
L_s = 1.12 y^{-1} (from eq. 7)
v = 2.77 m/y
Y = 10 m (CCME, 2006, Appendix I, p. 183)

$$0.00007 = \left(\frac{C_{gw}}{4}\right) exp\left\{\left(\frac{10}{2*1}\right)\left[1 - \left(1 + \frac{4*1.12*1}{2.77}\right)^{1/2}\right]\right\} erfc\left[\frac{10 - 2.77*5\left(1 + \frac{4*1.12*1}{2.77}\right)^{1/2}}{2(1*2.77*5)^{1/2}}\right]\left\{erf\left[\frac{(0+10/2)}{2*(0.1*10)^{1/2}}\right] - erf\left[\frac{0-10/2}{2(0.1*10)^{1/2}}\right]\right\}$$

$$C_{gw} = 0.0016\ mg/L$$

To calculate the mixing depth available due to infiltration rate and groundwater flow rate (s) (eq. 5), the following parameters are assumed:

d_a = 5 m (CCME, 2006, Appendix I, p. 183)
X = 10 m (CCME, 2006, Appendix I, p. 183)

I = 0.28 m/y (coarse-grained soils, CCME, 2006, Appendix I, p. 182)
K_H = 320 m/y (coarse-grained soils, CCME, 2006, Appendix I, p. 182)
i = 0.028 (CCME, 2006, Appendix I, p. 182)

$$s = 5\left\{1 - e^{-\frac{2.178*10*0.28}{320*0.028*5}}\right\} = 0.64\ m$$

To calculate the mixing depth available due to dispersion and diffusion (*r*) (eq. 4), the same *X* as in eq. 6 was assumed:

$$r = 0.01 * 10 = 0.1\ m$$

To calculate the average thickness of mixing zone (Z_d) (eq. 3), the following parameters are assumed:

s = 0.64 m (from eq. 5)
r = 0.1 m (from eq. 4)

$$Z_d = 0.1 + 0.64 = 0.74\ m$$

To calculate the allowable chemical concentration in leachate at the water table (C_Z) (eq. 2), the following parameters are assumed:

C_{gw} = 0.0016 mg/L (from eq. 6)
Z_d = 0.74 m (from eq. 3)
K_H = 320 m/y (coarse-grained soils, CCME, 2006, Appendix I, p. 182)
i = 0.028 (CCME, 2006, Appendix I, p. 182)
I = 0.28 m/y (coarse-grained soils, CCME, 2006, Appendix I, p. 182)
X = 10 m (CCME, 2006, Appendix I, p. 183)

$$C_z = 0.0016\left\{1 + \left(\frac{0.74 * 320 * 0.028}{0.28 * 10}\right)\right\} = 0.0053\ mg/L$$

Finally, to calculate the SQG_{FL} (eq. 1), the following parameters were assumed:

$C_L = C_Z$ = 0.0053 mg/L (from eq. 2)
$K_{d,diuron}$ = 1.7 cm^3/g (from eq. 11)
θ_w = 0.119 (coarse-grained soils, CCME, 2006, Appendix I, p. 183)
H_{diuron} = 1.97e-11 atm-m^3/mol (Table A2.1)
H'_{diuron} = H x 42.32 = 8.34e-10
θ_a = 0.241 (coarse-grained soils, CCME, 2006, Appendix I, p. 182)
ρ_b = 1.7 g/cm^3 (coarse-grained soils, CCME, 2006, Appendix I, p. 182)

$$\boldsymbol{SQG_{FL}} = 0.0053\left\{1.7 + \left(\frac{0.119 + 8.34e - 10 * 0.241}{1.7}\right)\right\}$$
$$= \boldsymbol{0.0093\ mg\ a.s./kg = 9.3\ \mu g\ a.s./kg}$$

Soil Quality Guidelines for Livestock Watering (SQG_{LW}) and for Irrigation Water (SQG_{IR})

For the agricultural land use, contamination that migrates to groundwater may affect the water quality in dugouts or water wells used for livestock watering or crop irrigation. For this reason, the SQG_{LW} and the SQG_{IR} should also be derived for agricultural soils.

The same model as the one used for the SQG_{FL} is used for the SQG_{LW} and the SQG_{IR}, but setting the allowable receptor concentration (C_w in eq. 6) equal to the livestock water and irrigation water guidelines,

respectively. No guidelines for livestock watering or irrigation water are derived in Switzerland and, in Canada, the number of substances for which those values are derived, is also limited. For diuron, no Water Quality Guidelines for the Protection of Agricultural Water Uses could be found (http://ceqg-rcqe.ccme.ca/en/index.html#void). Thus, in this case the SQG_{IR} cannot be calculated. According to the CCME (2006, p. 75), if a livestock water guideline is unavailable, a livestock water threshold value can still be calculated using the following formula:

$$LWT = \frac{DTED * BW}{WIR} \qquad \textit{Equation 12}$$

where,
LWT = calculated livestock water threshold value
DTED = Daily Threshold Effect Dose for lifestock (mg/kg bw/d)
BW = livestock body weight (kg)
WIR = livestock water ingestion rate (L/d)
As already mentioned in section 0 when deriving the SQG_I, the minimum requirements are not met to calculate a DTED. Therefore, in this case, the SQG_{LW} cannot be derived either.

1.6.1 Final soil protection value

According to the CCME (2006, p. 79), there must be at least sufficient data to calculate the SQG_{SC} in order to set an Environmental Soil Quality Guideline (SQG_E). For diuron, there was sufficient data to derive the SQG_{SC} (for coarse-grained soils) and the SQG_{FL}. The SQG_{SC} was much lower than the SQG_{FL} (1.1 and 9.3 µg/kg, respectively). For this reason, the **SQG_E** for diuron is equal to the SQG_{SC}, which is **1.1 µg a.s./kg d.w.**

1.7 United States of America – US EPA (2005)

1.7.1 Data evaluation

According to the US EPA (2005), data for plants, soil invertebrates, birds and mammals is considered for the derivation of soil protection values (Eco-SSLs). Microbes and soil microbial processes are not considered for the derivation of Eco-SSLs (US EPA, 2005, p.1-5). In the guidance, their importance within terrestrial systems is recognized, but it is mentioned that data is usually insufficient and the interpretation of test results too uncertain for establishing risk-based thresholds for risk screening purposes.

As mentioned in the section 4.1 “General considerations” of the main report the toxicity studies have to meet several validity steps in order to be finally scored and selected or not for the derivation of Eco-SSL. For diuron, the study with *E. fetida* and the formulation Diuron 80 % SC listed in Table A2.2 could not pass through step 1 (Literature Exclusion Criteria). The study failed the criterion 13 from the Literature Exclusion Criterion: “No effect reported for a biological test species”, since the study reported no effect at the maximum concentration tested. The rest of studies listed in Table A2.2 fulfilled the requirements to pass the Exclusion and Acceptance criteria (step 1 and 2). The evaluation criteria and the scoring (step 3) were applied these studies and are listed in Table A2.5. For practical reasons, the scoring was performed only to the most sensitive endpoint of each species and those, which shared criteria and scores were grouped together. A maximum score of 2 was given to a criterion when this showed no flaws according to the guideline. The full description of the scoring system for each criterion can be found in US EPA (2003, Attachment 3-2). For clarity, justifications of the scoring in Table A2.5 were given only for criteria with a score other than 2 (i.e., 0 or 1) (see footnotes in Table A2.5).

Soil bioavailability is considered in one of the criteria of the scoring system (see Table A2.5). According to US EPA (2005, p. 2-8), the primary soil parameters affecting bioavailability and toxicity of a substance are pH and organic matter content. For organic compounds, the combination of these two soil parameters and the log K_{ow} of the substance is used to categorize bioavailability into high, medium and low. Greater weight is given to those studies where soil parameters suggested higher bioavailability.

Table A2.5: Study evaluation criteria and scoring for the laboratory studies of Table A2.2. Scores: 2 = criterion fulfilled, 1 = partially fulfilled, 0 = not fulfilled. Abbreviations: s.e. = seedling emergence; v.v. = vegetative vigor.

Criteria	***E. fetida/andrei*** (Stäbler, 2001)	***F. candida*** (Luna, 2013)	***H. aculeifer*** (Ansaloni, 2013)	***A. cepa (s.e.), T. aestivum (v.v.), S. vulgare (v.v.), B. napus (v.v.), P. sativum (v.v.)*** (Heldreth & McKelvey, 1996) ***and G. max (v.v.), C. sativus (v.v.)*** (McKelvey & Kuratle, 1992)	***Z. mays (v.v.), B. vulgaris (v.v.) and L. esculentum (v.v.)*** (McKelvey & Kuratle, 1992)	***All plant species*** (Gimeno, 2013b)
Testing was Done Under Conditions of High Bioavailability (very high or high = 2, medium = 1, low or very low = 0)	1[54]	1[55]	1[55]	2	2	1[56]
Experimental Designs were Documented and Appropriate	2	2	2	2	2	2
Concentration of Substance of Interest in Soil was Reported	1[57]	1[57]	1[57]	not acceptable[58]	not acceptable[58]	not acceptable[58]
Control Responses were Acceptable	1[59]	2	2	1[59]	1[59]	2
Chronic or Life Cycle Test was Used	2	2	2	2	2	2
Contaminant Dosing Procedure was Reported and appropriate for Chemical and Test	0[60]	2	2	1[61]	1[61]	2
A Dose-Response Relationship is Reported or can be Established from Reported Data	2	2	2	2	1[62]	2
The Statistical Tests used to Calculate the Benchmark and the Level of Significance were Described	1[63]	2	2	2	2	1[63]
The Origin of the Test Organisms was Described	1[64]	2	1[64]	2	2	1[64]
Total score	**11**	**16**	**15**	**14 but not acceptable**	**13 but not acceptable**	**13 but not acceptable**

[54] Standard artificial soils with approx. 10 % OM, 20 % kaolinite, 69 % sand, 1 % $CaCO_3$ are assigned a medium bioavailability score of 1

[55] Standard artificial soil with 5 % organic matter
[56] Natural soil with low organic matter but high pH (pH=8.26)
[57] Toxicity values based on nominal concentrations (not measured)
[58] unacceptable to report the units only in application rates (e.g., lbs./acre)
[59] Results of negative control are not reported
[60] No information about the carrier to deliver the chemical, neither how the carrier is handled nor how the soil and chemical were mixed
[61] Information is missing about how the carrier was handled following dosing
[62] The vegetative vigor test for *Z. mays*, *B. vulgaris* and *L. esculentum* performed by Mc Kelvey and Kuratle (1992) showed a difference between the NOEC and the LOEC >3-fold but < 10-fold
[63] ANOVA was completed but no p-level was provided
[64] Not sufficient information about the commercial source was provided

Studies are deemed appropriate for deriving Eco-SSLs if they score above ten. This was the case for the earthworm, collembolan and mite studies. However, there is a knock-out criterion described in US EPA (2003, Attachment 3-2, p. A-4):

“It is unacceptable to report application rates (e.g., lbs./acre). Studies that only report application rates are not accepted and should not be used to derive an Eco-SSL.”

As mentioned in the Footnote 46 of Table A2.2, the original units reported for the plant studies were lbs. a.s./acre or g a.s./ha and no more information was provided in the original study in order to convert application rates to concentrations. For this reason, although the plant studies scored above ten, they were not accepted for the derivation of an Eco-SSL.

1.7.2 Derivation of soil protection value

Direct toxicity

Only the studies with soil invertebrates passed the criteria for the derivation of an Eco-SSL. A geometric mean of all the toxicity values at the highest relative bioavailability score should be performed. According to the guidance, the toxicity parameters that should be preferred are: EC_{20}, MATC and NOEC (in this order). Thus, the Eco-SSL for soil invertebrates is equal to the geometric mean of the MATC of the studies with earthworm and mite and the EC_{20} of the collembolan study:

$$\boldsymbol{Eco - SSL_{soil\ invertebrates}} = \sqrt[3]{17 * 49.65 * 463} = \boldsymbol{73\ mg\ a.s./kg\ d.w.}$$

Secondary poisoning

According to US EPA (2005), an Eco-SSL to protect wildlife should always be derived considering mammals and birds whose diet could be directly or indirectly exposed to soil. In order to derive those values, an extensive literature search and quality check should be performed, since this data was not available from the (re-)authorization report, no Eco-SSL Wildlife was derived.

1.7.3 Final soil protection value

Since the exposure route via secondary poisoning could not be calculated for diuron, a final Eco-SSL due to direct toxicity of 73 mg a.s./kg d.w. was suggested.

1.8 Australia – NEPC 2013

Before deriving an EIL, the level of protection should be defined and this will depend on the land use and the exposure pathways. For the case studies, we focused, only on the derivation of EIL applied in agricultural land use.

By using the preferred method to derive EIL, the SSD method, it is possible to protect a hypothetical percentage of species/ecological functions. For the agricultural land use, the aim is to protect crop species and, therefore, the level of protection for the crop and grass species is 95 %. However, it is mentioned in NEPC (2013) that the use of some agricultural practices (e.g., tillage, pesticides) make it unrealistic to protect soil invertebrates and microbial processes at the same level and, therefore, only 80 % of these will be protected.

