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Chemical risk indicator scoping study

Scoping study to develop an indicator on the risk of chemicals on ecosystems

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Executive Summary

This scoping study was conducted with the aim to develop indicators to support the assessment of the progress made in implementing the goals of the European Green Deal (EC, 2019), including key elements such as the *Chemical Strategy for Sustainability – towards a toxic-free environment*, the *Zero Pollution ambitions* as well as the Biodiversity strategy (EC, 2021c, EC, 2020a).

Thousands of chemicals resulting from human activities may be emitted into the environment which requires prioritisation actions for their safe management and reduce harm to human health and ecosystems. An estimation of potential harmful effects can be obtained from predicted risk or observed impacts on species or ecosystems, including changes in the diversity or size of the populations.

Under the existing regulatory framework addressing the placing on the market of substances such as plant protection products (PPPs), biocides, pharmaceuticals or industrial chemicals, a risk is defined as an exceedance of standardised thresholds, which are compared to expected concentrations of chemicals, based on a certain use of a single chemical. These assessments are standardised at European or at best at regional (north/south) levels and are meant to cover any ecosystems in EU, independently from multiple exposure of chemicals at one certain area. However, ecosystems differ and exhibit their own characteristics and specificities, and due to different land use types, sensitivity of organisms might change between different ecosystems and occurring mixtures of chemicals as well.

In this conceptual study, our leading approach is based on the risk, which can be summarised as a combination of hazard (toxicity) and exposure, but we introduce the specificities of a given habitat for both farmed and natural areas, by applying a protection factor within an indicator.

The report focuses on terrestrial ecosystems as an example, and identifies relevant methodologies and datasets related to chemical concentrations, their effects on ecosystems (habitats and species spatial distribution) to produce risk maps for chemicals that could be applied to various ecosystems.

A case study was developed to identify what would be the specification to calculate such an indicator or set of indicators. The key taxa are chosen on the basis on their importance to the ecology (*e.g.* plants as primary producers, and soil invertebrates for several ecosystem services within soils such as organic matter turnover), the availability of ecotoxicity data (on surrogate laboratory species) and the relevant biodiversity databases available. The spatial layers include information on ecosystems/habitats, including urban sites, agricultural lands, forests and protected habitats (rich in biodiversity) which were chosen as examples. These spatial layers are linked by 'connectors' which correspond to effect level data and occurrence data weighted with a specific factor defined as a protection factor, varying for different habitats. This protection factor is applied within the report as an example on how the indicator could emphasize the risk for a certain protection goal. The choice to protect a specific type of ecosystem is a policy decision that was not made during the project, but the use of the protection factor has demonstrated its flexibility in addressing different management questions.

1 Background and context

Human activities make use of thousands of chemicals which may be emitted into the environment, and thereby added to the legacy of synthetic or naturally occurring chemicals, of organic or metal nature.

In the last 3 years, the European Commission has proposed and adopted a corpus of ambitious strategies with the aim to ensure a better protection for human and ecosystems. The major milestone to tackle existential threats like environmental degradation was published by the Commission with the European Green Deal (EC, 2019). Key elements of the Green Deal such as the Biodiversity Strategy (EC, 2021c, EC, 2020a), with its legally binding Nature Restoration Law (EC, 2022), as well as the Soil Strategy (EC, 2021b, EC, 2021d), aim to protect and restore natural systems, habitats, species and soils. This aim is also addressed in the Farm to Fork Strategy, with the 50%-reduction target on the use and risk of pesticides by 2030 (EC, 2020c, EC, 2021a).

On the 14th October 2020, the European Commission adopted its *Chemicals' Strategy for Sustainability Towards a Toxic-Free Environment* (CSS) with the commitment to 'Develop a framework of indicators to monitor the drivers and impacts of chemical pollution and to measure the effectiveness of chemicals' legislation' (by 2024). This occurred in a context where **the threat and impact of chemicals on aquatic ecosystems, and especially on surface waters, is documented and recognized** (Malaj et al., 2014, Lemm et al., 2021, Posthuma et al., 2020), with diagnostic studies on the relative importance of chemical pollution as a driver for ecological alterations suggesting that – on average – one-fourth of such alterations are attributable to chemical pollution (Lemm et al., 2021).

For terrestrial environments, the same threat as well as the impact of chemicals are likely. However, **studies demonstrating the same magnitude of effect or impact are limited** (Corden et al., 2021).

The variety of land-use specific emission profiles and the approximately 350,000 compounds in global trade (Wang et al., 2020) are likely to result in highly variable and significant mixture exposures. Chemical prioritization is therefore needed and required by the Water Framework Directive (WFD) (EU, 2000) as well as the European Soil Strategy for 2030 (EC, 2021b, EC, 2021d). A first level is the relevance to the policy objective – *e.g.,* 'reduce harm to the environment'. Harm can be translated into predicted risk or observed health impacts on species or ecosystems, including changes in the diversity or size of the populations. The latter may be related to several other causes of variability than chemicals such as habitat characteristics or climate change.

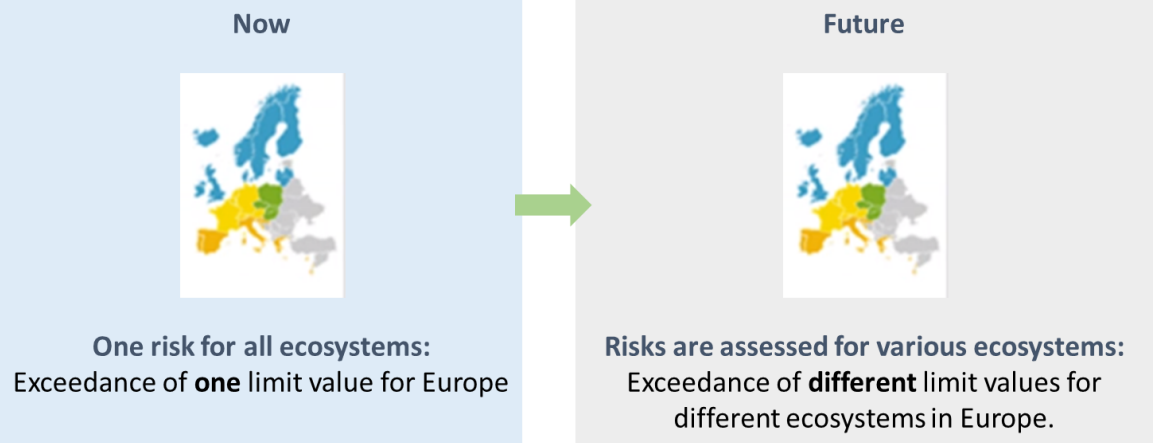
Although the focus is often on compounds both frequently encountered and exceeding their protective standards, it should be acknowledged that the overall chemical impacts are the consequence of exposure to mixtures.

2 Objectives

The aim of this scoping study is to outline *various options for methodologies* that can underpin *indicator(s) on the risk of (single/mixtures of) chemicals* on *various* types of ecosystems, habitats and species (Figure 2.1).

The risk is here defined as the ratio of chemical exposure to toxicity thresholds for surrogate species in combination with uncertainty and extrapolation factors. A high risk can thereby be driven by increased environmental concentrations and/or a low toxicity threshold and conversely for a low risk. However, whereas the risk is a quantitative expression defined in *ex ante* regulatory framework, the risk management for species within certain ecosystems depends on specific land use types, management practices, ecosystem types and additional information on sensitive species.

Figure 2.1: General objective of the methodology: developing a risk indicator which considers the specificity of a given ecosystem



Such indicators are called for to support the assessment of the progress to achieve the aims of the *Chemical Strategy for Sustainability – towards a toxic-free environment*, the *Zero Pollution ambitions* as well as the *aims of the Farm to Fork Strategy (EC, 2020b; EC, 2021a; EC 2020c)*. The report focuses on terrestrial ecosystems as an example, and will identify relevant datasets related to ecosystems (habitats and species), chemical concentrations and their effects.

The aim of the indicator is to provide a sufficient and indicative level of information for risk governance. It will inform governmental institutions, non-governmental organizations and the general public on to what extent terrestrial ecosystems, habitats, or species, are put at risk by the occurrence of chemicals in the environment.

In general, indicators have to fulfil multiple criteria as they need to:

- illustrate properly a specific phenomenon;
- be relevant for the policy aims/targets that they should shed light on;
- be easy to communicate towards the target audience;
- be updatable, which requires the availability of spatial and time trends.

This is illustrated by the extract of a concept paper in Annex 3, which was developed within the indicator framework for the Chemical Strategy for Sustainability, where indicators are used to monitor the drivers and impacts of chemical pollution.

There will always be trade-offs between these 4 criteria, and especially between the first and the last ones due to the lack of consistent data across, for example, chemicals and member states. For the present indicator, this may lead to choosing between considering a broad chemical, spatial, and time coverage but with a less precise methodology, or a narrow (incomplete) coverage but with in-depth precise analyses. Another trade-off may be between scientific complexity vs. communication to a non-expert audience.

These trade-offs result in some uncertainties in the calculation of indicators. They are deemed acceptable since the role of an indicator is not to measure precisely a specific phenomenon but to indicate a trend sufficiently well to support policy assessment and decisions.

With the aim to identify a risk or an impact on ecosystems, the approaches may differ:

- The most straightforward approach to identify a risk is to compare effect/impact (threshold) and exposure (environmental concentrations) leading to the calculation of a risk ratio which is an absolute value. This provides a binary answer i.e., the presence or absence of risk, which can sometimes be modulated, e.g. using a scale from low to high risk.
- Indicators can be more complex as they aim to answer specific questions within a context. Indicators may be built to show trends, the efficiency of measures or to set priorities. In their construction, more weight can be given to a certain parameter, as a function of the objective pursued (e.g. more weight for a certain protection goal, or certain hazard parameter such as mobility when prioritizing groundwater contaminants). Such indicators then inform on a relative change: whether the threat imposed by chemicals in specific regions is higher than in others, whether it evolves over time and according to the practices in place in these regions.