The importance of the exposure pathways can be determined by exploring the physicochemical properties of the substance (biodegradation time ($DT_{50,soil}$), Henry's law constant (K_H) and octanol-water partition coefficient (log K_{ow})). According to the categories described in NEPC (2013), diuron is a substance with a slow biodegradation in soil ($DT_{50,soil}$ > 45 days), not volatile (K_H dimensionless < 2.5e-7) and has low potential to biomagnify (log K_{ow} < 4) (A2.1). The two exposure routes that are considered most important after combining the three physicochemical properties are direct toxicity and metabolites (see NEPC, 2013, p.11 for further information). As mentioned in the main report, the toxicity of the metabolites was not considered for the case studies and only the direct toxicity with the parent compound was evaluated.

1.8.1 Data evaluation

According to the NEPC (2013), data for plants, soil invertebrates and microbial processes is considered for the derivation of soil protection values (EIL). Also, data for vertebrates is usually included, but this was not considered for the case studies. As mentioned in the section 4.1 "General considerations" of the main report, the toxicity studies have to meet several validity steps in order to be scored and selected for the derivation of EIL. For diuron, all the studies listed in Table A2.2 fulfilled the requirements to pass the Acceptance criteria (step 1). The scoring (step 2) was applied to the studies shown in Table of this report and are listed in Table A2.6. According to NEPC (2013) each experimentally derived toxicity datum should have its quality assessment. For practical reasons, and because the results from the two plant studies performed with the active substance presented in Table A2.2 resulted in the same rating, a unique score which represents all the plant species and endpoints of these two studies was performed.

According to NEPC (2013, p. 17) the test with microorganisms from Table A2.2 (C and N transformation) would not fulfil one of the validity steps: there is not a clear effect concentration (e.g., EC_{10}) or NOEC, LOEC given, since only two concentrations were tested. However, effects around 30 % could be observed for both tests at the highest concentration tested in loamy silt soils. To our understanding, the tests described in Table A2.2 are tests used for the authorization of PPPs, which are routinely performed with this particular experimental design and there is no reason to exclude them from the quality assessment. The experimental conditions of C and N transformation tests were almost the same and, therefore, the assessment had the same results for both tests. For this reason, the quality assessment in Table A2.6 can be referred to both tests.

The maximum score can be 3, 4, 5 or 10 depending on the criterion and was given when the test showed no flaws according to that criterion. For clarification, justifications of the scoring in Table A2.6 were given only for criteria with a score different than the maximum score (see footnotes in Table A2.6). In case, some of the questions did not proceed, because of the nature of the experimental conditions, we considered the question "not applicable" and the final score was re-calculated accordingly.

Table A2.6: Quality assessment performed according to NEPC (2013).

Question		***E. fetida/andrei*** (Stäbler, 2001)	***F. candida*** (Luna, 2013)	***H. aculeifer*** (Ansaloni, 2013)	**N-transformation** (Blumenstock, 1989)	**C-transformation** (Anderson, 1989)	**Plants** Heldreth & McKelvey, 1996 and McKelvey & Kuratle, 1992)	**Plants** (Gimeno, 2013b)
1	Was the duration of the exposure stated (e.g., 48 or 96 h)? (10 or 0 marks)	10	10	10	10	10	10	10
2	Was the biological end-point (e.g., immobilisation or population growth) stated and defined (10 marks)? Award 5 marks if only the biological endpoint is stated.	10	10	10	10	10	10	10
3	Was the biological effect stated (e.g., LC or NOEC)? (5 or 0 marks)	5	5	5	not applicable	not applicable	5	5
4	Was the biological effect quantified (e.g., 50% effect, 25% effect)? The effect for NOEC and LOEC data must be quantified. (5 or 0 marks)	5	5	5	5	5	5	5
5	Were appropriate controls (e.g., a no-toxicant control and/or solvent control) used? (5 or 0 marks)	5	5	5	5	5	5	5
6	Was each control and contaminant concentration at least duplicated? (5 or 0 marks)	5	5	5	5	5	5	5
7	Were test acceptability criteria stated (e.g., mortality in controls must not exceed a certain percentage) (5 marks)? or Were test acceptability criteria inferred (e.g., test method used (US EPA, OECD, ASTM etc.)) (award 2 marks). Note: Invalid data must not be included in the database.	2	5	5	2	2	2	5

Question		*E. fetida/andrei* (Stäbler, 2001)	*F. candida* (Luna, 2013)	*H. aculeifer* (Ansaloni, 2013)	N-transformation (Blumenstock, 1989)	C-transformation (Anderson, 1989)	Plants Heldreth & McKelvey, 1996 and McKelvey & Kuratle, 1992)	Plants (Gimeno, 2013b)
8	Were the characteristics of the test organism (e.g., length, mass, age) stated? (5 or 0 marks)	5	5	5	not applicable	not applicable	5	5
9	Was the type of test media used stated? (5 or 0 marks)	5	5	5	5	5	5	5
10	Were the contaminant concentrations measured? (4 or 0 marks)	0[68]	0[68]	0[68]	0[68]	0[68]	0[65]	0[65]
11	Were parallel reference toxicant toxicity tests conducted? (4 or 0 marks)	4	4	4	0[68]	0[68]	0[66]	0[66]
12	Was there a concentration–response relationship either observable or stated? (4 or 0 marks)	4	4	4	not applicable	not applicable	4	4
13	Was an appropriate statistical method or model used to determine the toxicity? (4 or 0 marks)	4	4	4	4	0[67]	4	4
14	For NOEC/LOEC data, was the significance level 0.05 or less? (4 or 0) or For LC/EC/BEC data, was an estimate of variability provided? (4 or 0)	4	4	4	not applicable	not applicable	4	4
15	Were the following parameters measured and stated? (3 marks if measured							
	and stated, 1 if just measured)	3	3	3	3	3	3	3
	pH (3, 1 or 0 marks)	3	3	3	3	3	3	3
	OM or OC content (3, 1 or 0 marks)	3	3	3	0[68]	0[68]		3

[65] Assuming that this question refers to measured concentrations in the soil. Only verifications of the nominal test concentrations were reported
[66] There is no mention of positive controls
[67] No statistics was reported

Question		*E. fetida/andrei* (Stäbler, 2001)	*F. candida* (Luna, 2013)	*H. aculeifer* (Ansaloni, 2013)	N-transformation (Blumenstock, 1989)	C-transformation (Anderson, 1989)	Plants Heldreth & McKelvey, 1996 and McKelvey & Kuratle, 1992)	Plants (Gimeno, 2013b)
	Clay content (3, 1 or 0 marks) CEC (3, 1 or 0 marks)	0[68]	0[68]	0[68]	0[68]	0[68]	0[68] 3	0[68]
16	Was the temperature measured and stated? (3 or 0 marks)	3	3	3	3	3	3	3
17	Was the grade or purity of the test contaminant stated? (3 or 0 marks)	3	3	3	3	3	3	3
18	Were other cations and/ or major soil elements measured? (3 or 0 marks) or Were known interacting elements on bioavailability measured (e.g., Mo for Cu and Cl for Cd)? (3 or 0 marks)	0[69]	0[69]	0[69]	0[69]	0[69]	0[69]	0[69]
19	For spiked soils with metal salts: were the soils leached after spiking? (3 or 0 marks)	not applicable	not applicable	not applicable	not applicable	not applicable	not applicable	not applicable
20	Were the incubation conditions and duration stated? (3, 1 or 0 marks)	3	3	3	3	3	3	3
	Total score ([Total score / 99 or 81] * 100)[70]	87 %	90 %	90 %	75 %	70 %	83 %	86 %
	Quality class (H ≥ 80 %, A 51 %–79 %, U ≤ 50 %)	H	H	H	A	A	H	H

[68] No information was given in the experimental conditions.
[69] No information of cations, major soil elements or other elements interacting on bioavailability were given.
[70] In the NEPC (2013) the maximum total score is 102. Because we considered some of the questions not applicable to the type of tests we were evaluating, the maximum total score applied is 99 for all studies except for the C- and N-transformation tests, which is 81. Quality class: H = high quality, A = acceptable, U = unacceptable.

The total score of our data is above 80 % for the tests with plants and soil invertebrates above 50 % for the microbial process tests, therefore the studies can be considered of high quality and acceptable, respectively. The last step (step 3) is the standardization of the toxicity data and the following factors:

- Measures of toxicity:
  Some conversions of the toxicity parameters should be applied in case data are expressed in different effect concentrations (e.g., EC_{50} and EC_{10}). Toxicity data that cause a 20 % to 40 % effect are considered in the same effect-group as LOEC data and are referred to throughout as LOEC and EC_{30} data. Only LOEC and EC_{30} are considered for the final derivation (NEPC, 2013, p. 20). Therefore, in case of having multiple toxicity parameters, those should be converted to EC_{30} or LOEC using conversion factors provided in the guidance. In case that EC_{30} data and LOEC are available from the same endpoint, EC_{30} data was preferred. Also, when different endpoints were described the lowest one was chosen. For the plant studies, EC_{25} were available and, since EC_{30}-type toxicity data are preferred over LOEC, they were chosen for the SSD. When different endpoints were described (seedling emergence and vegetative vigor), the lowest one was chosen. Plant tests with the same endpoint but different duration were not grouped together, since different exposure duration could exert an effect in the toxicity. Because the studies from collembolan and plant tests described EC_{20} and EC_{25}, respectively, and C- and N-transformation tests effects between 20 % and 40 % at the maximum concentration, no further conversion was necessary. For the studies where EC_x was not reported (earthworm and mite), the LOEC was taken instead.
- Duration of the exposures:
  Chronic data is preferred. In case there is data with acute exposure, acute to chronic conversions should be applied. For diuron, only chronic data is available, so no conversion was needed.

Two other standardization factors are described ("*Conversion from total to added concentrations"* and *"The use of toxicity data for endemic or overseas species"*) but they are considered not relevant for this case study.

According to NEPC (2013) aging and leaching factors should be applied to derive an EIL for aged contamination. Although these factors are relevant to evaluate the persistency of the chemical in the soil, this data was not provided in the (re-)authorization report, and therefore, not considered for the case studies.

1.8.2 Derivation of soil protection value

Direct toxicity and secondary poisoning

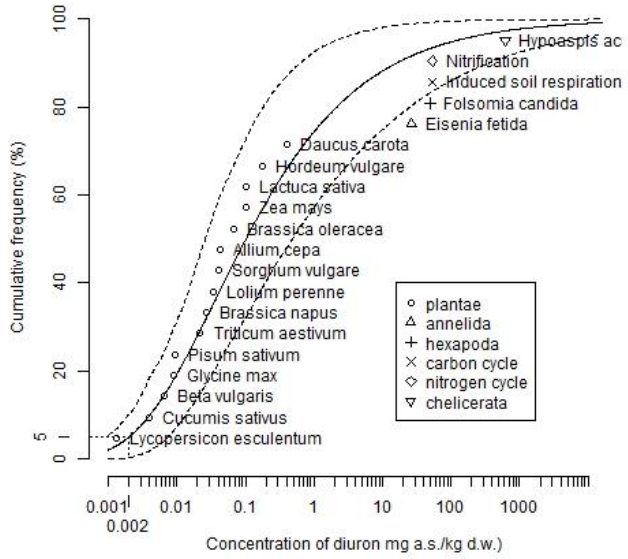
Normalization of the effect values to typical Australian soils should be done only in cases where normalization relationships for diuron have been described. Since no normalization relationship was found for the case studies, no normalization was applied. According to NEPC (2013, p. 34) in case normalization is not applied to the EIL the value is considered to be of moderate reliability.

The preferred methodology, if the data requirements are fulfilled, is the SSD using the Burr type III distribution. For diuron, there is data from 18 different species (invertebrates and plants) and two functional processes (C- and N-transformation processes), belonging to six different taxonomic or nutrient groups (Table A2.7). The SSD distribution is shown in Figure A2.3.

Table A2.7: List of species or functional processes, taxonomic or nutrients groups to which they belong and their corresponding LOEC or EC_{25}. List sorted in ascending order according to the LOEC and EC_{30} values.

Species or functional process	Taxonomic or nutrient group	LOEC and EC_{30} group (mg/kg d.w.)
Lycopersicon esculentum	plantae	0.0013
Cucumis sativus	plantae	0.0040
Beta vulgaris	plantae	0.0065
Glycine max	plantae	0.0090
Pisum sativum	plantae	0.0093
Triticum aestivum	plantae	0.022
Brassica napus	plantae	0.027
Lolium perenne	plantae	0.034
Sorghum vulgare	plantae	0.041
Allium cepa	plantae	0.043
Brassica oleracea	plantae	0.068
Zea mays	plantae	0.10
Lactuca sativa	plantae	0.10
Hordeum vulgare	plantae	0.18
Daucus carota	plantae	0.40
Eisenia fetida/andrei	annelida	26.7
Folsomia candida	hexapoda	49.65
Induced soil respiration	carbon cycle	53.3
Nitrification	nitrogen cycle	53.3
Hypoaspis aculeifer	chelicerata	621

Figure A2.3: SSD distribution of the effect data from Table A2.7 for diuron using the software BurrliOZ (Campbell et al., 2000). Dashed lines correspond the 95 % CI bounds and values extracted from the model for agricultural land use and 95 % confidential intervals associated to the values.