The conceptual scheme proposed in this scoping study will not be limited by lack of access or availability of data, whether it being country coverage, time trends or incompleteness of necessary chemicals data, effect levels or other parameters. However, it may highlight the need for securing access to various types of information.

Chemical mixtures are also in the scope of the methodology but will only be included in the case study to the extent that the data allows.

Within the development of the conceptual scheme, occurrence data of chemical exposure may come from monitoring or modelling, which may be based on monitored or reported statistical data. However, this study was initially designed to focus on monitoring data and includes a review of available relevant databases, which are used for the case study.

The indicator does not have the ambition to be accurate to the level of risk assessments, and therefore at this stage will not include specific information on fate and behaviour of chemicals (related to *e.g.* adsorption onto soil, uptake into biota (incl. plants), leaching with water, evaporation, biotic/abiotic degradation of the chemicals, or soil properties which may affect bioavailability). Neither will it try to assess the representativeness of the presence measured in the field vs. total presence of industrial and naturally occurring chemicals (including plant toxins and metals), due to current and legacy application/deposition of chemicals. It will only deal, to the extent possible, with legacy, accumulated and freshly applied contaminants.

The methodology will however be developed in a way that such refinements could be added in the future, *e.g.*, by replacing constants by a function of the relevant descriptors. Thus, precisions about the fate and behaviour in the environment could be included in future updates of the methodology.

Trophic interactions as well as cascade effects on biodiversity and ecosystem functioning cannot be fully displayed with this indicator, as existing data describing ecotoxicological effects on species and

species communities does not include this information. It is also to be noted that any differences in sensitivity between individual species, and between laboratory tests species and wildlife to determine effect levels can only be addressed as a level of variability and uncertainty. Furthermore, this conceptual study only aims at exploring how chemicals may affect different terrestrial ecosystems and does not at this stage assess the influence from multiple stressors – while recognizing their great significance and their tendency to increase the vulnerability and decrease the resilience of living organisms.

Considering that the evidence base at an EU level is patchy for data and to some extent also for the methodology, the indicator will most likely underestimate the risk of chemicals in a natural environment.

Overall, given that the scope of indicators is to support risk governance more broadly, and not specifically risk assessment, it is deemed to be scientifically correct for its purpose i.e., describing spatio-temporal trends to help prioritization of governance actions.

3 Methodology

3.1 Concept

3.1.1 Overall approach

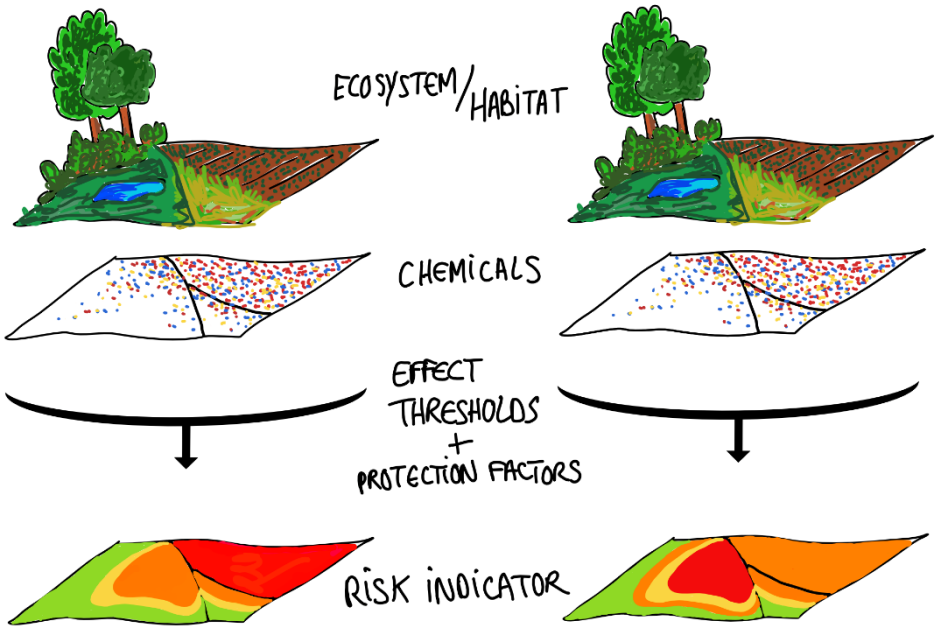
The scope of this indicator is to reflect the consequences of human activities (*e.g.,* farming) on ecosystems and should be designed to answer the very different needs coming from environmental policy and strategies. In principle, in this scoping study, the protection goal should both cover specific or protected habitats (or the relevant communities or species in these habitats), and also address intensively used areas such as agricultural landscapes, which are very relevant in terms of representativity.

In order to develop an indicator showing the risk of chemicals in specific ecosystems, habitats and species for both farmed and natural areas, this report takes the following approach:

A risk is defined as an exceedance of standardised thresholds, which are applied on the comparison of observed impacts on organisms with expected concentrations of chemicals. However, due to different land use types, sensitivity of organisms might change between different ecosystems. Moreover, the tolerable effect threshold might change between different kinds of ecosystems. This can be acknowledged by applying a protection factor within an indicator.

As illustrated in Figure 3.1, the methodological approach to calculate maps showing a specific risk, illustrated as different degrees of exceedance of tolerable effect thresholds, is to overlay and combine different layers of information on *which areas/habitats/ecosystems*, contain *which species*, that are exposed to *which amounts of chemicals*. Information on the sensitivity of the species towards different toxicological effects, and how sensitive the species are to the applied chemicals, is used as 'connectors' between the different layers of spatial information. In practical terms, these may be constants (or functions) in the equations used to calculate the maps.

Figure 3.1: Overlaying and connecting different layers of spatial information on habitats, species and chemical occurrence to produce risk maps



Notes: The habitat map shows an example of protected land (left), farmed land (right) and land without any legal status (lower triangle). The chemical contamination is highest where chemicals are applied, but may drift with air, aerosols, dust or water into areas with no deliberate application of chemicals. In figure 3.1a (left) there is no difference in the protection factor applied to farmed land vs, protected habitat leading to most risk in the areas where chemicals are applied (red colour). In figure 3.1b (right) the farmed land has a lower protection factor, and the protected land has a higher protection factor, leading to a higher risk (red) in the protected non-sprayed area, compared to the farmed area where chemicals are sprayed. The lower triangle is an area with no specific status or protection factor.

Which spatial areas the indicator should cover is a choice, which may be informed by the policy objectives set for various types of land use or occurrence of sensitive habitats. This could be broad ecosystem types, specific habitats related to more detailed habitat typologies, or protected and representative species communities they support.

For each layer there are also choices related to different priorities for what is found relevant to protect, such as habitats, ecosystems, species, etc. Other choices relate to which descriptors, such as types of chemicals, soil types etc., that are considered the most relevant to include, by which methodology, *e.g.,* monitoring vs. modelling, or using which effect threshold. Another consideration relates to whether data currently is or can be expected to become available.

The EU Green Deal includes a pioneering proposal to restore Europe's nature and a concurrent commitment to reduce the use and risk of chemical pesticides by 50 % by 2030. This proposal, also embedded in the Biodiversity, Soil and Farm to Fork strategies, particularly aims to mitigate the impact of declining soil health and pesticide-induced pollinator loss (EC, 2020a, EC, 2021c, EC 2020c). With this respect, agricultural areas, which cover circa 50 % of the European land, and the use of pesticides in protected areas in accordance with the management rules of the Natura 2000 sites, as well as any ecologically sensitive area are highly relevant.

Therefore, depending on the context in which the indicator is developed, the parameters to be included may need to be chosen to fit to purpose (ex. individual species, communities, habitats), and their relevance assessed for the goal pursued. The same would apply to other features expected from

this indicator such as the spatial (*e.g.*, local, EU wide, planet boundaries) and temporal (*e.g.*, current or long-term effects including accumulation and chronic effects) features.

Attempts made to adapt the risk assessment to regional or local conditions are usually driven by the environmental fate and behaviour of compounds leading to exposure. For instance, Urionabarrenetxea et al. (2022) used the PERSAM model to integrate spatially explicit predicted environmental concentrations (PECs) to estimate the risk quotient (exposure to toxicity ratio) of four active substances of plant protection products (PPPs) accounting for European landscape and agricultural variability. Predicted concentrations in soil varied depending on climatic conditions (*e.g.* low temperatures affecting degradation, precipitation affecting leaching, pH and organic matter affecting bioavailability) and crop cultures. However, in this study as in existing regulatory risk assessment schemes for chemicals, effect data are not modified as a function of habitats or species and does not allow for the identification of sensitive or specific local/regional conditions based on the absence or presence of certain species.

This result illustrates the importance of environmental factors and soil characteristics in modifying exposure locally, including bioavailability (see section 3.3) but the approach does not fulfil all the objectives of the indicator.

In order to improve the current paradigm for risk assessment and develop an indicator able to take into account the variety of habitats, the main components of the indicator should cover three lines of information:

- Two of them relate to the risk associated to chemical pollution and belong to the Risk ratio type of approach:
    - Line 1: Chemical occurrence/exposure assessment, which includes the nature and amounts of chemicals to which organisms can be exposed e.g., measured or predicted environmental concentrations.
    - Line 2: Chemical hazard (which can be toxicity threshold) assessment for specific species, including uncertainties.

- One refers to the characteristics of ecosystems and is not directly related to chemicals:
    - Line 3: Ecological information, related to the ecosystems/habitats which can be affected, and to their characteristics (e.g., key or hosted species).

These 3 lines of information need to be considered together, yet the way to combine these data is still to be defined. Line 3 can take the form of:

- a management factor to modulate the accepted threat towards wildlife. For instance, certain threat towards non-target species is accepted within agricultural land, whereby threats for natural, protected areas would not be accepted.
- or a data-informed factor based on the sensitivity of species living in protected areas as compared to agricultural land.

As an example, the WFD collects information about these two kinds of information but has not managed to provide an aquatic ecosystem indicator, due both to scientific / technical issues and structural reasons.

All three lines can be described using different sources of information and methodological approaches (Line 1 and 2 are described under 3.2). For Line 3, these are described below.

3.1.2 Ecosystems and habitat

An “ecosystem” is usually defined according to three main components. It is a complex of living organisms (biotic components), with their physical environment (abiotic components) and their mutual relations (ecological and physical processes and interactions), within a specified area (Bland, 2017). The Convention on Biological Diversity is also defining ecosystems as ‘dynamic complex of plant, animal and micro-organism communities and their non-living environment, interacting as a functional unit" (United Nations, 1992).

An ecosystem therefore considers equally the biological and physical features, as well as how they are interacting, while an “habitat” is primarily characterized by its physical features (topography, vegetation type, plant or animal physiognomy, soil characteristics, climate, water quality etc.), and by the particular species of plants and animals that live there (Davies et al., 2004). Plant species are however the main indicator species to identify different habitats (Hall et al., 1997). Indeed, the very strong link that binds plant communities to their natural environment means that they are excellent indicators of the physical parameters of this environment (climate, type of soil, influence of animals, etc.).

The conservation and management of ecosystems has never been more central to the future of biodiversity and human well-being. The UN Sustainable Development Goals from 2015, and now the post-2020 agenda of the Convention on Biological Diversity (CBD), are mandating global action that depends on ecosystem assessments, and information infrastructures are being rapidly developed to support these global policy initiatives, like the UN System of Environmental, Economic Accounting – Experimental Ecosystem Accounting (SEEA EEA), the criteria for the International Union for Conservation of Nature (IUCN) Red List of Ecosystems (RLE) or Standards and criteria for Key Biodiversity Areas (KBA). All of these require a standardised, globally consistent, spatially explicit typology and terminology for managing the world’s ecosystems and their services (IUCN Global Ecosystem Typology, 2020).

Still, efforts to identify threatened ecosystems are at a much earlier stage of development than approaches for identifying taxonomic groups that are threatened with extinction, now well established, using methods like the one developed by the IUCN Red List of Threatened Species (RLTS). One of the reasons is that there are still limited or non-existent data on the spatial distribution or the temporal intensity changes of many stressors to ecosystems, as well as on the interactions between those stressors and their relationships with ecosystem condition, which may often be non-linear (Newton, 2021). And it is definitely the case for risk assessment for terrestrial ecosystems, which represents a great challenge due to their ecological complexity (Tarazona and Vega, 2002). Assessing specifically the risk of chemical exposure to ecosystems should require defining the different “ecological receptors”, which have strong ecological role in ecosystem functioning and for which knowledge on effects of chemical exposure are available. Terrestrial vertebrates, soil–ground–foliar dwelling invertebrates, plant species, and soil micro-organisms are the main “ecological receptors” to be considered. “Exposures routes” should also be considered, meaning the consideration of direct and indirect exposure. Direct exposures cover those related to the emissions during the life cycle of the chemical substance, while indirect exposures focus on those occurring after the emission, related to the fate and behaviour of the molecule in the environment, including cocktail effect and mixtures (United Nations, 1992).

3.1.3 Including pesticide protection in Nature Conservation

The IPBES (Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services), in its 2019 Global Assessment Report on Biodiversity and Ecosystem Services (IPBES, 2019), estimated that about 1 million species are at risk of extinction — more than ever before in human history. In addition,

global indicators of ecosystem extent and condition show a reduction of about half or their estimated natural baselines, with many continuing to decline. The loss of clean air, drinkable water, pollinating insects, forests, and species pose as big of a threat to species survival as climate change, and many experts are already describing what is the sixth "mass extinction event" since half-billion years.

Current European reports are also documenting the strong decline of biodiversity in the EU, like the European Environment State and Outlook (EEA, 2020), the last State of Nature Report showing the assessment of species and habitats protected under the Habitats and Birds Directives (EC, 2020d), the report on the state and trend of European forest ecosystems (EEA, 2016) or the report on the state of knowledge on soil biodiversity of the FAO (FAO, 2020). All those reports are underlining the urgent need for actions to protect and enhance species, habitat and ecosystem condition within the European Union, and have identified pollution and chemical contamination as one of the main drivers of biodiversity loss.

New EU political actions aiming to preserve and improve the biological state of ecosystems have been taken for the current 2020-2030 decade, as part of the EU Green deal presented in 2019. Among others, the biodiversity strategy for 2030 was published in 2020 together with the Farm to Fork Strategy, the Soil strategy for 2030 was published in 2021, and the Regulation proposal for a legally binding Nature restoration law (NRL) was finally published in 2022 (EC, 2020; EC, 2022). All those recent policies are aiming to protect and restore nature within the EU within and outside existing and future protected areas, with the objective or reversing biodiversity loss and bringing back nature to a good condition.

The European Soil Strategy for 2030 is setting the target of achieving 100 % healthy soils by 2050, and announces also a legally binding Soil Health Law for 2023. In addition, the latest version of the proposed Regulation on the Sustainable Use of PPPs includes the main goals from the Farm to fork strategy, that is the reduction of pesticide use and risk by 50 % until 2030, in addition to a ban on the use of PPP in sensitive areas([1]), and within 3 meters of such areas (EU, 2022b). To fulfil political decisions, requirements as well as strategies, the impact of chemicals on ecosystems and habitats needs to be measured as well as displayed. For this purpose, vulnerability of ecosystems and habitats will be linked within this study to chemical exposure. The protection of habitats and ecosystems from chemical pollution can be based on the risk assessment of single species, repealing the current risk assessment scheme for chemicals, as chemical threats are observed on indicator species. The predicted effect on similar species, as well as on the overall biodiversity and ecological functioning within one habitat or ecosystem is then assumed by applying assessment factors (*e.g.* EC, 2002). Depending on the land-use and based on the vulnerability as well as sensitivity of habitats, different protection goals are in place from different legislation frameworks. These protection goals underlying the different legislations have a different focus and provide a different level of protection. Consequently, and in practice, spatial differentiation in the protection level of habitats is the general approach in the European landscape. Some examples are given below.

Nature reserves or protected areas are often designated based on the occurrence of vulnerable as well as sensitive habitats, species or communities. However, the level of protection varies depending on the regulatory frame, and so does the nature of human activities allowed. Protected areas can be distinguished with regard to their size, their protective purpose and their protection objectives, and by the resulting restrictions on use and human activities. The main categories of protected areas can be defined according to the system developed by the IUCN to create protected area management categories. This system includes 6 Categories, from "Strict nature reserve" where all human disturbances except scientific study, environmental monitoring and education are prohibited, to "Protected area with sustainable use of natural resources", of which human involvement is a large

([1]) sensitive areas are not necessarily natural areas (e.g. Natura 2000 sites) but may include urban parks, playgrounds, among others.

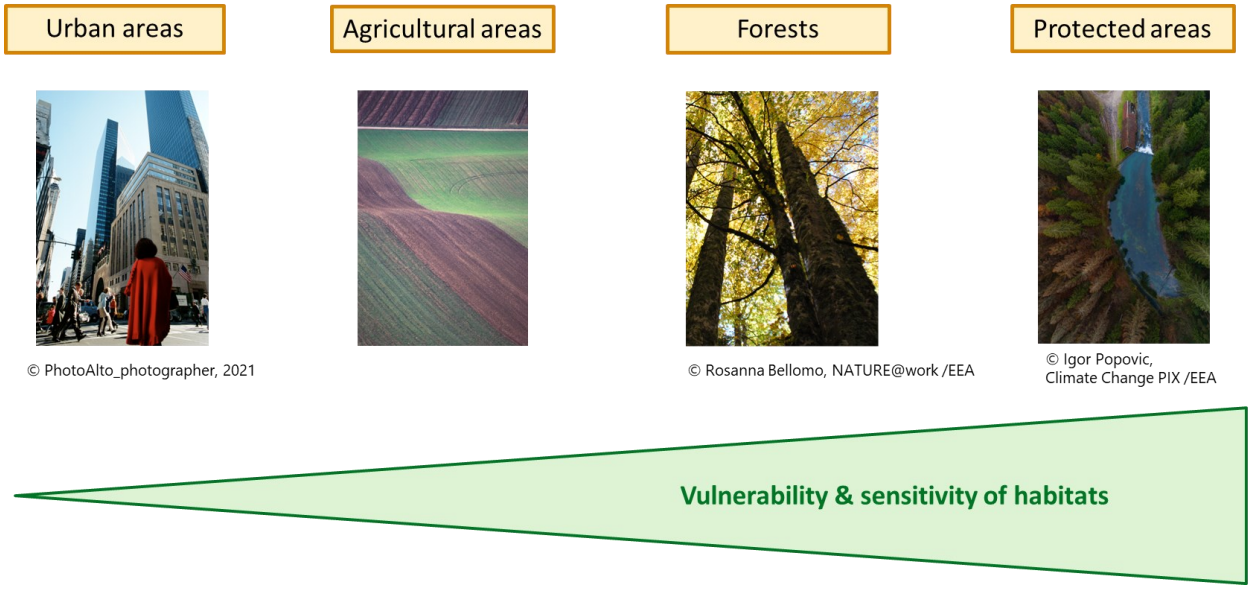
factor in their management. The EU also have the NATURA 2000 network, dedicated to ensure the long-term survival of Europe's most valuable and threatened species and habitats, listed under both the Birds Directive and the Habitats Directive.