	Results	
	Value (mg a.s. / kg d.w.)	95 % Confidence interval
95 % - protection of crops	0.002	0.00083 - 0.0069
80 % - protection of soil invertebrates and microbial processes	0.011	0.0047 - 0.037

According to NEPC (2013) the percentage of species or soil processes to protect for agricultural uses is 80 % for soil invertebrates and microbial processes and 95 % for crops. According the guidance no additional assessment factor should be applied to the SSD. However, under certain circumstances, the confidence that the final EIL may be sufficiently protective may be questioned. The way of increasing

this confidence is by increasing the percentage of species to be protected in the SSD. Thus, this percentage should be modified in these two cases:

- if a contaminant biomagnifies (log K_{ow} > 4)
- if the number of species or soil processes is limited (e.g., if there is only 5 – 8 species or functional processes)

Diuron has a log K_{ow} of 2.78 and more than eight species could be represented in the SSD. Thus, there was no need to increase the percentage of species or soil processes to be protected.

1.8.3 Final soil protection value

The final EIL for agricultural land use is **0.002 mg a.s./kg d.w.** to protect the crop and grass species related to this land use and **0.011 mg a.s./kg d.w.** to protect soil processes and soil invertebrates.

1.9 Summary of soil protection values for diuron

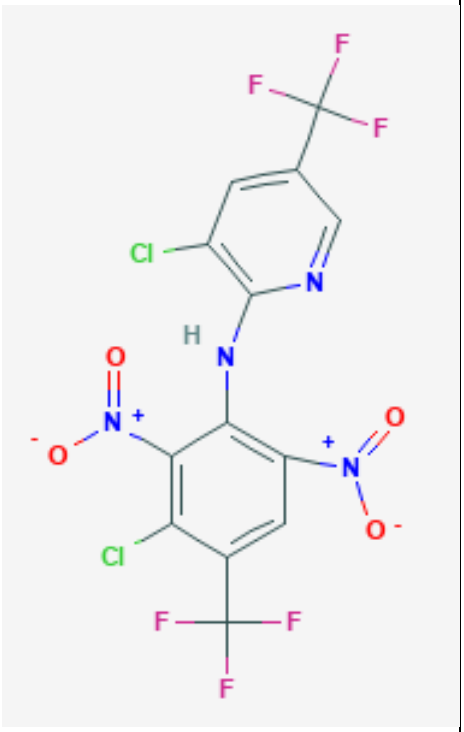
Region – Methodology	Soil protection values	Diuron (mg a.s./kg d.w.)
EFSA	RAC	1.07
EC TGD (2003)	$PNEC_{soil}$	0.000075 (not normalized) 0.00015 (norm. to 3.4 % OM)
The Netherlands – RIVM (2007)	$MPC_{eco,soil}$	0.000075 (not normalized) 0.00044 (norm. to 10 % OM)
Canada – CCME (2006)	SQG_E	0.0011
USA – US EPA (2005)	Eco-SSL	73
Australia – NEPC (2013)	EIL	0.002 (crop species) 0.011 (soil invertebrates and microbial processes)

2 Case study for the fungicide fluazinam

2.1 General data

Fluazinam is a fungicide which acts as uncoupler of oxidative phosphorylation in mitochondria, inhibiting fungal spore germination, hyphal penetration, growth and sporulation. It has also high reactivity with thiols (Tomlin, 2009; EC DRAR, 2019, Vol. 1, p. 16).

Table A2.8: General information for fluazinam.

IUPAC Name	3-chloro-N-[3-chloro-2,6-dinitro-4-(trifluoromethyl)phenyl]-5-(trifluoromethyl)pyridin-2-amine	
CAS registry number	79622-59-6	
EU Number	616-712-5	
Molecular formula	$C_{13}H_4Cl_2F_6N_4O_4$	
Code SMILES	C1=C(C=NC(=C1Cl)NC2=C(C=C(C(=C2[N+](=O)[O-])Cl)C(F)(F)F)[N+](=O)[O-])C(F)(F)F	
Pesticide Category	Fungicide, family 2,6-dinitroaniline	
Molecular weight	465.09 g/mol	
pK_a	7.34 (20°C) (EC DRAR, 2019, Vol. 3 B2 p. 38)	
Log K_{ow}	4.5, 5 (20, 22°C) (EC DRAR, 2019, Vol. 1 p. 42)	
K_{oc}	920 (EFSA Scientific Report 2008, p. 64)	
Water solubility	0.106, 0.135 and 2.72 mg/L (20°C at pH 5, 7 and 9 respectively) (EC DRAR, 2019, Vol.3 B2 p. 34)	
Henry's law constant	5.93 ×10^{-2} Pa m^3/mol (20 °C)(EC DRAR, 2019 Vol. 3 B2 p.27) K_H dimentionless [71]= 2.43e-5	
$DT_{50,soil}$	26.5 days (Tomlin, 2009), 17.1-226 days (geom. mean 72.5 days) (EFSA, 2008, p. 64)	
$DT_{90,soil}$	210 – 873 days (EFSA, 2008, p. 64)	
EU Classification	Acute Tox.4 – H322; Eye Dam.1 – H318; Skin Sens. 1A – H317; Aquatic Chronic 1 – H410; Aquatic Acute 1 – H400; Repr. 2– H361d[72] (EU Pesticides database. Status: July 2020)	

2.2 Ecotoxicological data

Ecotoxicological values available for fluazinam are presented in Table A2.9. The ecotoxicological data was collected from the Draft Renewal Assessment Report (EC DRAR, 2019) for the reauthorization of fluazinam as a PPP and from the Draft Assessment Report (EC DAR, 2006).

All studies shown in Table A2.9 were performed either with the active substance, i.e., fluazinam technical grade with purities ranging from 97.3 % to 99.7 %, or with the representative formulations (Trade names: IKF-1216 500 SC, TIFC 500 SC (also named Fluazinam 500 SC or Fluazinam 500 SC Novafito) and MCW 465 500 SC). The following studies/endpoints from the EC RAR (2019) have not been considered valid, and thus not shown in the table, due to the following reasons:

[71] Henry's law constant dimensionless calculated with EPA On-line Tools for Site Assessment Calculation (https://www3.epa.gov/ceampubl/learn2model/part-two/onsite/henryslaw.html)

[72] H332: Harmful if inhaled; H318: Causes serious eye damage; H317: May cause an allergic skin reaction; H410: Very toxic to aquatic life with long lasting effects; H400: Very toxic to aquatic life; H361d: Suspected of damaging the unborn child.

- Crosby (1995) cited in EC DRAR (2019) Vol. 3 CA B9, p. 302: The RMS considered the study not valid because of the phytotoxic effects in the controls.
- Scheerbaum (2006), amendment Scheerbaum (2016), cited in EC DRAR (2019) Vol. 3 CP B9 – MCW 465 500 SC, p. 227: Study considered “not acceptable” by the RMS.

Table A2.9: Soil ecotoxicological data for fluazinam from EC DAR (2006) and EC DRAR (2019). Values resulting from calculations are rounded to two significant figures. Some unit conversion and/or calculations are specific for some methodologies. In order to improve the clarity of which data was used for each methodology, the methodology (EC TGD, 2003; NEPC, 2013; RIVM, 2007; US EPA, 2005; RAC-EFSA and CCME, 2006) is specified in parenthesis. Abbreviations: Conc.=concentration, OM=organic matter, Appl. = application, a.s.=active substance, WHC= water holding capacity.

Species & Taxonomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parameter**	**Appl. rates** (original units for plant studies in g a.s./ha)	**Conc. mg a.s./kg d.w.** (EC TGD, 2003; NEPC, 2013; RIVM, 2007; US EPA, 2005)	**Corrected values**[73] (RAC-EFSA)	**Normalized conc. mg/kg d.w., 3.4 % OM** (EC TGD, 2003)	**Normalized conc. mg/kg d.w., 10 % OM** (RIVM, 2007)	**Conc. mg/kg d.w.** (CCME, 2006)	**Soil type**	**Source**
Eisenia fetida (earthworm)	Fluazinam techn. (97.3 % a.s.)	mortality	14 days	LC_{50}	-	> 1000	> 500	> 428	> 1258	> 1000	artificial soil: 70 % fine silica sand, 20% kaolinite clay, 10 % sedge peat (79.5 % OM) and 10 mg/kg $CaCO_3$. pH 7.0 ± 0.2. OM in soil ~ 8 %[74]	Edwards & Coulson, 1985 cited in EC DAR, 2006, Vol.3 CA B9, p.532
		Behavior and weight	28 days	NOEC	-	10	5	4.3	13	10		
				LOEC	-	100	50	43	126	100		
				MATC	-	32	16	14	40	32		
	MCW-465 500 SC (39.48 % a.s.)	reproduction and weight	56 days	NOEC	-	≥ 3.9	≥ 2.0	≥ 1.3	≥ 3.9	≥ 3.9	artificial soil: 69 % quartz sand, 20 % kaolin clay, 10 % sphagnum peat	Winkelmann, 2016 cited in EC DRAR, 2019, Vol. 3 CP B9 -

[73] According to SANCO/10329/2002 (EC SANCO, 2002), tests performed with artificial soils, which usually contain higher organic carbon content than many natural soils, should be corrected if the log K_{ow} of the substance is greater than 2. This correction was applied to earthworm, mite and collembolan tests, but not to microorganism transformation tests. Plants are not included in the RAC derivation, therefore, no value was shown in the table.

[74] Soil organic matter calculated assuming that the only source of organic matter in the artificial soil was from the sedge peat and that the organic matter content of the sedge peat is 79.5 %.

Species & Taxo-nomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parame-ter**	**Appl. rates** (original units for plant stud-ies in g a.s./ha)	**Conc. mg a.s./kg d.w.** (EC TGD, 2003; NEPC, 2013; RIVM, 2007; US EPA, 2005)	**Corrected values**[73] (RAC-EFSA)	**Normalized conc. mg/kg d.w., 3.4 % OM** (EC TGD, 2003)	**Normalized conc. mg/kg d.w., 10 % OM** (RIVM, 2007)	**Conc. mg/kg d.w.** (CCME, 2006)	**Soil type**	**Source**
											and 0.38 % CaCO3. pH 6.0 ± 0.5	MCW 465 500 SC, p. 180
	Fluazinam 500 SC (38.4 % a.s.)	mortality	14 days	LC_{50}	-	> 682	> 341	> 232	> 682	> 682	artificial soil: 70 % fine silica sand, 20 % kaolin clay, 10 % peat and 5 g CaCO3/kg. pH 6.0 ± 0.2	Yearsdon et al., 1991 cited in EC DRAR, 2019, Vol. 3 CP B9 - IKF-1216 500 SC, p. 145
Eisenia andrei (earthworm)	Fluazinam 500 SC (39.4 % a.s.)	reproduction	56 days	NOEC	-	< 0.35	< 0.175	< 0.12	< 0.35	< 0.35	artificial soil: 68-69 % fine quartz sand, 20 % kaolin clay, 10 % peat and 1 % $CaCO_3$. pH 6.0 ± 0.5. pH 6.0 ± 0.5	Römbke & Moser, 1999 cited in EC DRAR, 2019, Vol. 3 CP B9 - IKF-1216 500 SC, p. 146
		weight		NOEC	-	≥ 35.0	≥ 17.5	≥ 11.9	≥ 35.0	≥ 35.0		
Folsomia candida (collembolan)	MCW-465 500 SC (39.48 % a.s.)	mortality	28 days	LC_{50}	-	> 10.8	> 5.4	> 7.3	> 21.6	> 10.8	artificial soil ISO 1167: 74.8 % fine quartz sand, 20 % kaolin clay, 5 % Sphagnum peat and 0.2 % $CaCO_3$. pH 6.0 ± 0.5	Lührs, 2008, amend-ment Lührs, 2016 cited in EC DRAR, 2019, Vol. 3 CP B9 - MCW 465 500 SC, p. 211
		reproduction		EC_{50}	-	8.74	4.37	5.9	17.5	8.74		
		mortality and reproduction		NOEC[75]	-	5.4	2.7	3.7	10.8	5.4		
				LOEC	-	10.8	5.4	7.3	21.6	10.8		
				MATC	-	7.6	3.8	5.2	15.3	7.6		

[75] An EC_{10} of 5.617 mg a.s./kg d.w. was reported, but the RMS preferred the NOEC.