In certain countries, agricultural activities can take place in a significant proportion of all Natura 2000 areas while farmland in general can be protected under the Habitats and Birds Directives. Therefore regulatory frameworks and protection goals may overlap and sometime conflict in these areas. The societal decision to allow the agricultural use of PPPs implies the acceptance of effects of chemicals on pest organisms while, at the same time, prevent certain effects of these chemicals on non-target populations of natural species in the agroecosystem (Brock et al., 2006). However, the approval criteria for PPPs request that the use of PPPs in agricultural areas shall have no unacceptable effects on the environment, with particular regards to its fate and distribution in different environmental media, impact on non-target species, and impact on biodiversity and the ecosystem (EU, 2009b). This implies that the application of PPP should also not lead to adverse effects in nature reserves (*e.g.*, Natura 2000 habitats) or further downstream in aquatic ecosystems. For this reason, the Water Framework Directive has different protection goals compared to the PPPs regulation 1107/2009 (Brock et al., 2006); the Water Framework Directive (WFD) (2000/60/EC) has the main objective to protect and enhance the ecological status of aquatic ecosystems and to promote sustainable water use (EU, 2000), while the protection goals of the PPPs regulation 1107/2009 are defined very broadly and generally, *i.e.,* "no adverse effects of the use of pesticides in the environment". Therefore, EFSA is working on the elaboration of this general protection goal into more specific protection goals (see next section).

As shown above, based on the vulnerability as well as sensitivity of different habitats, different regulations have different levels of protection for habitats but also for species.

Within this study, we suggest focusing on different types of landscapes and ecosystems: Protected areas, forests, agroecosystems (which may also be part of protected areas, see case study) as well as urban areas (Figure 3.2). As stated above, certain areas can be both agricultural areas and protected areas, and the level of protection, and hence the protection factors to be applied can be questioned. The extent to which different types of lands should be protected is a political decision. However, the way the indicator can discriminate this kind of overlap will be studied in the Case Study (see section 5).

Figure 3.2: Illustrative context indicating the vulnerability as well as sensitivity of the protected habitat. Protected areas, like Natura 2000 areas cover also special sites within urban areas, agricultural sites as well as forests



3.2 Components of the indicator

3.2.1 Protected ecosystems: Identification of surrogate species

In the context of this study, the indicator aims to inform on the risk caused by chemicals to habitats and communities of wild species. In general, in order to gain information on the toxicity of a given chemical to a defined species, two options are possible:

- Bioassays using relevant species to obtain more knowledge on the toxicity of defined chemicals
- Field data where impacts can be evidenced when compared to reference conditions.

With a focus on the risk rather than on the impact, the indicator can rely on existing laboratory data and therefore on effect levels measured for test species, rather than wild species, and vary according to the different protection goals.

In the risk assessment for chemicals, a challenge is that protection goals outlined in legislation are often too general and broad to be directly applicable for environmental risk assessments (ERAs). Therefore, EFSA is already working on the operationalization of protection goals by applying the ecosystem services approach (EFSA, 2016). Such an approach intends to account for biodiversity and ecosystem services and to make general protection goals operational for use in all risk assessment areas. More recently, EFSA aims to define of more holistic environmental protection goals as part of its roadmap towards a more systems-based environmental risk assessment (Sousa et al., 2022) and has launch a European partnership in order to develop an improved methodological framework to allow for this change of paradigm.

Comparatively in the context of industrial chemicals, the REACH regulation addresses the environment as a whole without specifying any particular ecosystemic or biodiversity protection goals. The precursor of the new guidance document developed in application of REACH chemicals (ECHA, 2017) recognizes the complexity, heterogeneity and diversity of soil ecosystems as the major challenge when

assessing potential adverse effects of substances on soil organisms. The overarching hypothesis is that protecting the most sensitive taxon, with an appropriate uncertainty factor allowing for the extrapolation from a few test species, used in monospecies laboratory experiments, to field species, will allow to maintain the structure and then the functions of natural ecosystems.

The guidance proposes however that as a minimum, due to the complexity and diversity of the terrestrial environment, a comprehensive effect assessment for the whole compartment can only be achieved by a set of assessment endpoints covering (i) the different routes by which terrestrial organisms may be exposed to substances (i.e. air, food, pore water, bulk-soil) and (ii) the most relevant taxonomic and functional groups of terrestrial organisms (micro-organism, plants, invertebrates, vertebrates) being potentially affected. It is however also recognised that only higher full fauna tier studies, such as (terrestrial) field studies or terrestrial model ecosystems, designed to observe effects on more than one taxonomic group may address the effects on ecosystem structure and function which is not usually possible with single species tests.

Under REACH, the actual scoping of the effect assessment for the terrestrial environment does not include terrestrial invertebrates living above-ground (*e.g.,* ground-dwelling beetles). With this respect the requirements set out for the regulation on PPPs are more stringent due to the broad application and emission of PPPs into the environment. For the terrestrial environment, proposed protection goals by EFSA (2017) for agricultural used sites have not been set by the European Commission, yet.

We base our approach on the data requirements for PPPs as laid down in legislation (EU, 2009b). In contrast to other chemicals which enter the environment not purposely or by accident, PPPs are applied to the environment directly with the aim to control weeds, insects or fungi. Therefore, the data requirements for PPPs include much more species at different trophic levels as well as time scales than other regulations for chemicals (*e.g.*, REACH, biocides or pharmaceuticals).

In the following, it is described which organisms need to be assessed in the risk assessment for PPPs and at which level (individual, population, functional). For the soil compartment we include in our analysis other regulatory frameworks than PPP which also request data on terrestrial plants, earthworms and microorganisms.

Birds and mammals: In the risk assessment for PPPs, birds and mammals are assessed at the individual level by acute and chronic tests. While the acute tests aim to identify lethal effects from short exposure, chronic tests aim to identify effects on reproduction as well as development of offspring. Data is used to predict individual as well as population effects.

Terrestrial plants: In the risk assessment for chemicals, terrestrial plants are assessed at the population level by a seedling emergence test (which has a link to soil) and a vegetative vigour test (which has a link to spray drift thus exposure via air).

Earthworms: Depending on the regulatory topic, the risk assessment for chemicals requires an acute or a chronic test on earthworms. While the risk assessment for PPPs is based on a chronic test on earthworms, other regulations base the risk assessment mainly on acute data. Effects on population level are estimated by underlying data describing effects on abundance, reproduction or biomass.

Soil mesofauna: The risk assessment for PPPs requires chronic tests on springtails and mites. Within those chronic tests the reproduction success of test organisms is observed and effects on population level are estimated by underlying data describing effects on abundance and reproduction.

Microorganisms: In the risk assessment for chemicals, the function of micro-organisms is assessed by the nitrification transformation as well as the carbon cycle.

Pollinators: In the risk assessment for chemicals, bees need to be assessed at the population level in a honeybee larval toxicity test (in the laboratory in the first step of the risk assessment) or in semi-field or field tests in a higher tier step. Honeybees are one the most well studied indicator of insect health, and they are economically important for crop pollination, honey production, and wild plant pollination

(DiBartolomeis et al., 2019). For PPPs, non-target arthropods are also used as indicator species, by testing lethal effects as well as reproduction success in the laboratory in the first step of the risk assessment or at a higher tier level in the field.

According to DiBartolomeis et al. (2019) the honey bee (*Apis mellifera*) is generally considered to be relatively sensitive to pesticides when compared to other bee species, but there has also been some concern that the honey bee is not a good indicator for other bees or other beneficial insects because of species differences in autecology and sensitivity. Information being developed on the toxicity of insecticides to pollinators other than honeybees, notably bumble bees (*Bombus species*) and several solitary bee species remains insufficient to extrapolate to all chemicals. In DiBartolomeis et al.'s study, although there were significant inter-species differences that varied through time, overall, the magnitude of these differences was generally within an acceptable two-fold range indicating that an assessment factor of 10 could be sufficient (DiBartolomeis et al., 2019).

Food-chain: For industrial chemicals and PPPs a similar approach is followed in order to cover the risk linked to the trophic transfer of contaminant through the food chain. For substances showing a high lipophilicity (indicated by a log Pow above 3), a risk assessment for the 'secondary poisoning' exposure for birds and mammals is required. The aquatic food chain is simulated by a food intake of fishes from terrestrial birds and mammals. The simulation of a contaminated fish is based on experimental data, a Bioaccumulation test on fishes. For the terrestrial food chain, the food intake of contaminated earthworms from terrestrial birds and mammals is calculated by standard assumptions regarding accumulation of substances in earthworms. If the following risk assessment fails, the conduction of a bioaccumulation test on earthworms can be provided (EFSA, 2009). Thus, experimental data for fishes are available for substances showing a high lipophilicity (log pow >3), whereby experimental data on earthworms describing the bioaccumulation factor are not requested by current data requirements for chemicals. These assessments are meant to use conservative assumptions, but do not describe any specific secondary consumer species, birds or mammals being describe as generic taxon with generic food consumption habits. For substances being (very) persistent, (very) bioaccumulative and toxic (PBT or vPvB according to the criteria laid down in REACH annex XIII), higher predators in the food chain may require a dedicated assessment.

3.2.2 Selection of effect level criteria

In this scoping study, the indicator aims to reflect the risk on specific species and habitats linked to a chemical or chemical mixture. The level of aggregation to be chosen for the hazard part of the indicator, *i.e.,* the effect level criteria, is highly dependent of the particular application context of the indicator.

When considering a sensitive or representative individual species, it seems relevant to use an equivalent surrogate species to determine the effect criteria. On the other hand, the monospecific approach does not reflect the complex interactions and function that take place in an ecosystem. With this respect, threshold criteria based on multispecies approach would appear to be more appropriate.

The effect level criteria available and their relevance in the scope of the indicator are discussed hereafter.

Monospecies approaches

Deterministic interpretation of acute and chronic test data

Ecotoxicological tests can be done by following standardised guidelines, which are provided *e.g.*, by the Organisation for Economic Co-operation and Development (OECD). A huge advantage of following a standardized test protocol is the comparability of produced data. The description of risks can be done for acute as well as chronic data.

- Acute data describes mainly lethal or growth effects and aims to identify a 50 % effect level, expressed as effect concentration (EC50) or lethal concentration (LC50) and therefore species loss or harm on non-target species;
- Chronic data aims to detect effects on reproduction and also covers effects on mortality and aims to derive a so called 'No Effect Concentration Level (NOEC)';
- Alternatively, a surrogate describing a 10 % (adverse) effect concentration (EC10) can also be used, which is considered to be within the normal biological variability.

For in-soil organisms like springtails, mites, earthworms and microorganisms, only chronic tests are required for the evaluation of effects of PPPs under current legal data requirements (EC No 283/2013 and EC No 284/2014, see EU, 2013a, EU, 2013b). Still, a major advantage of chronic data is the high significance for population effects and the target to determine the concentration without effects on tested species.

Both observation levels – acute and chronic - could be used for the demonstration of chemical risk within an indicator. However, the use of chronic level is more protective as the endpoint aims to find no effects, or just small effects of 10 %. In any case, acute and chronic risks must be calculated and presented separately and should be combined with an assessment or safety factor.

Threshold derivation including extrapolation and uncertainties: Regulatory acceptable concentrations (RAC)

The regulatory acceptable concentration (RAC) is derived by applying safety or assessment factors on ecotoxicological data, derived from surrogate species in laboratory tests.

$$\text{Regulatory acceptable concentration (RAC)} = \frac{Ecotoxicological\ effect\ value\ (ECx\ or\ NOEC)}{\text{Assessment factor (AF)}}$$

The assessment or so-called safety factors are used within regulatory frameworks to address existing uncertainty. Ecotoxicological endpoints of the first step of the terrestrial risk assessment are derived from lab tests on single species level by testing so called 'surrogate' species in artificial media (*e.g.*, soil or in between glass plates). Safety factors cover the extrapolation from standard lab species in standardised lab tests conducted in (mostly) artificial soils towards other labs, as well as other organisms and communities in field conditions i.e., with natural soils and interaction between species. Standardized assessment factors are described in respective Guidance Documents (*e.g.*, EC, 2002) as well as in European regulations (*e.g.,* EU No 546/2011, EU, 2011) and are applied on species level.

For terrestrial organisms, a safety (or assessment) factor of 10 is used for acute data, whereby a safety factor of 5 is used for chronic data within the regulation of PPPs (EC, 2002). The RAC can be derived on single species level as well as for species within one compartment in a multispecies approach (*e.g.*, water bodies or soils). Within the regulatory framework for PPP, the RAC is derived for the soil compartment by choosing the lowest available RAC for one substance based on ecotoxicological data

for earthworms, springtails and mites. Microorganisms as well as terrestrial plants are assessed separately within the regulatory framework of PPPs (EC, 2002). For microorganisms the endpoint is different from the other taxonomic groups mentioned above, as the protection level here is the functional level (e.g., microbial respiration) and not the structural level as for the other taxonomic groups.

It should be noted that the risk assessment conducted for PPP is not literally monospecific, but rather covers individual taxonomic groups (plant, invertebrates, microorganisms).

Multispecies approaches

To overcome the risk demonstration at mono-species and individual taxonomic group level (ECx/NOEC approach), multispecies methods could be used if respective data on several organisms are available, namely the species sensitivity distributions (SSD's) for the statistical interpretation of a data set for several (mono-) species (Posthuma et al., 2002), the conduction of micro- mesocosms or field studies, as well as the Predicted No Effect concentration (PNEC) or the Environmental Quality Standards (EQS) approaches for threshold values can be considered (ECHA, 2008, EC, 2018).

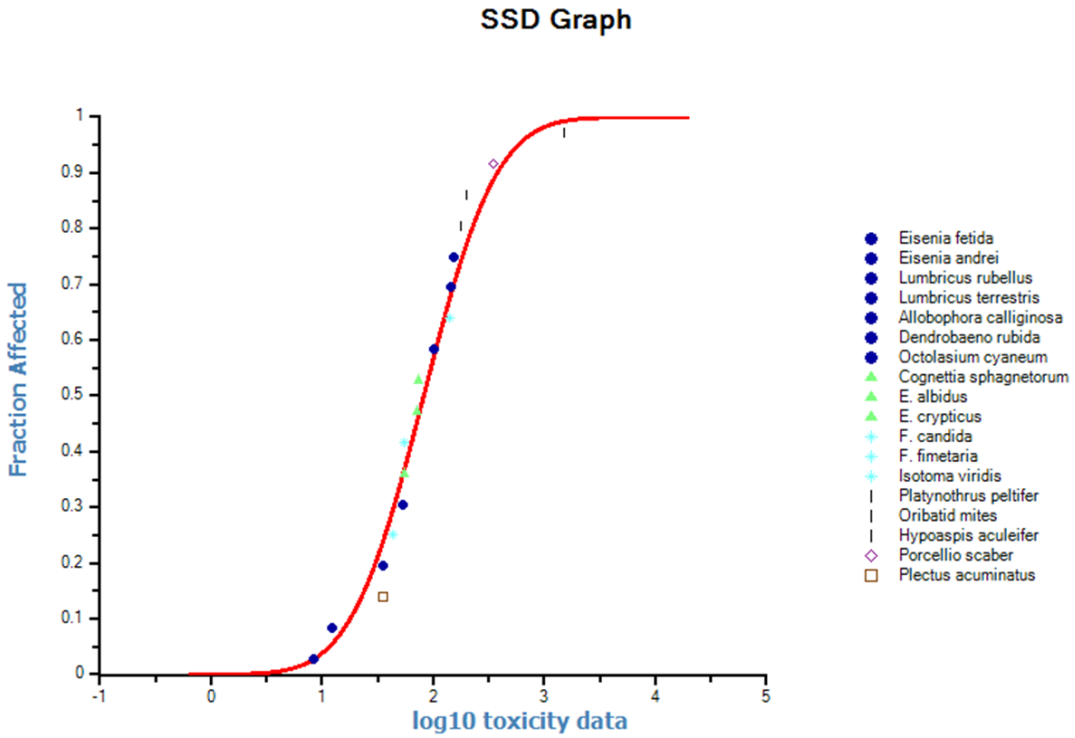
Statistical interpretation of test data: Species Sensitivity Distributions (SSD)

The SSD approach combines ecotoxicological effect values from different taxa. For the risk assessment of chemicals, the 5^{th} percentile of the species distribution is calculated, aiming to identify the concentration, where 95 % of species is 'safe', or 5 percent of species is 'at risk' (Hazard Concentration 5, HC5). Based on the statistical evaluation of the produced curve, assessment factors might also be necessary or, alternatively, the lower limit of the HC5 is used for regulatory processes.

When displaying the risk of chemicals, the quality of the derived HC5 must be assessed *e.g.,* by the Goodness of fit of the curve, and decisions about the expressive power need to be taken.

Figure 3.3 shows an example of SSD graph for 18 species of in-soil organisms, exposed to copper compounds, calculated with the calculation tool ETX 2.2 (Aldenberg and Jaworkska (2000) with amendments from Aldenberg and Luttik (2002), 2002). The resulting HC5 is 11.18 mg/kg soil dry weight (DW) (lower limit HC5 = 4.42 mg/kg soil DW; upper limit HC5 = 20.79 mg/kg soil DW). Assumption of normality for the datapoints was successfully tested.

Figure 3.3: Species sensitivity distribution based on 18 species of in-soil organisms for copper compounds, calculated with ETX 2.1. Blue dots= earthworms, green triangles = enchytraids, blue diamonds = springtails, black lines = mites; purple open diamonds = isopoda; brown squares = nematoda. Datasource: List of endpoints for Copper, Appendix to List of endpoints (EFSA, 2018)



The application of the SSD approach in terms of grouping species as well as applying assessment factors differs between chemical regulations. While the guidance document for REACH chemicals suggests to include at least eight species from different groups independently in combination with an assessment factor of 1 to 5 for the calculation of an SSD (ECHA, 2008), corresponding guidance documents for the risk assessment of PPPs for aquatic organisms (EFSA, 2013) separate differing taxonomic groups of aquatic organisms for the calculation of an SSD. According to EFSA (2013), separate SSDs for fish, aquatic invertebrates, algae and aquatic higher plants are to be conducted. For vertebrates (e.g., fish) a minimum number of 5 species is mentioned whereby for invertebrates (*e.g.*, daphnids or algae) a minimum number of 8 species is recommended. The suggested safety factors range from 3 to 6 depending on the quality of the curve. SSD's can be calculated with the software's ETX 2.2, Mosaic or with an Excel tool, provided by UBA (Dose_Response_SSD_BCF Tool). Under the WFD, a combined approach is followed for a substance exerting a specific mode of action: SSD's should be constructed using first the entire dataset, so that the relative sensitivities of taxa can be examined and second, using only those taxa that are expected to be particularly sensitive (*e.g.*, for an herbicide acting by photosynthetic inhibition, only data for higher plants and algae would be used) (EC, 2018).

For PPPs and for terrestrial organisms, the combination of different trophic levels (*e.g.,* vertebrates and plants) is not recommended as both the application and expression of endpoints differs. Ideally, an SSD is based on the same endpoint. While vertebrates are mainly exposed by food and ecotoxicological effects values are expressed in mg/kg bodyweight, plants or soil surfaces are sprayed with test chemicals and endpoints are expressed in g/ha. Soil organisms like microorganisms,

earthworms, springtails and mites as well as soil-related organisms like plants can however be combined when endpoints are similar, *e.g.,* effect concentration based on g/ha.