Species & Taxo-nomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parame-ter**	**Appl. rates** (original units for plant stud-ies in g a.s./ha)	**Conc. mg a.s./kg d.w.** (EC TGD, 2003; NEPC, 2013; RIVM, 2007; US EPA, 2005)	**Corrected values**[73] (RAC-EFSA)	**Normalized conc. mg/kg d.w., 3.4 % OM** (EC TGD, 2003)	**Normalized conc. mg/kg d.w., 10 % OM** (RIVM, 2007)	**Conc. mg/kg d.w.** (CCME, 2006)	**Soil type**	**Source**
	Fluazinam 500 SC (39.4 % a.s.)	mortality	28 days	LC_{50}	-	14.0	7.0	4.7	14.0	14.0	artificial soil: 69.5 % fine quartz sand, 20 % kaolin clay, 10 % sphag-num peat and 0.5 % $CaCO_3$. pH 6.0 ± 0.5	Klein, 2002 cited in EC DRAR, 2019, Vol. 3 CP B9 - IKF-1216 500 SC, p. 166
		reproduction		EC_{50}	-	11.9	6.0	4.1	11.9	11.9		
				EC_{10}	-	4.5	2.25	1.5	4.5	4.5		
		mortality and reproduction		NOEC	-	< 1.2	< 0.6	< 0.42	< 1.2	< 1.2		
	TIFC 500 SC (40.2 % a.s.)	reproduction	28 days	EC_{50}	-	9.1	4.6	6.2	18	9.1	artificial soil: 75 % industrial quartz sand, 20 % kaolin clay, 5 % sphag-num peat. pH 6.26	Neri, 2015 cited in EC DRAR, 2019, Vol. 3 CP B9 - TIFC 500 SC, p. 100
				EC_{10}[76]	-	5.63	2.82	3.8	11	5.63		
		Mortality and reproduction		NOEC	-	6.9	3.5	4.7	14	6.9		
				LOEC	-	12.4	6.2	8.4	25	12.4		
				MATC	-	9.2	4.6	6.3	18	9.2		
Hypoaspis acu-leifer (mite)	Fluazinam techn. (99.52 % a.s.)	mortality	14 days	LC_{50}	-	> 110	> 55	> 75	> 220	> 110	artificial soil: 5 % sphagnum peat, 20 % kaolin clay, 74.7 % industrial quartz sand, 0.2 % calcium car-bonate. pH 5.6-5.9,	Schulz, 2016 cited in EC DRAR, 2019, Vol 3 CA B9, p.259
		reproduction	14 days	NOEC	-	≥ 110	≥ 55	≥ 75	> 220	≥ 110		

[76] RMS considered the EC_{10} value as the relevant reproduction endpoint.

Species & Taxo-nomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parame-ter**	**Appl. rates** (original units for plant stud-ies in g a.s./ha)	**Conc. mg a.s./kg d.w.** (EC TGD, 2003; NEPC, 2013; RIVM, 2007; US EPA, 2005)	**Corrected values**[73] (RAC-EFSA)	**Normalized conc. mg/kg d.w., 3.4 % OM** (EC TGD, 2003)	**Normalized conc. mg/kg d.w., 10 % OM** (RIVM, 2007)	**Conc. mg/kg d.w.** (CCME, 2006)	**Soil type**	**Source**
											OM 5 %[77]	
	TIFC 500 SC (40.2 % a.s.)	reproduction	14 days	EC_{50}	-	2595	1298	1764	5189	2595	artificial soil: 75 % industrial quartz sand, 20 % kaolin clay, 5 % sphag-num peat. pH 6.4	Colli, 2015 cited in EC DRAR, 2019, Vol. 3 CP B9 - TIFC 500 SC, p. 103
				EC_{10}[78]	-	47	24	32	94	47		
micro-organisms	Fluazinam 500 SC (39.49 % a.s.)	nitrogen transfor-mation	28 days	54.9 % stimula-tion	-	0.27	0.27	0.40	1.2	0.27	natural soil: sam-ple from Rossdorf (Germany), loamy sandy soil (10.3 % clay, 37.5 % silt, 52.2 % sand), TOC 1.34 %, CEC: 14.1 mval Ba/100 g dw, total N 1.84 mg/100 mg dw, max WHC 48 ml water/100 g soil. pH 7.4	Reis, 2002 cited in EC DRAR, 2019, Vol. 3 CP B9 - IKF-1216 500 SC, p. 181
				112 % stimula-tion	-	2.27	2.27	3.4	10	2.27		
		carbon trans-formation		6.05 % inhibition	-	0.27	0.27	0.40	1.2	0.27		
				2.89 % inhibition	-	2.27	2.27	3.4	10	2.27		

[77] Soil organic matter content estimated assuming that the only source of organic matter in the artificial soil comes from the sphagnum peat and that the organic matter content of the Sphagnum peat is approximately 100 %

[78] The reliability of the EC_{10} is considered poor, but the RMS decided that it should be considered for risk assessment since it was not possible to determine a reliable NOEC (effects > 15 %)

Species & Taxonomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parameter**	**Appl. rates** (original units for plant studies in g a.s./ha)	**Conc. mg a.s./kg d.w.** (EC TGD, 2003; NEPC, 2013; RIVM, 2007; US EPA, 2005)	**Corrected values**[73] (RAC-EFSA)	**Normalized conc. mg/kg d.w., 3.4 % OM** (EC TGD, 2003)	**Normalized conc. mg/kg d.w., 10 % OM** (RIVM, 2007)	**Conc. mg/kg d.w.** (CCME, 2006)	**Soil type**	**Source**
Zea mays *Avena sativa* *Allium cepa* *Sorghum bicolor* *Fagopyrum esculentum* *Cucumis sativus* *Brassica kaber* *Raphanus sativus* *Glycine max* *Lycopersicon esculentum* (Terrestrial plant)	Fluazinam techn. (97.3% a.s.)	vegetative vigor (phytotoxicity and fresh weight)	14 days	ER_{50}	≥ 1500	≥ 1	-	- [79]	- [79]	- [80]	soilless commercial growing medium (Redi-Earth-Peat-Lite Mix)	Backus, 1993b cited in EC DRAR, 2019, Vol 3 CA B9, p.299
Zea mays *Avena sativa* *Allium cepa* *Sorghum bicolor* *Fagopyrum esculentum* *Cucumis sativus*	Fluazinam techn. (97.3% a.s.)	seedling emergence (emergence and fresh weight)[81]	14 days	ER_{50}	≥ 1500	≥ 1	-	- [79]	- [79]	≥ 0.88[82]	natural soil amended with 50 % silica sand and supplemental nutrients	Backus, 1993a cited in EC DRAR, 2019, Vol 3 CA B9, p.296

[79] No information about the organic matter content was provided in the test, therefore data could not be normalized.
[80] No information about the soil texture was provided in the test, so no conversion to mg/kg d.w. could be applied according to CCME (2006).
[81] Two different methods were tested in this study: Petri dish seed germination method and pre-emergence bioassay method. Only the last one was included in the table, since no soil was used for the petri dish test.
[82] According to the CCME (2006): "Coarse-grained soils: Soil which contains greater than 50 % by mass particles greater than 75 µm mean diameter (D50 > 75 µm)." The soil was amended with 50 % sand, therefore, we considered the soil coarse-grained and used the standard bulk soil for coarse-grained soils of 1.7 g/cm^3 (CCME, 2006, p. 182) and 10 cm depth for the conversion from g/ha to mg/kg d.w.

Species & Taxo-nomic group	**Substance tested**	**Test type & Endpoint**	**Duration**	**Parame-ter**	**Appl. rates** (original units for plant stud-ies in g a.s./ha)	**Conc. mg a.s./kg d.w.** (EC TGD, 2003; NEPC, 2013; RIVM, 2007; US EPA, 2005)	**Corrected values**[73] (RAC-EFSA)	**Normalized conc. mg/kg d.w., 3.4 % OM** (EC TGD, 2003)	**Normalized conc. mg/kg d.w., 10 % OM** (RIVM, 2007)	**Conc. mg/kg d.w.** (CCME, 2006)	**Soil type**	**Source**
Brassica kaber *Raphanus sativus* *Glycine max* *Lycopersicon esculentum* (terrestrial plant)												
Avena sativa *Allium cepa* *Beta vulgaris* *Brassica napus* *Daucus carota* *Glycine max* (terrestrial plant)	MCW-465 500 SC	vegetative vigor (phyto-toxic effects and fresh weight)	21 days	ER_{50}	≥ 1500	≥ 1	-	≥ 2	≥ 5.8	≥ 0.88	Certified LUFA soil (No. 2.3, loamy sand, TOC = 1.02)	Fiebig, 2006 cited in EC DRAR, 2019, Vol. 3 CP B9 - MCW 465 500 SC, p. 231

2.3 RAC values - EFSA

2.3.1 Data evaluation

The quality assessment from the studies was based on the evaluation performed by the RMS and no further assessment was needed for the acceptance of the studies.

2.3.2 Derivation of soil protection value

Direct toxicity

In Table A2.9 tests with fluazinam on earthworms, collembolans, mites, microorganisms and plants are summarized. As mentioned for the case study with diuron, plants are not considered for the derivation of RAC values. The tests with microorganisms (N- transformation), showed significant effects after 28 days. Although the study was considered valid, it was not further considered for risk assessment by the RMS due its low reliability (according to the SANCO/10329/2002, effects should be below 25 % after 100 days and, in this case, the duration was only 28 days). For this reason, and assuming that the same principles would apply for the RAC derivation, the N-transformation study was not considered. The lowest chronic endpoint is for the study with the earthworm *E. fetida*, which has a NOEC < 0.35 mg/kg d.w. Due to the observed toxicity for earthworms in the laboratory tests, a higher tier field study with earthworms was required for the (re-) authorisation of fluazinam. A valid earthworm field study was described in the EC DRAR (2019) by Krück (2009). This study showed that there were no effects on endogeic, anecic and epigeic species due to the treatment with fluazinam at the end of the experiment (8 months after the application) at a maximum concentration of 1.544 mg a.s./kg d.w. Thus, the effects observed in the laboratory studies with earthworms could be refined with the field study. However, this was not the case for the collembolan study with *F. candida*, which presented a NOEC < 1.2 mg a.s./kg d.w. and no further valid higher test studies were submitted. For this reason, the study with *F. candida* from Klein (2002) was selected as the most sensitive study and was used for the RAC derivation. Because the log K_{ow} from fluazinam is larger than 2 (log K_{ow} = 4.5 - 5), the toxicity value was divided by a factor of 2 and the corrected NOEC for *F. candida* would be < 0.6 mg a.s./kg d.w. In order to derive a RAC value, the NOEC is divided by 5[83]:

$$\boldsymbol{RAC} = \frac{NOEC}{trigger\ value} = \frac{< 0.6}{5} = \boldsymbol{< 0.12\ mg\ a.s./kg\ d.w.}$$

Secondary poisoning

For substances with a log K_{ow} ≥ 3 the bioaccumulation potential may be triggered (EFSA, 2009). Fluazinam has a log K_{ow} of 5 (worst case scenario) and, therefore, the risk for secondary poisoning should be assessed. A full guidance of how to derive a RAC based on biomagnification for the food chain from earthworm to earthworm-eating birds and mammals is not yet available. However, following the recommendations from the EFSA opinion on how to derive RAC in water for secondary poisoning (EFSA, 2013) and the guidance of EFSA for the Risk Assessment for birds and mammals (EFSA, 2009) the following approach could be proposed:

$$RAC_{sp} = \frac{NOAEL_{bird\ or\ mammal}}{AF * MF * BCF_{earthworm}}$$

where,

RAC_{sp} = regulatory acceptable concentration in soil for secondary poisoning (mg/kg d.w.)

NOAEL = relevant long-term no-adverse-effect level for birds or mammals (mg/kg b.w./day)

AF = Assessment Factor, a value of 5 applies for chronic risk assessments (EFSA, 2009, 2013)

MF = Multiplication Factor are based on a 10-g mammal eating 12.8 g worms (fresh) per day, and a 100-g bird eating 104.6 g per day. The multiplication factors are 1.28 and 1.05 for mammals and birds, respectively (EFSA, 2009, p.72)

[83] Five is the trigger value for the chronic exposure of macro-organisms, which is compared with the toxicity exposure ratio (TER) for the risk assessment according to the Uniform Principles (Commission Regulation (EU) No 546/2011, EC 2011).

$BCF_{earthworm}$ = bioconcentration factor for earthworms on dry weight basis ($kg_{soil\ d.w.}/kg_{\ earthworm\ fresh\ weight}$), which can be estimated using the following formula:

$$BCF_{earthworm} = \frac{0.84 + 0.012 * K_{ow}}{f_{oc} * K_{oc}} = \frac{0.84 + 0.012 * 100000}{0.02 * 920} = 65$$

where,
K_{ow} = 100000 (Table A2.8, worst case scenario with a log K_{ow} of 5)
f_{oc} = organic carbon content of soil. Default value = 0.02 (EFSA 2009)
K_{oc} = organic carbon adsorption coefficient = 920 (Table A2.8)

For the calculation of the RAC_{sp}, a NOAEL of 1.12 mg/kg b.w./day from a long-term toxicity study with mice (Unknown, 1988/96, cited in the EC DRAR, 2019, Vol 3 B6, p. 96) was selected as the most relevant. The study lasted 104 weeks (over 2 years) and the endpoint was incidence of liver cell tumors. No studies were reported for birds, so only the value for mammals could be derived.