The unit of g/ha can also be converted to mg/kg soil DW by using standard transformation assumptions described in . As an example, a NOEC of 375 g/ha can also be expressed as a NOEC of 0.5 mg/kg soil dry weight.

This transformation is usually not needed under REACH (although possible) because direct soil exposure is considered as more relevant than spray for industrial chemicals, and data are generated according to the intended use of chemicals. Nevertheless, for industrial chemicals, the data requirement for soil organisms is limited, and is a function of the tonnage placed on the market. The availability of data generated is poor and the derivation of an HC_5 based on SSD is limited. To overcome this issue, Posthuma et al. (2019b) have proposed to calculate SSDs with a reduced set of data *e.g.,* using extrapolation from acute to chronic data and QSAR taking note that the quality of the SSD has to be ranked in this case.

Micro- mesocosms, field studies and terrestrial model ecosystems

The highest step in the risk assessment of chemicals includes tests with more than one species. For the aquatic compartment, micro- or mesocosms in artificial ponds (standing water) or streams (running water) are conducted. Based on the mode of action of the tested chemicals, they also include more than one trophic level *e.g.*, primary producers, invertebrates of several functional groups (herbivores, carnivores and detritivores) and in some cases (but not preferable in mesocosms) also fish. One major advantage of higher tier field studies is the possible detection of interspecies interactions as the decline or harm of one species affects another, the so-called indirect effects. For example, primary producers might also harm organisms at higher trophic levels *e.g.*, (in-)vertebrates. Within the regulation of PPPs, micro- or mesocosm tests are designed and used to identify ecological threshold option (ETO) values as well as ecological recovery option (ERO) values. Both values can be used to set the RAC but they need different assessment factors in terms of the precautionary principle (EFSA, 2013).

For the terrestrial compartment, field or semi-field studies or terrestrial model ecosystem (TME's) are common. Examples are *e.g.*, field studies on earthworms, non-target arthropods or bees. One major drawback of existing higher tier studies on terrestrial organisms is the observation of only one organism group. Higher-Tier Studies including effects on microorganisms, in-soil fauna and NTAs (non-target Arthropoda) and plants (*e.g.,* effects of pesticides on plants in a plant strip) are currently not used in the current ERA schemes.

Higher tier studies on terrestrial organisms are available only for some substances as they are used within regulation of chemicals for two purposes: To avoid a non-authorisation or to reduce necessary risk mitigation measurements. For the purpose of demonstrating risks of chemicals with a chemical indicator, in combination with the identification of substances mainly driving the risk as well as demonstrating European reduction targets, the use of higher tier data makes the picture unbalanced as they are not available for all chemicals. Comparability of risk between numerous chemicals is not given if higher tier data is used within a chemical indicator.

Predicted No Effect Concentration (PNEC)

Within the regulation of industrial chemicals, the PNEC is used for the risk assessment, which is in principle comparable to the RAC. According to the REACH guidance (ECHA, 2008), PNEC can be derived from the lowest experimental NOEC based on a monospecies approach or from SSDs by applying assessment factors on ecotoxicological data. An assessment factor allows to extrapolate from single-

species laboratory data to a multispecies ecosystem. The size of the assessment factor is a function of both uncertainties, variability and extrapolations, notably:

- intra- and inter-laboratory variation of toxicity data;
- intra- and inter-species variations (biological variance);
- short-term to long-term toxicity extrapolation;
- laboratory data to field impact extrapolation.

In contrast to the regulation of PPPs, assessment factors vary depending on the quantity of available data which depends on the intended sales of the assessed chemical (ECHA, 2008).

Within REACH, individual PNECs are available in the terrestrial environment for:

- PNECsoil, meant to protect all soil living organisms (based on 1) the lowest ecotoxicity data among plants, earthworms, and microorganisms, and an assessment factor when using the deterministic approach or 2) based on the HC5 divided by an assessment factor when using the probabilistic approach);
- PNECoral, which will protect in theory all types of predators (i.e. birds, mammals) exposed through secondary poisoning due to for example the ingestion of contaminated preys. In this case, the lowest experimental endpoint observed in birds or mammals is also divided by an assessment factor to derive the PNECoral.

Environmental quality standards (EQS)

In the previous sections, *ecotoxicity data* or *thresholds* relate to monospecies, monotaxonomic or pluritaxonomic groups, but only for species of a particular position in ecosystems. Both PPPs Regulation and REACH distinguish:

- Species with a link to soil: terrestrial plants, earthworms, microorganisms;
- Species in the food chain depending on soil organisms: pollinators (depending on flowering terrestrial plants), predators of soil organisms, etc.

These threshold values are derived for one specific protection goal, being a taxon (*e.g.,* plants) or combine several taxa, as for instance soil organisms.

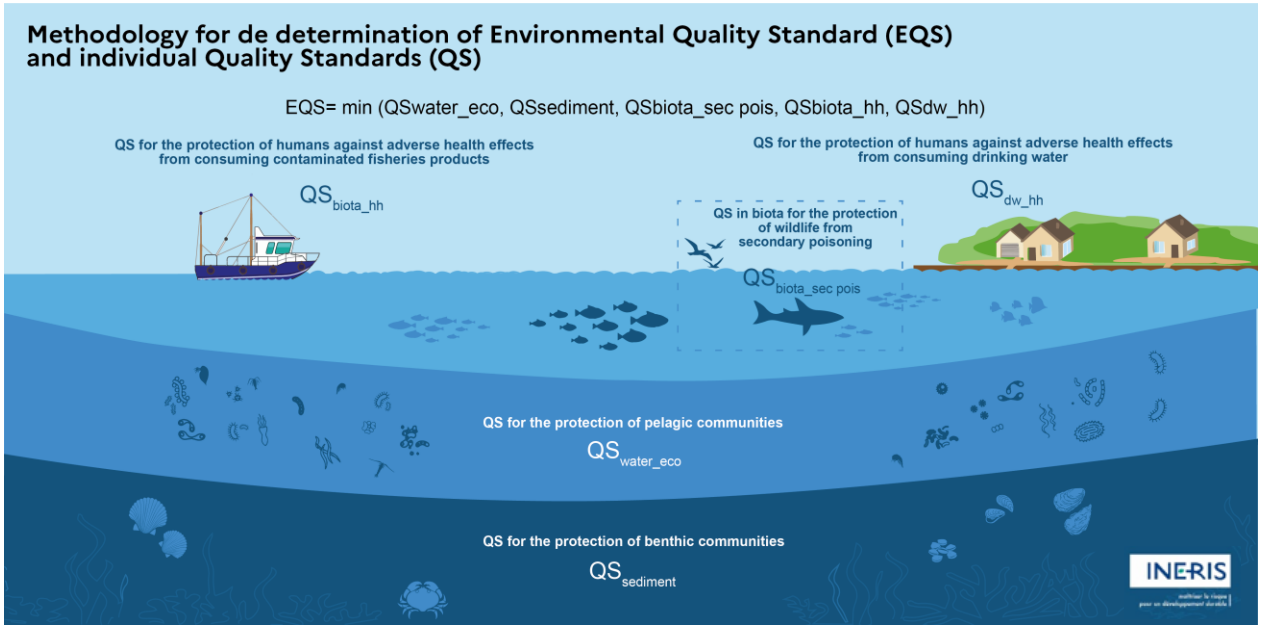
In the WFD (EU, 2000), the concept of EQS which has been proposed is an overall threshold that protects all receptors and routes of exposure that does not normally apply in thresholds developed for other regulatory schemes. EQSs should protect freshwater and marine ecosystems from possible adverse effects of chemicals as well as human health via drinking water or ingestion of food originating from aquatic environments.

Five distinct protection goals (Figure 3.4) are considered for the EQS:

- For the protection of ecosystems:
    - QSwater,eco: quality standard in the water column based on direct aquatic ecotoxicity
    - QSsediment: quality standard in sediment
    - QDbiota,secpois: quality standard in biota to protect against the secondary poisoning of predators

- For the protection of human health:
    - QSbiota,hh: quality standard in biota for the protection of human health based on human consumption of fishery products
    - QSwater,dw: quality standard for the abstraction of drinking water

Figure 3.4: Methodology for the determination of Environmental Quality Standard (EQS) adapted from EC (2018)



The EQS is then defined as the most stringent quality standard among the 5 protection goals.

EQSwater = min (QS_{water_eco}, $QS_{sediment}$, $QS_{biota\_sec\ pois}$, QS_{biota_hh}, QS_{water,dw_hh})

It is to be noted that in order to be able to compare the different QSs and determine the most stringent among the different protection goals, it is necessary to express all the individual QSs using the same unit. The technical guidance document on EQS derivation (EC, 2018) provides extensive guidance and methods to convert individual thresholds.

By construction, EQSs represent a higher level of integration than PNEC since they combine several protection goals. EQSs have not been described for the terrestrial compartment but have a regulatory definition under the WFD. A similar approach to the one used in the WFD could be followed in order to propose for the indicator a component for effect that could be integrative of the protection goals.

An example of the EQS concept applicability for the indicator could be:

$EQS_{terrestrial}$ = **min** (QS_{plants}, $QS_{soil\ invertebrates}$, $QS_{microorganisms}$, $QS_{pollinators}$, $QS_{biota\_sec\ pois}$, etc.)

Alternatively, with an aggregation for soil organisms:

$EQS_{soil\ organisms}$ = **min** ($QS_{earthworms}$, $QS_{collembola}$, $QS_{microorganisms}$, etc.)

As mentioned above, the comparison of individual QSs implies that they are expressed in the same unit. Some examples have been provided above in the section dedicated to SSDs that could also be applied here.

Discussion/uncertainties of choice of effect levels

The diversity of species and functions to be considered to protect biodiversity led to a level of complexity that regulators had to overcome by relying widely on monospecies laboratory testing, and the use of assessment factors. This level of complexity must be recognised, and the residual uncertainties identified.