Thus the RAC_{sp} is calculated as follows:

$$\boldsymbol{RAC_{sp}} = \frac{1.12}{5 * 1.28 * 65} = \mathbf{0.0027\ mg\ a.s./kg\ d.w.}$$

2.3.3 Final soil protection value

Considering direct toxicity to soil organisms, a RAC < 0.12 mg a.s./kg d.w. was obtained. Due to the potential bioaccumulation of fluazinam, a RAC_{sp} of 0.0027 mg a.s./kg d.w. was also calculated for secondary poisoning. Since the RAC value for direct toxicity was an unbound value and because the RAC_{sp} was much lower than the RAC for direct toxicity, a final RAC of 0.0027 mg a.s/kg d.w. was proposed for fluazinam.

2.4 European Chemical Agency (ECHA)

2.4.1 Data evaluation

The quality assessment from the studies was based on the evaluation performed by the RMS and no further assessment was needed for the acceptance of the studies.

2.4.2 Derivation of soil protection value

Direct toxicity

Conversion of concentrations to a standard OM content of 3.4 % could be calculated for all studies except for the terrestrial plant tests from Backus (1993a, 1993b). No information about the OM content was provided for those tests and the EC TGD (2003) is unclear about how to treat results, which cannot be normalized. For this reason, the study with terrestrial plants from Fiebig (2006) was preferred.

According to the ECHA (2017, p. 149), if in a two-concentration test with microorganisms, statistical differences are found and effects are > 15 %, no NOEC can be derived and the test cannot be used for risk assessment. This is the case for the N-transformation test from Reis (2002). However, the test provides critical information about the high sensitivity of N-transformation processes towards fluazinam. Therefore, a lower-than NOEC, with the lowest concentration tested is listed among the critical toxicity data for fluazinam (Table A2.10). For the C-transformation test, statistical differences were detected at the highest concentration tested but the lowest concentration did not show differences to the control and the effects were below 15 %. For this reason, a NOEC of 0.40 mg. a.s/kg d.w. was determined for the C-transformation test.

The appropriate derivation method, according to the data availability, is the assessment factor method (EC TGD, 2003, p. 116).

Table A2.10: Critical toxicological data of the terrestrial organisms for fluazinam. If critical values were unbound, they are shown in the table with the appropriate sign. If possible, alternative exact values for the same species/trophic level are also shown in parenthesis.

Group	Species	Parameter	Conc. in mg/kg d.w.*	Literature
Primary producer	*Avena sativa* *Allium cepa* *Beta vulgaris* *Brassica napus* *Daucus carota* *Glycine max*	ER_{50}	≥ 2	Fiebig, 2006 cited in EC DRAR, 2019, Vol. 3 CA B9, p.296
Decomposer (nutrient transformer)	Microorganisms Nitrogen mineralization (Carbon transformation)	NOEC	< 0.40 (0.40)	Reis, 2002 cited in EC DRAR, 2019, Vol. 3 CP B9 – IKF -1216 500 SC, p.181
Decomposer (litter transformer)/Primary consumer	*Eisenia andrei* *(Eisenia fetida)*	NOEC	< 0.12 (4.3)	Römbke & Moser, 1999 cited in EC DRAR, 2019, Vol. 3 CP B9 – IKF -1216 500 SC, p.146 (Edwards & Coulson, 1985 cited in EC DAR, 2006, Vol. 3 CA B9, p.532)

	Folsomia candida	NOEC	< 0.42 (Geometric mean = 2.8; from NOEC = 3.7, EC_{10} = 1.5 and EC_{10} = 3.8)	Klein, 2002 cited in EC DRAR, 2019, Vol. 3 CP B9 – IKF -1216 500 SC, p.166 (Studies for the geometric mean: Lührs, 2016 cited in EC DRAR, 2019, Vol. 3 CP B9 – MCW 465 500 SC, p.211 Klein, 2002 cited in EC DRAR, 2019, Vol. 3 CP B9 – IKF -1216 500 SC, p.166 Neri, 2015 cited in EC DRAR, 2019, Vol. 3 CP B9 – TIFC 500 SC, p.100)
Consumer (Secondary consumer)	*Hypoaspis aculeifer*	NOEC	32	Colli, 2015 cited in EC DRAR, 2019, Vol. 3 CP B9 – TIFC 500 SC, p.103

**Concentrations normalized to 3.4 % organic matter*

According to the EC TGD (2003, p. 118), if there are NOECs for three long-term toxicity tests (from different groups of organisms) an AF of 10 can be used. In Table A2.10, there are NOECs for primary producers, decomposers, decomposers/primary consumers and consumers. For two of the trophic levels (decomposer and decomposer/primary consumer), the NOECs showed < values and for one trophic level (primary producer), the ER_{50} showed ≥ values. For plants, no NOER was reported but a decrease in growth of 20 % was observed for *A. cepa*, which would suggest a NOER lower than the single concentration tested in the study. Although lower than values should be considered the most critical ones, unbounded values should not be used in the calculations of the $PNEC_{soil}$. For this reason, only reliable exact values from Table A2.10 (in parenthesis) were considered for the derivation of $PNEC_{soil}$ but the AF was increased from 10 to 50. In case that more than one toxicity value from different studies for the same species, endpoint and duration exists, a geometric mean of those values should be calculated. This was the case for *F. candida*, and the geometric mean of three studies was provided in Table A2.10[84]. The most sensitive group of organisms (considering only the exact values) were the microorganisms (C-transformation) with a NOEC of 0.40 mg a.s./kg d.w. According to the deterministic method (or AF method), this results in a $PNEC_{soil}$ of:

$$\boldsymbol{PNEC_{soil}} = \frac{NOEC_{norm.}}{AF} = \frac{0.40}{50} = \mathbf{0.008\ mg\ a.s./kg\ d.w.}$$

According to the EC TGD (2003), a normalization to 3.4 % organic matter should be applied to all studies prior the $PNEC_{soil}$ derivation, as it was done in the previous equation. However, in order to compare the results with other methodologies, which do not apply this kind of normalizations, a $PNEC_{soil}$ with the toxicity value of the same organism and endpoint, but not normalized, and with the same AF is also shown:

$$\boldsymbol{PNEC_{soil-not\ normalized}} = \frac{NOEC_{not-norm.}}{AF} = \frac{0.27}{50} = \mathbf{0.0054\ mg\ a.s./kg\ d.w.}$$

Secondary poisoning

According to the EC TGD (2003, p. 123) a substance is potentially bioaccumulative if it has a log K_{ow} > 3. As shown in Table A2.8, fluazinam has a log K_{ow} between 4.5 and 5. The log K_{ow} of fluazinam is higher than the trigger value proposed in the EC TGD (2003) and, therefore, a further evaluation of secondary poisoning is necessary.

Only toxicity studies reporting on dietary and oral exposure are relevant as the pathway for secondary poisoning is referring exclusively to the uptake via the food chain. Results from long-term studies are strongly preferred, such as NOECs for mortality, reproduction or growth (EC TGD, 2003, p. 128).

[84] An EC_{10} for a long-term test which is obtained by extrapolation using appropriate statistics (e.g. probit analysis) can be considered as a NOEC (EC TGD, 2003, p. 98). For this reason, EC_{10} and NOEC have been combined for the geometric mean.

For the calculation of the $PNEC_{oral}$, a NOEC (as a concentration in the food (mg/kg_{food})) from a long-term toxicity study with mouse (Unknown, 1988/96, cited in the EC DRAR, 2019, Vol 3 B6, p. 96) was used. The study lasted 104 weeks (over 2 years) and the endpoint was incidence of liver cell tumors. The study reported a $NOEC_{oral}$ of 10 mg/kg_{food}. Based on the EC TGD (2003, p. 130) an AF of 30 should be applied to the $NOEC_{oral}$:

$$PNEC_{oral} = \frac{TOX_{oral}}{AF_{oral}} = \frac{10\ mg/kg_{food}}{30} = 0.33\ mg/kg_{food} \qquad \textit{Equation 17}$$

Normally, the $PNEC_{oral}$ is expressed in mg/kg_{food} as a soil protection value for worm-eating birds or mammals. Concentration in the food corresponds in this case to the concentration in the earthworms. The total concentration of a substance in the worm is the result of bioaccumulation in worm tissues and the adsorption of the substance to the soil present in the earthworm gut. Since birds and mammals consume earthworms including their gut contents, the concentration of the substance in the predator may be affected by the amount of substance that is in the soil. The $PNEC_{oral}$ calculated above could therefore be converted into a soil concentration ($PNEC_{oral,soil}$). This can be achieved by doing a back calculation equivalent to what is used to estimate the $PEC_{oral,predator}$ in chemical risk assessment (EC TGD, 2003, p. 131). For the back calculation, it is assumed that the concentration of the substance in the earthworm ($C_{earthworm}$) is equal to the $PNEC_{oral}$

$$PNEC_{oral} = C_{earthworm}$$

where,

$C_{earthworm}$ = total concentration of the substance in the worm as a result of bioaccumulation in worm tissues and the adsorption of the substance to the soil present in the gut ($mg/kg_{wet\ earthworm}$)

Consequently, the resulting concentration of the substance in the soil (C_{soil}) should be equivalent to the $PNEC_{oral,soil}$

$$C_{soil} = PNEC_{oral,soil}$$

The total concentration in a full worm can be calculated as the weighted average of the worm's tissues (through bioconcentration factor (BCF) and pore water) and gut contents (through soil concentration). However, it is mentioned in EC TGD (2003, p. 132) that, when measured data on bioconcentration in worms is available, the measured data can be used instead of the calculations via bioconcentration factor (BCF) and pore water. This is the case for fluazinam, in which a bioaccumulation experiment from Winkelmann (2015) was submitted in the EC DRAR (2019, Vol. 3 CP B9 – MCW 465 500 SC, p. 199) and considered valid by the RMS. The guidance provided in the TGD (2003) on how to proceed with data obtained from experimental bioaccumulation studies is very limited. In order to complete the information, the RIVM (2007, p. 94), which used the same approach, was also consulted and the following equation was applied:

$$PNEC_{oral,soil} = \frac{C_{earthworm} * (1 + F_{gut} * CONV_{soil})}{BAF_{earthworm} + F_{gut}} \qquad \textit{Equation 18}$$

where,

$C_{earthworm}$ = total concentration of the substance in the worm as a result of bioaccumulation in worm tissues and the adsorption of the substance to the soil present in the gut ($mg/kg_{wet\ earthworm}$)

F_{gut} = fraction of gut loading in worm (kg_{ww}/kg_{dw})

$CONV_{soil}$ = conversion factor for soil concentration wet-dry weight soil (kg_{ww}/kg_{dw})

$BAF_{earthworm}$[85] = Bioaccumulation factor ($kg_{dw\ soil}/kg_{ww\ earthworm}$)

In order to use the results from experimental bioaccumulation studies with earthworms, the Bioaccumulation Factor (BAF) should be provided and expressed as the ratio between the concentration in

[85] The terminology used for bioaccumulation experiments is differently applied by RIVM (2007) and the EC DRAR (2019) (which, in turn, this last one uses the terms of the OECD guideline 317 (OECD, 2010)). The term "BAF" used in the EC DRAR (2019) corresponds to the "BSAF" mentioned in RIVM (2007). In this section the terminology used in the EC DRAR (2019), and thus in the OECD guideline 317, has been applied and the terms in the RIVM equations changed accordingly.

soil based on dry weight and the concentration in worms based on wet weight. The experiment provided the results in dry weight as well as in wet weight, for both earthworm and soil (BAFk dw = 0.452 kgsoil/kgearthworm and BAFk fw = 0.0909 kgsoil/kgearthworm). Therefore, some unit transformations have been first applied according to information given in the study:

Equation 19

$$BAF_k = BAF_{k\,dw} * ratio\ WDW{:}WFW = 0.452 * 0.158 = 0.0714\ kg_{dw\ soil}/kg_{ww\ earthworm}$$

where,

BAF_k = kinetic bioaccumulation factor[86] ($kg_{dw\ soil}/kg_{ww\ earthworm}$)

$BAF_{k\,dw}$ = kinetic bioaccumulation factor on dry weight basis ($kg_{dw\ soil}/kg_{dw\ earthworm}$)
= 0.452 $kg_{dw\ soil}/kg_{dw\ earthworm}$ (Winkelmann, 2015, cited in EC DRAR, 2019, Vol. 3 CP B9 – MCW 465 500 SC, p.206)

ratio WDW:WFW = mean ratio of the average of worm dry weight (WDW) and fresh weight (WFW) from control replicates ($kg_{dw\ earthworm}/kg_{ww\ earthworm}$)
= 0.158 $kg_{dw\ earthworm}/kg_{ww\ earthworm}$ (Winkelmann, 2015, cited in EC DRAR, 2019, Vol. 3 CP B9 – MCW 465 500 SC, p.202)

In RIVM (2007) it is mentioned that the results from the bioaccumulation studies should be normalized to the standard soil of the EC TGD (2003), i.e., to 2 % of soil organic carbon. In order to perform the normalization according to the RIVM (2007, p. 104), the BAF was recalculated as follows:

Equation 20

$$BAF_{earthworm} = BAF_k * \frac{Foc_{soil\ TGD}}{Foc_{soil\ exp}} = 0.0714 * \frac{0.02}{0.03} = 0.0476\ kg_{dw\ soil}/kg_{ww\ earthworm}$$

where,

$BAF_{earthworm}$ = Bioaccumulation factor ($kg_{dw\ soil}/kg_{wwt\ earthworm}$)

BAF_k = kinetic bioaccumulation factor on dry weight basis ($kg_{dw\ soil}/kg_{dw\ earthworm}$)
= 0.0714 $kg_{dw\ soil}/kg_{ww\ earthworm}$ (eq. 14)

$Foc_{soil\ exp}$ = weight fraction of organic carbon in the soil compartment from the experiment ($kg_{OC}/kg_{dw\ soil}$) = 0.03 $kg_{OC}/kg_{dw\ soil}$ (Winkelmann, 2015, cited in EC DRAR, 2019, Vol. 3 CP B9 – MCW 465 500 SC, p.207)

$Foc_{soil\ TGD}$ = weight fraction of organic carbon in the soil compartment for standard soil according to the EC TGD (2003) ($kg_{OC}/kg_{dw\ soil}$) = 0.02 $kg_{OC}/kg_{dw\ soil}$ (EC TGD, 2003, p. 43)

$CONV_{soil}$ can be calculated using the following equation (EC TGD, 2003, p. 132):

Equation 21

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid\ soil} * RHO_{solid}} = \frac{1700}{0.6 * 2500} = 1.1\ kg_{ww}/kg_{dw}$$

where,

RHO_{soil} = bulk density of wet soil (kg_{ww}/m^3) = 1700 kg_{ww}/m^3 (EC TGD, 2003, p.44)

RHO_{solid} = density of the solid phase ($kg_{dw\ solid}/m_{solid}^3$) = 2500 kg_{dw}/m^3 (EC TGD, 2003, p.43)

$F_{solid\ soil}$ = volume fraction of solids in soil (m_{solid}^3/m_{soil}^3) = 0.6 m^3/m^3 (EC TGD, 2003, p.43)

The following parameters can be assumed to calculate the $PNEC_{oral,soil}$:

$BAF_{earthworm}$ = 0.0476 $kg_{dwt\ soil}/kg_{wwt\ earthworm}$ (from eq. 15)

F_{gut} = fraction of gut loading in earthworm = 0.1 kg_{dw}/kg_{ww} (EC TGD, 2003, p. 132)

$CONV_{soil}$ = 1.1 kg_{ww}/kg_{dw} (from eq. 16)

$C_{earthworm}$ = $PNEC_{oral}$ = 0.33 mg/kg_{food} (from eq. 12)

[86]There are two types of BAF. If the steady state is reached during the uptake phase, the steady state bioaccumulation factor (BAF_{ss}) should be calculated. In case that the steady state is not reached, like in the study from Winkelmann (2015), the kinetic bioaccumulation factor (BAF_k), determined from the uptake and elimination rate constants, should be provided instead (OECD guideline 317 (OECD, 2010)).

$$\boldsymbol{PNEC_{oral,soil}} = \frac{C_{earthworm} * (1 + F_{gut} * CONV_{soil})}{BAF_{earthworm} + F_{gut}} = \frac{0.33(1 + 0.1 * 1.1)}{0.0476 + 0.1} = \boldsymbol{2.48\ mg\ a.s./kg_{dw}}$$

2.4.3 Final soil protection value

A $PNEC_{soil}$ of 0.008 mg a.s./kg d.w. from direct toxicity to soil organisms was obtained. It should be mentioned that no test with the potentially most sensitive group of organisms (fungi since fluazinam is a fungicide) was reported an assessment with additional studies with fungi could presumably change the $PNEC_{soil}$. Due to the potential bioaccumulation of fluazinam, a $PNEC_{soil}$ of 2.48 mg a.s./kg d.w. was also calculated for secondary poisoning. Although there is no clear mention of which strategy to follow when two $PNEC_{soil}$ with different exposure pathways (direct exposure and secondary poisoning) can be derived, it seems reasonable to choose the lowest value. In this case, in order to protect in-soil organisms from direct toxicity, a final **$PNEC_{soil}$ of 0.008 mg a.s./kg d.w.** has been chosen for fluazinam.

2.5 The Netherlands – RIVM (2007)

2.5.1 Data evaluation

In general, the quality assessment from the studies follows the system developed by (Klimisch et al. (1997). However, since there has been already an evaluation from RMS and the quality assessment would bring to similar results, no re-evaluation has been performed and the validity from RMS regarded as face value.

2.5.2 Derivation of soil protection value

Direct toxicity

For this case study, exactly the same considerations as the ones applied for the EC TGD (2003) could be assumed. Only the considerations for the microorganism studies were different (as mentioned already in the case study of diuron). In this case, only the C-transformation study was considered, since the N-transformation test had one concentration with an effect > 70 %. Because the two tested concentrations had a difference between the effect concentrations smaller than 15 % (6.05 % - 2.89 % = 3.16 %), the average of the two concentrations is suggested as the NOEC. This results in a NOEC of 5.6 mg a.s./kg d.w. when values are normalized to 10 % of organic matter. In this case, microorganisms would also be the most sensitive organisms, since the geometric mean for *F. candida* from the studies by Lührs (2008), Klein (2002) and Neri (2015), which is the following lowest value, gives a NOEC of 8.1 mg a.s./kg d.w. (geometric mean of 10.8, 4.5 and 11 mg a.s./kg d.w.). For this reason, the same procedure as the one applied for the $PNEC_{soil}$ was used but with the data normalized to 10 % organic matter (recommended for the Dutch standard soils). The final $MPC_{eco,soil}$ for fluazinam is:

$$\boldsymbol{MPC_{eco,soil}} = \frac{NOEC_{norm.}}{AF} = \frac{5.6}{50} = \mathbf{0.11\ mg\ a.s./kg\ d.w.}$$

According to the RIVM (2007), a normalization to 10 % organic matter should be applied to all studies prior the $MPC_{eco,soil}$ derivation, as it was done in the previous equation. However, in order to compare the results with other methodologies, which do not apply this kind of normalizations, a $MPC_{eco,soil}$ with the toxicity value of the same organism and endpoint, but not normalized, and with the same AF is also shown:

$$\boldsymbol{MPC_{eco,soil-not\ normalized}} = \frac{NOEC_{not-norm.}}{AF} = \frac{1.27}{50} = \mathbf{0.025\ mg\ a.s./kg\ d.w.}$$

Secondary poisoning

The assessment of secondary poisoning follows the EC TGD (2003). Therefore, the process described in section 2.3.2 can be applied here as well. Differently to the EC TGD (2003) where the calculations for the $PNEC_{oral,soil}$ assumed a soil organic carbon content of 2 %, a correction has to be applied to adapt the MPC for secondary poisoning in soil ($MPC_{sp,soil}$) to a standard Dutch soil with a soil organic carbon content of 5.88 %. So the final $MPC_{sp,soil}$ follows this equation[87] from RIVM (2007, p. 95 and 104):

$$MPC_{sp,soil} = \frac{Foc_{Dutch\ standard\ soil}}{Foc_{soil,TGD}} * PNEC_{oral,soil}$$

where,

$MPC_{sp,soil}$ = Maximum Permissible Concentration for secondary poisoning in soil (mg/kg d.w.)

$Foc_{Dutch\ standard\ soil}$ = fraction of organic carbon in Dutch standard soil (kg/kg) = 0.0588 kg/kg

$Foc_{soil,TGD}$ = weight fraction of organic carbon in soil as defined in the EC TGD (2003) (kg/kg) = 0.02 kg/kg

$PNEC_{oral,soil}$ = Predicted no Effect concentrations for secondary poisoning in soil as defined in the EC TGD (2003) = 2.48 mg a.s./kg d.w.

[87] For clarity, this equation has been slightly modified for this report.

Thus the $MPC_{sp,soil}$ can be calculated as follows:

$$\boldsymbol{MPC_{sp,soil}} = \frac{0.0588}{0.02} * 2.48 = \boldsymbol{7.3\ mg\ a.s./kg\ d.w.}$$

2.5.3 Final soil protection value

Since there was no change in the methodology, the same situation as for the EC TGD (2003) took place. The MPC for direct toxicity in soil was lower than the MPC for secondary poisoning. Therefore, a **final $MPC_{eco,soil}$ of 0.11 mg a.s./kg d.w.** was proposed.

2.6 Canada – CCME (2006)

As mentioned in the case study for diuron, only the exposure pathways for the agricultural land use will be described in this chapter.

2.6.1 Data evaluation

Studies should be screened according to whether they should be considered “acceptable” or “unacceptable” for the derivation of the soil protection values. The exhaustive assessment performed by the RMS was considered sufficient and comparable and no further re-assessment was considered necessary.

2.6.2 Derivation of soil protection value

The protection values we considered for fluazinam for agricultural soils are: soil contact (SQG_{SC}), and soil and food ingestion procedure (SQG_{I}). For fluazinam, the soil to groundwater pathway was not considered, since this substance has low solubility (from 0.106 to 2.72 mg/L (Table A2.8)). Therefore, the SQG for freshwater live (SQG_{FL}), livestock watering (SQG_{LW}) and irrigation water (SQG_{IR}) were not derived. There was insufficient data on microbial transformation processes. For this reason, the nutrient and energy cycling check (SQG_{NEC}) could not be derived either.

Soil Quality Guideline for Soil contact (SQG_{SC})

Data selection according to soil type and bioavailability considerations

The terrestrial tests for earthworms, collembolans, mites and plants (seedling emergence test) described in Table A2.9 were performed with similar soil textures. Although no exact information about the final texture of the soil is given for the tests performed with artificial soils, it was assumed, as a worst-case scenario, that the sand used for the tests was coarse. Therefore, a single SQG_{SC} for coarse-grained soils was derived.

The bioavailability conditions of the studies listed in Table A2.9 were assessed. The organic carbon content and pH of studies with soil invertebrates were within the range of acceptable studies for the derivation of SQG_{SC}. For plants, only the study from Fiebig (2006) reported the type of soil used (LUFA No. 2.3), which it is also in the range of acceptable bioavailability conditions. No information on the bioavailability conditions could be derived from the other plant studies listed in Table A2.9.

Derivation of the Soil Quality Guideline for Soil Contact (SQG_{SC})

Derivation of the Threshold Effects Concentration (TEC)

In Table A2.9, there are more than ten data points from three different studies, which is the minimum data requirement for the “weight of evidence” method. The preferred toxicity parameter would be EC_{25}. Since there were no EC_{25} described in the toxicity tests of Table A2.9, the LOEC, NOEC or EC_{50} (in this order of preference) could be used instead. Eight data points are from soil invertebrates and 13 from plants. Although the minimum requirements are met for the “weight of evidence” method, there is no mention in the CCME (2006) how to proceed with unbound data. For fluazinam, only few studies showed exact data. For this reason, expert judgement was applied and the “lowest observed effect concentration” method with exact data was used instead. In order to apply this method, a minimum of three studies including one invertebrate and one plant study should be present. Three plant studies were listed in Table A2.9 for fluazinam. However, since there are no exact values for endpoints from plants, plant studies were not considered for the TEC derivation but the minimum data requirements to apply this method were still considered fulfilled.

For the “lowest observed effect concentration” method the lowest effect concentration (LOEC) divided by an uncertainty factor (UF) (if needed) is used to derive the TEC. In this case, the collembolan *F. candida* showed the lowest effect concentrations. Because there are two reproduction studies with exact LOECs for *F. candida* (studies from Lührs, 2008 and Neri, 2015) a geometric mean of 12 mg a.s./kg d.w. from the two LOECs has been proposed for the TEC derivation. According to the CCME (2006, p. 55) the magnitude of the UF is determined by expert judgement. In this case, although there are the

minimum number of studies (three) representing different taxonomic orders and the LOEC for earthworms is taken from a chronic study, there is only three exact LOEC, two of them for the same species, and no exact values for plants in the dataset. Therefore, the maximum UF of 5 is applied:

$$TEC = \frac{lowest\ LOEC}{UF} = \frac{12\ mg\ a.s./kg\ d.w.}{5} = 2.4\ mg\ a.s./kg\ d.w.$$

Derivation of the Soil Quality Guideline for Nutrient and Energy Cycling (SQG_{NEC})

In the CCME (2006, p.135), there are several methods described to calculate the SQG_{NEC}. Data on nitrogen-fixation and nitrification is preferred but data on nitrogen mineralization and carbon cycling may be used as well. For fluazinam, there are two reliable studies, one on carbon transformation and one on nitrogen mineralization (Reis, 2002). However, a minimum of three studies is required to derive a SQG_{NEC} using any of the methods mentioned in the guideline. Due to insufficient data, no SQG_{NEC} could be derived for fluazinam.