The effect levels will especially depend on the test system, i.e.:

- how the chemical is 'delivered' to the organism i.e., the exposure route, such as uptake via direct contact (e.g., foliage uptake or soil contact for earthworms), water (e.g., root uptake in plants), air, soil, and/or food (e.g., ingestion of contaminated material).
- the physical-chemical parameters of the media such as soil (type, porosity, pH, organic carbon, cation exchange capacity) and plants (waxiness of the leaves and stage of the development of the plant);
- the characteristics of the chemical itself, which affect its fate as well as bioavailability *e.g.,* water solubility, hydrophobicity/fat solubility, if the chemical can be ionized to positively or negatively charged chemicals;
- various conditions affecting the growth and health of the living organisms *e.g.*, seasonal weather variation, the presence of other chemicals causing mixture effects, and the presence of other living organisms, which may modulate the organism's sensitivity.

All of these parameters affect not only the fraction of the loaded chemical that is bioavailable to the organism, but also its uptake and sensitivity.

The sensitivity of laboratory species compared to naturally occurring species living in natural habitats therefore requires extrapolations from laboratory to field and from species to populations and communities. This is accompanied with uncertainty as sensitivity may differ according to species, habitat and chemical. As it can be argued that laboratory species are selected to be easily bred, it can also be put forward that field species may be adapted to certain conditions, including already existing chemical pressure. Uncertainties are solved by applying Assessment Factors, the size of which differ among regulations.

The US-EPA (2019) is currently revising its methodology for National Level Endangered Species Risk Assessment Process for Biological Evaluations of Pesticides (US-EPA, 2022) to classify them as:

- "may affect, but is not likely to adversely affect" the species or designated critical habitat (NLAA); or
- "may affect and is likely to adversely affect" the species or designated critical habitat (LAA)

The US EPA has collected information about species sensitivities and provides an Interspecies correlation estimation calculator, which may help to extrapolate from laboratory species to wild and/or protected species. This is yet available for aquatic organisms and birds/mammals only (Willming et al., 2016).

Moreover, lab tests on in-soil organisms as well as terrestrial plants are conducted in an **artificial soil mixture**, defined by the OECD, **independently from occurring soil types in natural habitats**. One of the main influencing parameters in the test medium is the organic carbon content in soils (Römbke and Sousa, 2017). In addition, Römbke and Sousa (2017) showed a large variation in ecotoxicological effect values from lab tests conducted with earthworms and collembolans in standardized natural soils, as well as artificial OECD soils, depending on the test chemical as well as the tested organism, which is not covered by the current safety factors (Kotschik et al., 2018). The extrapolation from ecotoxicity data generated in the lab in artificial soils towards natural conditions in the field is connected with high uncertainty, which must be covered by sufficient assessment factors.

The RAC definition for PPPs for aquatic systems refers to thresholds as well as recovery options, which values can only be observed with higher tier tests (like mesocoms) (EFSA, 2013). They are infrequent in the data set but they could have relevance for field conditions. They have however to be considered with cautions with regards to the adequation of exposure condition.

The statistical analysis of SSDs, as described above, has been considered to express the sensitivity of ecosystem/habitats. Regarding the ecological relevance of this approach, it is to be reminded that the SSD gives a robust estimate of the range of sensitivities to be encountered in an ecosystem, but it is still based on single species data, and species-interactions at the ecosystem level are not covered (TGD-EQS, EC, 2018).

Posthuma et al. (2019b) propose nevertheless an ecological interpretation of risk quotients calculated on the basis of two types of SSDs:

- One based on EC50: an impact is expected, thus the derived HC5 is interpreted as a concentration leading to 'species loss' if no safety factor is applied.
- One based on NOEC: interpreted as sufficiently protected.

This review of effect level criteria underlines the importance of the choice to be made when selecting the type of ecotoxicity data and their interpretation in the indicator. **Whereas acute toxicity (EC_{50}) data are more frequent in the databases, chronic data (NOEC) are more relevant for the protection of ecosystems, especially if they cover functioning or multigenerational endpoints.** The lack of chronic data may be overcome with the use of a default acute-to-chronic ratio to convert acute into estimated chronic values (Posthuma et al., 2019b).

In addition, when considering the number of species tested to fulfil the legal requirements under the main chemical regulations (mainly in this case REACH and PPPR), it appears that the **number of required species tested as a function of the chemical use** i**s more important for pesticides**, due to their desired toxic action against target species and wide dispersive use on soil. Soil species tested under REACH regulation are limited to the plant / earthworm / microorganism taxa. In addition, in the REACH Chemical Safety Assessment reports, testing on soil organisms is required only when the production volume exceed a certain annual tonnage, or certain exposure condition. For these two reasons, the number of soil ecotoxicity data generated under REACH are limited.

Metals in soil are assessed differently to other pollutants, because besides their use as PPPs (such as copper as fungicide) or industrial chemicals, they are also naturally occurring substances with various spatial distribution. In agricultural areas, it is to be noted that metals may originate from additional sources, such as fertilizers or sludge application. Because of this and of their long-lasting use in human activities in combination with high persistency, they are of particular concern also for polluted soil management. More ecotoxicity data for metals are usually available than for other chemicals, including field studies, local species and bioavailability. The counterpart is a high variability in the results that need statistical analysis before being used.

In the next paragraphs we will further elaborate on how an indicator covering different chemical classes and focusing on the terrestrial habitats could look like, given all limitations and possibilities.

3.2.3 Chemical pressures on ecosystems

Environmental policies may aim for reducing the negative effects of chemicals on ecosystems in various ways. The 7th Environment Action Programme (EAP) hence seeks to ensure that 'The use of PPPs does not have any harmful effects on human health or unacceptable influence on the environment, and such products are used sustainably', while the Marine Strategy Framework Directive (MSFD) has the objective that 'Contaminants are not at a level giving rise to pollution effects' (SOER2020, Chapter 10, Table 10.1).

These aims are hence connected to environmental concentrations which may lead to adverse effects in organisms depending on the level of exposure and uptake during their life cycle i.e., internal chemical concentrations.

In practice, there is seldom monitoring data on the internal concentrations in biota (with some exemptions of chemicals in marine biota, bees and some plants). Rather chemical occurrences in the external environment are linked to expected internal concentrations, or observed effects from *e.g.,* laboratory *in-vitro* or *in-vivo* studies. The added (loaded/spiked) concentration at which some (unwanted) effects are observed refers to the 'effect level' previously introduced. As an example, in the pesticide environmental risk assessment (ERA), effects on so-called 'non-target organisms', is assessed by spiking a chemical in some concentration(s) in surrounding soil or residues on surfaces like glass plates or leaves. These are used to describe effects on invertebrates like earthworms, springtails, mites as well as microorganisms, terrestrial plants and non-target above ground arthropods. The effect levels or ecotoxicological endpoints are expressed as soil concentrations or loads.

This introduces some methodological challenges, where it is important to keep track of whether occurrence data are compared to the right effect levels. Some typical contributions to uncertainties in occurrence data are:

- Chemical occurrence may follow a certain distribution over time and space. This raises the question about which concentration to compare the ecotoxicological effect levels with. In the environment, the amount of chemical(s) loaded onto a soil or biota is typically not known – rather, the amount (or residues) can be measured in the environmental matrices afterwards e.g., in the soil, plants or animals. While such occurrence data inform on the current risk for soil organisms, they do not allow to assess the chemical stress organisms were subject to by the initial load. Therefore, the chemical concentration in soil should in principle be 'linked' back to the amount that was most likely loaded, to assess whether the effect levels were exceeded or not.
  The average concentrations are typically compared to chronic effects that are influenced by long-time (average) exposures. For acute effects, it is however the maximum concentration that may trigger effects (death, growth reduction) and therefore they will typically be compared to the $Conc_{P95}$, $Conc_{P99}$. In other cases, the $Conc_{P75}$ is used (reference to EFSA guidance, communication with Jean-Lou Dorne).
- The derivation of occurrence data from statistical data on *e.g.*, sales, application or load data using models and information on typical uses in agricultural or industrial practices. If there is no information on where or for which crop the chemical is used, averages of typical application rates are typically used. This introduces a risk to assume uses where they have not been used, or, on the contrary, to underestimate the uses, where the pesticide actually has been used in higher amounts than assumed.

In the following section, some general considerations on which chemicals may be relevant to look for are described, as well as the pros and cons of monitored vs. modelled data, and some reflections on soil properties that may link soil occurrences to exposure of terrestrial organisms.

Chemicals (substances) of concern

Given that tens, if not hundreds of thousands of chemicals are used (EEA, 2020, chapter 10), it is necessary to prioritise which chemicals to include in the assessments, which are *most likely* to be of risk to ecosystem health. In the CSS, chemicals have been categorized into whether they are 'Substances of concern', based on their intrinsic properties, mainly linked to their chronic risks to human and environmental health (Patinha Caldeira et al., 2022).

The risk is defined as the combination of exposure to the chemical and hazard from this chemical i.e., how toxic the chemical is. Below is provided a non-exhaustive list of considerations, that may inform on how relevant the chemicals are to be included in the occurrence data:

Exposure

- *How likely is it that a chemical is present on a specific land?*
  Depending on the land use – *e.g.* agricultural land, forests, industrial area, urban or rural land, it may be assessed if specific chemicals have been applied or deposited there by various air, water or dust transport mechanisms. Such lists have been made for *e.g.,* agriculture depending on crop type and temporal zone (see for example the maps provided by RIVM on the Atlas Natural Capital, RIVM, 2022), records of which inorganic/organic fertilizers that are applied to specific lands, mapping of certain businesses and risks of inorganic and organic pollutants (*e.g.,* oil spills, chlorinated solvents, fungicides used in wood preservation, PFAS production plants or air bases where they have been used).