Derivation of the SQG_{SC}

A comparison between the TEC and the SQG_{NEC} was not possible, since no value for the SQG_{NEC} could be derived for fluazinam. For this reason, the SQG_{SC} is equal to the TEC:

SQG_{SC} = 2.4 mg a.s./kg d.w.

Soil Quality Guideline for Soil and Food Ingestion (SQG_I)

Fluazinam has a log K_{ow} of 5 (worst case-scenario described in Table A2.8, equivalent to a K_{ow} of 10^5). A $K_{ow} > 10^5$ is, according to the CCME (2006, p. 13), the trigger value to include, not only herbivores grazing on agricultural lands, but also wildlife in the derivation of SQG_I. Therefore, wildlife should also be considered in the derivation of the SQG_I.

According to the CCME (2006, p.57), oral toxicological data should be used for the derivation of the SQG_I. The minimum data requirements are:

- A minimum of three studies
- At least two of the studies must be oral mammalian studies and one oral avian study
- A maximum of one laboratory rodent study can be used
- A grazing herbivore (e.g., ungulates) with a high ingestion rate to body weight ration should be considered

For fluazinam, no feeding studies with ruminants were submitted in the EC DRAR (2019, Vol. 1, p. 59). In the report, it is mentioned that, the calculated dietary burden for livestock did not exceed the trigger value and, therefore, no feeding studies were required.
By lacking a grazing herbivore study, the minimum data requirements to determine the Daily Threshold Effects Dose (DTED) could not be met and therefore the derivation of a SQG_I for fluazinam was not possible.

2.6.3 Final soil protection value

According to the CCME (2006, p. 79), there must be at least sufficient data points to calculate the SQG_{SC} in order to set a SQG_E. Moreover, if the contaminant biomagnifies, the pathway Soil and Food Ingestion becomes a required pathway and its evaluation is essential for the derivation of the SQG_E. Although a SQG_{SC} (for coarse-grained soils) of 2.4 mg a.s./kg d.w. could be derived, for the reasons previously mentioned, no final SQG_E could be proposed for fluazinam.

2.7 United States of America – US EPA (2005)

2.7.1 Data evaluation

A detailed description of the application of the US EPA (2005) study evaluation process is described previously in section 4.1 “General considerations” of the main report and for the case study of diuron. Similar to diuron, some of the studies listed in Table A2.9 for fluazinam could not pass step 1 (Literature Exclusion Criteria). The studies with *E. fetida* (Winkelmann, 2016), *E. andrei* (Römbke & Moser, 1999), *H. aculeifer* (Schulz, 2016) and with terrestrial plants (Backus, 1993 a and b and Fiebig, 2006) failed the criterion 13 from the Literature Exclusion Criterion: “No effect reported for a biological test species”. These studies reported only unbound values and thus, no exact effect could be extracted from them. The studies listed in Table A2.11 are the ones that passed step 1 and 2 and could be scored according to the Study Evaluation Criteria.

As indicated in US EPA (2005, p. 3-4), if a study presented multiple endpoints and/or toxicity parameters, only the most relevant one should be recorded. Justifications are provided in Table A2.11 if criteria were scored with 1 or 0.

Table A2.11: Study evaluation criteria and scoring for the studies of Table .

Criteria	***E. fetida (weight)*** (Edwards & Coulson, 1985)	***F. candida (reproduction)*** (Lührs, 2008)	***F. candida (reproduction)*** (Klein, 2002)	***F. candida (reproduction)*** (Neri, 2015)	***H. aculeifer (reproduction)*** (Colli, 2015)
Testing was Done Under Conditions of High Bioavailability (very high or high = 2, medium = 1, low or very low = 0)	1[88]	1[89]	1[88]	1[89]	1[89]
Experimental Designs were Documented and Appropriate	1[90]	2	2	2	2
Concentration of Substance of Interest in Soil was Reported	1[91]	1[91]	1[91]	1[91]	1[91]
Control Responses were Acceptable	1[92]	2	2	2	2
Chronic or Life Cycle Test was Used	2	2	2	2	2
Chemical Dosing Procedure was Reported and appropriate for Chemical and Test	0[93]	0[93]	0[93]	0[93]	0[93]
A Dose-Response Relationship is Reported or can be Established from Reported Data	1[94]	2	2	2	2
The Statistical Tests used to Calculate the Benchmark and the Level of Significance were Described	1[95]	2	2	2	2
The Origin of the Test Organisms was Described	1[96]	2	2	2	2
Total score	**9**	**14**	**14**	**14**	**14**

[88] Standard artificial soils with approx. 10 % OM, 20 % kaolinite, 69 % sand, 1 % CaCO3 are assigned a medium bioavailability score of 1
[89] Standard artificial soils with approx. 5 % OM
[90] Only four concentrations tested (including the control)
[91] Toxicity values based on nominal concentrations
[92] Results of negative controls not reported
[93] No information of the carrier or vehicle used to deliver the chemical
[94] Difference between the NOEC and LOEC is 10-fold
[95] ANOVA was performed but p-level was not provided
[96] Sufficient information about the organisms was not provided

Studies are deemed appropriate for deriving Eco-SSLs if they score above ten. The earthworm study was the only study that scored below 10. Consequently, this study was not considered for the derivation of an Eco-SSL.

2.7.2 Derivation of soil protection value

Direct toxicity

More than three acceptable studies for soil invertebrates were available for fluazinam. Therefore, the geometric mean of the following data points was used for the derivation of the Eco-SSL for soil invertebrates:

Study	Parameter
F. candida (reproduction) (Lührs, 2008)	MATC = 7.6 mg a.s./kg d.w.
F. candida (reproduction) (Klein, 2002)	EC_{10} = 4.5 mg a.s./kg d.w.
F. candida (reproduction) (Neri, 2015)	MATC = 9.2 mg a.s./kg d.w.
H. aculeifer (reproduction) (Colli, 2015)	EC_{10} = 47 mg a.s./kg d.w.

$$\boldsymbol{Eco - SSL_{soil\ invertebrates}} = \sqrt[4]{7.6 * 4.5 * 9.2 * 47} = \boldsymbol{11\ mg\ a.s./kg\ d.w.}$$

Secondary poisoning (Eco-SSL Wildlife)

As mentioned for the case study of diuron, Eco-SSL Wildlife was not derived in this report.

2.7.3 Final soil protection value

Since the exposure route via secondary poisoning could not be calculated for fluazinam, a final **Eco-SSL** due to direct toxicity of **11 mg a.s./kg d.w.** was suggested.

2.8 Australia – NEPC 2013

As already mentioned in the case study for diuron, only the soil protection values for the agricultural land use will be derived in this chapter.

According to the categories described in NEPC (2013), fluazinam is a substance with a slow biodegradation in soil ($DT_{50,soil}$ > 45 days (if the average of the two values listed in Table A2.8 is taken), moderate volatility (K_H dimensionless: between 2.5e-3 and 2.5e-7) and has high potential to biomagnify (log K_{ow} ≥ 4) (Table A2.8). Thus, the two exposure routes that are considered the most important after combining the three physicochemical properties are biomagnification and direct toxicity (see NEPC, 2013, p.11 for further information). Both exposure routes were evaluated.

2.8.1 Data evaluation

A detailed description of the application of the study evaluation process is described previously in section "4.1 General considerations" of main report and for the case study of diuron.

One of the criteria to consider a study acceptable (step 1) is that the difference between tested concentrations cannot be greater than five-fold. The studies with *E. fetida* (Edwards & Coulson, 1985; Yearsdon et al., 1991) had a difference of more than five-fold between the concentrations. For this reason, they could not be considered further in the study evaluation process. The studies with microorganisms (Reis, 2002) and with the terrestrial plants (Backus, 1993a and b; Fiebig, 2006) were part of the first tier in the registration process for PPP, in which only two concentrations and one concentration were tested, respectively. Similar to what was described for diuron, there are not really clear statements of what to do in case of standard studies performed with only one or two concentrations instead of with a range of concentrations. However, this kind of test designs are recommended by the OECD guidelines for the testing of PPP with microorganisms (OECD, 2000a, 2000b) and with terrestrial plants (OECD, 2006a, 2006b). As they represent standard test designs used for PPPs, they were accepted for the derivation of an EIL. Due to the single concentration tested for terrestrial plants, the same EC_{50} was determined for all 13 plant species. In this case, it would not make sense to include all the plant species in the SSD and, instead, the species will be grouped according to their sensitivity (accounted as percentage of effect) for the representation. The studies with earthworms *E. fetida* (Winkelmann, 2016) and *E. andrei* (Römbke & Moser, 1999), the collembolan *F. candida* (Klein, 2002; Lührs, 2008; Neri, 2015), and the mite *H. aculeifer* (Colli, 2015; Schulz, 2016) fulfilled all the criteria, and were therefore considered acceptable. The following quality assessment for the studies with earthworms, collembolans, mites, microorganisms, and plants are shown in Table A2.12.

As indicated in the diuron case study, justifications are provided in Table A2.12 if criteria were not scored with the maximum score. In case, some of the questions did not proceed because of the nature of the experimental conditions, we considered the question "not applicable" and the final score was re-calculated accordingly.

Table A2.12: Quality assessment performed according to NEPC (2013) for the studies with earthworms E. fetida *(Winkelmann, 2016) and* E. andrei *(Römbke & Moser, 1999), the collembolan* F. candida *(Klein, 2002; Lührs, 2008; Neri, 2015), the mite* H. aculeifer *(Colli, 2015; Schulz, 2016), microorganisms (Reis, 2002) and terrestrial plants (Backus, 1993a and b; Fiebig, 2006) (EC DRAR, 2019).*

Question		***E. fetida*** (Winkelmann, 2016)	***E. andrei*** (Römbke & Moser, 1999)	***F. candida*** (Klein, 2002)	***F. candida*** (Lührs, 2008)	***F. candida*** (Neri, 2015)	***H. aculeifer*** (Colli, 2015)	***H. aculeifer*** (Schulz, 2016)	**C- and N-transformation** (Reis, 2002)	**Plants** (Backus, 1993a and b)	**Plants** (Fiebig, 2006)
1	Was the duration of the exposure stated (e.g., 48 or 96 h)? (10 or 0 marks)	10	10	10	10	10	10	10	10	10	10
2	Was the biological end-point (e.g., immobilisation or population growth) stated and defined (10 marks)? Award 5 marks if only the biological endpoint is stated.	10	10	10	10	10	10	10	10	10	10
3	Was the biological effect stated (e.g., LC or NOEC)? (5 or 0 marks)	5	5	5	5	5	5	5	not applicable	5	5
4	Was the biological effect quantified (e.g., 50% effect, 25% effect)? The effect for NOEC and LOEC data must be quantified. (5 or 0 marks)	5	5	5	5	5	5	5	5	not applicable	not applicable
5	Were appropriate controls (e.g., a non-toxicant control and/or solvent control) used? (5 or 0 marks)	5	5	5	5	5	5	5	5	5	5
6	Was each control and contaminant concentration at least duplicated? (5 or 0 marks)	5	5	5	5	5	5	5	5	5	5
7	Were test acceptability criteria stated (e.g., mortality in controls must not exceed a certain percentage) (5 marks)? or Were test acceptability criteria inferred (e.g., test method used (US EPA, OECD,	2	2	2	2	2	2	2	2	2	2

	Question	*E. fetida* (Winkelmann, 2016)	*E. andrei* (Römbke & Moser, 1999)	*F. candida* (Klein, 2002)	*F. candida* (Lührs, 2008)	*F. candida* (Neri, 2015)	*H. aculeifer* (Colli, 2015)	*H. aculeifer* (Schulz, 2016)	**C- and N-transformation** (Reis, 2002)	**Plants** (Backus, 1993a and b)	**Plants** (Fiebig, 2006)
	ASTM etc.)) (award 2 marks). Note: Invalid data must not be included in the database.										
8	Were the characteristics of the test organism (e.g., length, mass, age) stated? (5 or 0 marks)	5	5	5	5	5	5	5	not applicable	5	5
9	Was the type of test media used stated? (5 or 0 marks)	5	5	5	5	5	5	5	5	5	5
10	Were the contaminant concentrations measured? (4 or 0 marks)	0[97]	0[97]	0[97]	0[97]	0[97]	0[97]	0[97]	0[97]	0[97]	4
11	Were parallel reference toxicant toxicity tests conducted? (4 or 0 marks)	4	4	4	4	4	4	4	4	0[98]	0[58]
12	Was there a concentration–response relationship either observable or stated? (4 or 0 marks)	0[99]	4	4	4	4	4	0[99]	not applicable	0[99]	0[99]
13	Was an appropriate statistical method or model used to determine the toxicity? (4 or 0 marks)	4	4	4	4	4	4	4	4	4	4
14	For NOEC/LOEC data, was the significance level 0.05 or less? (4 or 0) or For LC/EC/BEC data, was an estimate of variability provided? (4 or 0)	0[100]	4	4	4	4	4	0[100]	not applicable	0[100]	0[100]
15	Were the following parameters measured and stated? (3 marks if measured and stated, 1 if just measured) pH (3, 1 or 0 marks)										

[97] Only nominal concentrations.
[98] Referent toxicant tests not performed.
[99] Concentration-response relationship was not observed, since there was no effect at the maximum effect concentration (earthworms (Winkelmann, 2016), mites (Schulz, 2016)) or at the single application (plants (Backus, 1993a and b; Fiebig, 2006)).

Question		***E. fetida*** (Winkelmann, 2016)	***E. andrei*** (Römbke & Moser, 1999)	***F. candida*** (Klein, 2002)	***F. candida*** (Lührs, 2008)	***F. candida*** (Neri, 2015)	***H. aculeifer*** (Colli, 2015)	***H. aculeifer*** (Schulz, 2016)	**C- and N-transformation** (Reis, 2002)	**Plants** (Backus, 1993a and b)	**Plants** (Fiebig, 2006)
	OM or OC content (3, 1 or 0 marks)	3	3	3	3	3	3	3	3	0[100]	0[100]
	Clay content (3, 1 or 0 marks)	3	3	3	3	3	3	3	3	0[100]	3
	CEC (3, 1 or 0 marks)	3	3	3	3	3	3	3	3	0[100]	0[100]
		0[100]	0[100]	0[100]	0[100]	0[100]	0[100]	0[100]	3	0[100]	0[100]
16	Was the temperature measured and stated? (3 or 0 marks)	3	3	3	3	3	3	3	3	3	3
17	Was the grade or purity of the test contaminant stated? (3 or 0 marks)	3	3	3	3	3	3	3	3	3	3
18	Were other cations and/ or major soil elements measured? (3 or 0 marks) or Were known interacting elements on bioavailability measured (e.g., Mo for Cu and Cl for Cd)? (3 or 0 marks)	0[101]	0[101]	0[101]	0[101]	0[101]	0[101]	0[101]	0[101]	0[101]	0[101]
19	For spiked soils with metal salts: were the soils leached after spiking? (3 or 0 marks)	not applicable	not applicable	not applicable	not applicable	not applicable	not applicable	not applicable	not applicable	not applicable	not applicable
20	Were the incubation conditions and duration stated? (3, 1 or 0 marks)	3	3	3	3	3	3	3	3	3	3
	Total score ([Total score / 99, 81 or 94] * 100)[102]	79 %	87 %	87 %	87 %	87 %	87 %	79 %	88 %	64 %	71 %
	Quality class (H ≥ 80 %, A 51 %–79 %, U ≤ 50 %)	A	H	H	H	H	H	A	H	A	A

[100] No information was given in the experimental conditions.
[101] No information of cations, major soil elements or other elements interacting on bioavailability were given.
[102] In the NEPC (2013) the maximum total score is 102. Because we considered some of the questions not applicable for the evaluated tests, the maximum total score applied is 99 for *E. fetida* (Winkelmann, 2016), *E. andrei* (Römbke & Moser, 1999), *F. candida* (Klein, 2002, Lührs, 2008, Neri, 2015) and *H. aculeifer* (Colli, 2015, Schulz, 2016), 94 for the plant tests (Backus, 1993a and b; Fiebig, 2006), and 81 for the C- and N-transformation tests (Reis, 2002). Quality class: H = high quality, A = acceptable, U = unacceptable.

The total score of the data is higher than 80 % for all studies, except for the plant studies, the study with *E. fetida* and the mite study from Schulz (2016), which had scores between 51 and 79 %. Therefore, the studies can be considered of high quality or acceptable. The last step (step 3) is the standardisation of the toxicity data according to the following factors:

- Measures of toxicity:
  According to the guidance, toxicity data should be grouped according to the percentage of the effect caused at the given concentration in the following way: NOEC and EC_{10} group, if the effect ranges from 0 % to <19%; LOEC and EC_{30} group, if the effect ranges from 20 % to 40%; or EC_{50} group, if the effect ranges from > 40 % to 60%. In Table A2.13, the original toxicity parameters and the respective group according to the percentage of the effect are described.
  Unbounded values either with no effects at the highest tested concentrations (> values) or with effects already at the lowest concentration tested (< values) can be used for the SSD and were treated similarly. The percentage of the effect at that concentration was examined and grouped according to the effect ranges, as mentioned above.

  Values in the LOEC and EC_{30} group should be preferred and, in case that they are not available and other toxicity parameters are reported, they could be converted to this group by applying some conversion factors, which according to the guidance, were initially used for metals. The equivalences for the conversions are the following and were applied, if needed, to the toxicity parameters in Table A2.13:

  $$LOEC\ or\ EC_{30} = \frac{EC_{50}}{2}$$

  $$LOEC\ or\ EC_{30} = NOEC\ or\ EC_{10} * 2.5$$

  For plant species, the magnitude of the adverse effect was checked for each plant species. According to NEPC (2013, p. 27), in case there are several endpoints for the same species, the most sensitive endpoint should be use. Thus, only the most sensitive endpoint of each plant species was used for the SSD. Two groups of effects could be detected for plants: more sensitive plants (group 1) with effect concentrations between 20 % and 40 % effect; and less sensitive plants (group 2) with effect concentrations below 19 % effect (Table A2.13). In case that more than one toxicity value from different studies for the same species, endpoint and duration existed, a geometric mean of those values was calculated (NEPC, 2013, p. 27). This was the case for *F. candida* and *H. aculeifer*.

- Duration of the exposures:
  All studies are considered chronic, so no conversion is needed.

Other two standardization factors are described “Conversion from total to added concentrations” and “The use of toxicity data for endemic or overseas species” but they are considered not relevant for this case.

Table A2.13: List of studies selected for the EIL derivation. For each study the following information was reported: the species or functional process, the taxonomic or nutrients group, toxicity parameters reported in the original source with the effect concentration in parenthesis, group of toxicity data, and value converted into LOECs or EC_{30} group (in parenthesis it is indicated if the value is the result of a conversion factor or a geometric mean). Abbreviations: CF= Conversion Factor (applied to the original toxicity parameter).

Species or functional process (study)	**Taxonomic or nutrient group**	**Toxicity parameter (mg a.s./kg d.w.)**	**Group**	**LOEC and EC_{30} group (mg a.s /kg d.w.)**
Eisenia fetida (Winkelmann, 2016)	Annelida	NOEC ≥ 3.9 (13.2 % effect)	NOEC and EC_{10}	LOEC > 9.8 (CF: 2.5)
Eisenia andrei (Römbke & Moser, 1999*)*	Annelida	NOEC < 0.35 (54.3 % effect)	EC_{50}	LOEC < 0.18 (CF: 0.5)
Folsomia candida (Lührs, 2008)	Hexapoda	LOEC = 10.8 (29 % effect)	LOEC and EC_{30}	LOEC = 10.8
Folsomia candida (Klein, 2002)	Hexapoda	NOEC < 1.2 (7.7 % effect)	NOEC and EC_{10}	LOEC < 3.0 (CF: 2.5)
Folsomia candida (Neri, 2015)	Hexapoda	LOEC = 12.4 (19.5 % effect)	LOEC and EC_{30}	LOEC = 12.4
Folsomia candida (all three studies)	Hexapoda	-	-	LOEC = 7.4 (geometric mean)
Hypoaspis aculeifer (Schulz, 2016)	Chelicerata	NOEC ≥ 110 (7.1 % effect)	NOEC and EC_{10}	LOEC > 275 (CF: 2.5)
Hypoaspis aculeifer (Colli, 2015)	Chelicerata	EC_{10} = 47 (10 % effect)	NOEC and EC_{10}	LOEC = 118 (CF: 2.5)
Hypoaspis aculeifer (both studies)	Chelicerata	-	-	LOEC = 180 (geometric mean)
Induced soil respiration (Reis, 2002)	carbon cycle	0.27 (6.05 % effect)	NOEC and EC_{10}	LOEC = 0.68 (CF: 2.5)
Nitrification (Reis, 2002)	nitrogen cycle	0.27 (54.9 % effect)	EC_{50}	LOEC = 0.14 (CF: 0.5)
Allium cepa (Fiebig, 2006) *Lycopersicon esculentum* (Backus, 1993b) *Cucumis sativus* (Backus, 1993b)	plantae (group 1)	EC50 > 1 (effect 20 to 40%)	LOEC and EC_{30}	LOEC > 1

Species or functional process (study)	Taxonomic or nutrient group	Toxicity parameter (mg a.s./kg d.w.)	Group	LOEC and EC_{30} group (mg a.s /kg d.w.)
Zea mays (Backus, 1993a,b) *Avena sativa* (Backus, 1993a,b; Fiebig, 2006) *Beta vulgaris* (Fiebig, 2006) *Brassica napus* (Fiebig, 2006) *Daucus carota* (Fiebig, 2006) *Sorghum bicolor* (Backus, 1993a,b) *Fagopyrum esculentum* (Backus, 1993a,b) *Brassica kaber* (Backus, 1993a,b) *Raphanus sativus* (Backus, 1993a,b) *Glycine max* (Backus, 1993a,b; Fiebig 2006)	plantae (group 2)	EC50 > 1 (effects < 19 %)	NOEC and EC_{10}	LOEC > 2.5 (CF: 2.5)

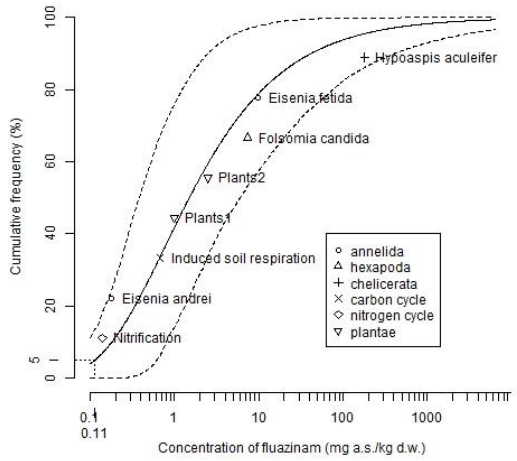
2.8.2 Derivation of soil protection value

Direct toxicity and secondary poisoning

No normalization relationships could be found for this substance. Therefore, the EIL is considered to be of medium reliability.

The preferred methodology, if the data requirements are fulfilled, is the SSD using the Burr type III distribution followed by the AF method. For fluazinam, there is data from 17 different species (invertebrates and plants) and two functional processes (C- and N-transformation processes), belonging to six different taxonomic or nutrient groups (Table A2.13). However, since most plant species had a similar effect at the same concentration and in order to avoid a bias towards the plant data, only two values for plants were used. This resulted in a total of eight data points for the SSD. The SSD distribution is shown in Figure A2.4.

Figure A2.4: SSD distribution of the effect data from Table A2.13 for fluazinam using the software BurrliOZ (Campbell et al., 2000). Dashed lines correspond the 95% CI bounds. Results extracted from the model for agricultural land use and 95 % confidential intervals associated to the values.



	Results	
	Value (mg a.s./kg d.w.)	**95 % Confidence interval**
98 % - protection of crops including bio-magnification protec-tion	0.071	0.035 - 0.571
85 % - protection of soil organisms and microbial processes including biomagnifi-cation protection	0.25	0.130 - 1.360

According to NEPC (2013) the percentage of species or soil processes should be modified in two cases:

- if a contaminant biomagnifies (log K_{ow} > 4)
- if the number of species or soil processes is limited (e.g., if there is only 5 – 8 species or functional processes)

Fluazinam has a log Kow of 4.5 to 5, which would trigger bioaccumulation to higher trophic levels (log K_{ow} > 4). According to NEPC (2013, p. 30) the final soil protection value should account for the risk of secondary poisoning by increasing the percentage of protection up to 98 % and 85 %, for the protection of crop and grass species, and of soil processes and soil invertebrates, respectively (biomagnification protection) (Figure A2.4).

Although the SSD was only performed with eight data points, the sensitivity of 17 species and two functional groups towards fluazinam are represented in the SSD. Therefore, no further increase in the percentage of species to protect was applied.

2.8.3 Final soil protection value

The final EIL for agricultural land use, including secondary poisoning, is **0.071 mg a.s./kg d.w.** to protect the crop and grass species and **0.25 mg a.s./kg d.w.** to protect soil processes and soil invertebrates.

2.9 Summary of soil protection values for fluazinam

Region – Methodology	Soil protection value	Fluazinam (mg a.s./kg d.w.)
EFSA	RAC	0.0027
EC TGD (2003)	$PNEC_{soil}$	0.0054 (not normalized) 0.008 (norm. to 3.4 % OM)
The Netherlands – RIVM (2007)	$MPC_{eco,soil}$	0.025 (not normalized) 0.11 (norm. to 10 % OM)
Canada – CCME (2006)	SQG_E	-
USA – US EPA (2005)	Eco-SSL	11
Australia – NEPC (2013)	EIL	0.071 (crop species) 0.25 (soil invertebrates and microbial processes)

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