- *Which volumes of chemicals are used or deposited on the land and how often?*
  Chemicals that are used in higher volumes, and over long periods of time are more likely to lead to high exposures that can be of risk to the biota. Chemicals repetitively applied on land in intensive agriculture, voluntarily or not, such as pesticides (active ingredients and adjuvants), pollutants in organic fertilizers (veterinary drugs including certain metals such as Zn, endemic hormones, industrial chemicals, etc.) as well as metals in inorganic fertilizers, are examples of highly used chemicals in scope of the prioritization.

- *What is the distance to the point of emission?*
  The closer to a point source, *e.g.* where the chemical has been used, handled (*e.g.,* filling or cleaning of containers/tanks), produced, manufactured or emitted (*e.g.,* waste water treatment plant), the higher the concentration tends to be. Dominant streams of air or water may also affect the spreading of the pollution.

- *Are the chemicals persistent?*
  Persistent chemicals only degrade slowly and therefore accumulate in biota and in the environment to which they spread. Current and historic uses of persistent chemicals may therefore be relevant in the prioritization.

- *Do the chemical bioconcentrate or bioaccumulate?*
  Chemicals that bioconcentrate within a single organism (*e.g.,* in the leaves due to evaporation of water), or bioaccumulate (across trophic levels) will be riskier, since exposures over time will increase to levels, that might exceed the effect levels.

- *Are the chemicals bioavailable to the biota*?
  Chemicals that are in direct contact with the biota will typically lead to higher exposures. Examples may be soil organisms like earthworms or nematodes which can absorb chemicals through the skin, and which ingest soil, pollinators being exposed to sprayed flowers, and plants that are oversprayed and additionally exposed by uptake of water soluble chemicals with the water, or where seeds and roots are directly exposed to chemicals in soil. Surfactant chemicals also tend to be stratified, *i.e.* have non-homogeneous concentrations in media, and distribute to surfaces of sea and surface water, or bind to sludge and protein rich media. Biota living in these specific environments are more at risk to get high exposures. Depending on the organism and the route of exposure (through water, dermal/through the leaves, ingestion, sediment, air or affecting routes) the most risky chemicals will depend on the intrinsic

properties of the chemical. It will also depend on the properties for the environmental media, being soil, water or plants. For each combination of environmental medium and species there may therefore be more or less risky chemicals.

- *Have the chemicals been applied or distributed at sensitive times of development*?
  Chemicals that enter environment at critical times of biological development, such as seedling and insect development from eggs to larva may be more relevant both in terms of the exposure, but also related to how toxic they are.

Hazard

- *Which effects do the chemical have on an organism?*
  Different species have different sensitivities towards chemicals. Whereas aquatic species may be sensitive to surfactant effects on their gills interfering with their uptake of oxygen, collembolans and non-target arthropods are sensitive towards insecticides and plants to phytotoxic chemicals interfering with the conversion of light into energy.

- *How toxic (potent) are the chemicals?*
  Chemicals which are designed to be bioactive, or which just happen to be so, and which are toxic at low doses, are often those that drive the risk. In ecosystems these tend to be pesticides, biocides, pharmaceuticals, metals, but also biotoxins which are produced by plants/fungi/algae to limit the growth of other biota. During different stages in a biota lifecycle, the biota may have different vulnerability to exposure to chemicals, which means that the potency 'changes' over time as previously mentioned. Chemicals that are developmentally toxic (endocrine disruptors, neurotoxic, immunotoxic, metabolic toxic) would typically fall in this category.

- *Do the chemicals have intergenerational effects?*
  Some chemicals impair not just the growth or mortality of the exposed organisms, but also the reproductive and overall health and resilience of subsequent generations. Such long-term effects can lead to decreases of the populations, generation by generation to levels that put the species at risk from being extinct in affected habitats.

In this conceptual study we have chosen to deal with complex processes that often lack information to be applied across Europe so that factors or functions can be used rather than calculating the actual number for each chemical. An example is bioavailability. While the data may be available for some soils and relevant for some metals, it is not the case across organic pollutant and species. Factors between 0-1 can however be set, where 0 is no bioavailability, and 1 is if all the applied chemical is bioavailable to the organism.

Based on the above considerations, the following groups of chemicals have been identified as being of priority for various types of terrestrial land cover/land use.

Agricultural soils:

- Pesticides, synthetic and plant toxins used as biopesticides;
- Metals present in inorganic fertilizers (*e.g.,* Cd), organic fertilizers (*e.g.,* Zn), naturally occurring, or used as pesticides (*e.g.,* Cu);
- Industrial chemicals present in organic fertilizers (*e.g.,* POPs in sludge and manure);
- Pharmaceuticals (veterinary or human) present in organic fertilizers (*e.g.,* antibiotics and pain killers in sludge and manure);
- Biocides in organic fertilizers;

- Persistent chemicals that bioaccumulate or form mobile degradation products, including industrial POPs and pesticides.

For brownfields affected by industrial pollution, the following chemicals may be relevant:

- Oil and fuel pollutants, including PAHs and BTEXN (benzene, toluene, ethylbenzene and xylene);
- Chlorinated solvents, from *e.g.,* cleaning agents, car and printing shops;
- Organochlorine and other persistent pesticides, from *e.g.,* greenhouses;
- Brominated and other organo-halogen flame retardants;
- Per- and polyfluoroalkyl substances (PFAS);
- Phenols, from *e.g.,* fungicide treatment of wood;
- Metals.

Industrial/Urban sites:

- Aerial deposition of dust or rain from industrial sites and traffic;
- Emissions from building and product stock;
- Surface runoff from roads (e.g., Cr, front shield detergents, abrasion from metal, and waxes from cars and combustion fuels);
- Organic pollutants from consumer products and from use/production (also including long range transport).

Forests and parks, including golf courses:

- Pesticides and fungicides applied;
- Fertilizers;
- Aerial deposition of dust or rain from industrial sites.

Protected habitats:

- Pesticides and fertilizers, also applied within protected areas (e.g., Natura 2000) and nearby agricultural areas;
- Aerial deposition of dust or rain, and water and soil run-off from industrial sites as well as agricultural used sites.

A challenge for metals and other naturally occurring chemicals (*e.g.,* plant toxins) is to determine what the 'naturally occurring background level' is and which level is therefore acceptable, even if it exceeds effect levels, such as in areas with high naturally occurring metal concentrations. For anthropogenic pollutants, such as PFAS, which are now spread globally (Cousins et al., 2022) and have contaminated most if not all ecosystems, discussions evolve around whether 'background' concentrations should be set to zero (because the chemicals are not natural), or what their current actual 'baseline' levels are.

Combined exposure of terrestrial organisms to chemical mixtures

For the time being, effects of chemicals are separated in different regulations for PPPs, industrial chemicals, biocides as well as pharmaceuticals and cleaning detergents. However, multiple exposure of terrestrial organisms occurs due to current land use practices. Agricultural areas are exposed to PPPs by direct exposure several times during the growing season (Knillmann et al., 2021), but also to pharmaceuticals, biocides and industrial chemicals reaching agricultural areas by fertilization using sewage sludge or manure. Silva et al. (2019), Humann-Guilleminot et al. (2019), Leisner et al. (2020), and Kosubová et al. (2020), or Riedo et al. (2021) observed multiple residues of active substances used as PPPs in agricultural land. This reality is not addressed by the current regulations as well as guidance

documents for the risk assessment of chemicals but could be addressed within a chemical indicator by using a mixtox approach (EFSA, 2019a).

In practice, the question is addressed, mainly using approached relying on Concentration Addition (CA) using *e.g.,* NOEC and PNEC (Backhaus and Faust, 2012, EFSA, 2019a). Posthuma et al. (2019a) proposed an improved component-based method to predict impacts from pollution with complex mixtures. This approach includes all occurring (or predicted) substances, independently from the availability of Environmental Quality Standards. In a first step, toxic units are summed as well as risk quotients. Moreover, species sensitivity distributions (SSDs) are used to identify mixture toxic pressures. If ecotoxicity data is not available, the QSAR approach as well as read across data can be used to identify the toxic units.

Occurrence /Monitoring data

By occurrence data we mean monitoring data of chemicals present in soil or biota. The use of data on chemical occurrence from European-wide surveys is beneficial, given uniformity in sampling procedures, analysis, and quality control, and thus comparability of data. An ideal dataset has the following criteria fulfilled: High spatial resolution, wide range of land-use categories and available soil property data available. In chapter 4.1, a review of occurrence datasets is performed and includes both soil monitoring data from pan European or national monitoring programs, and biota monitoring data.

Depending on the organism and the soil, the connection between the occurrence and exposure will differ due to chemical bioavailability, which is driven by the binding affinity of the chemical as well as occurring soil type. Occurring soil types within Europe are described in EFSA (2021) as well as in Annex 1 of this document and vary in pH as well as organic carbon content. Up to now, factors addressing the standardization of soil types are not available.

Tiktak et al. (2013) define two types of ecotoxicologically relevant concentrations: the concentration in total soil (absorbed plus dissolved) and the concentration in the soil liquid phase to be ecotoxicologically relevant. Soil monitoring concentrations often correspond to the total concentration in soil. Such data are likely to overestimate the exposure to chemicals of in-soil organisms living in water films (e.g., nematodes) and plant uptake through the roots.

For terrestrial plants, data expressed as total concentration in soil are relevant for seed development and roots exposure, even if the bioavailable fraction of chemicals that potentially could be uptaken through roots and translocated into the aerial parts is the most likely to be responsible of the ecotoxicity. On the other hand, data expressed as load of sprayed chemical is highly relevant for leaves.

For in-soil organisms like earthworms, collembolas or mites, the total concentration in soil as well as the pore water fraction is relevant. In-soil organisms might be directly exposed but are also able to absorb chemicals upon ingestion of soil particles. For chemicals with a high Koc/low water solubility the trophic route may supersede direct exposure (EC, 2018).

Because monitoring data are limited to specific locations, chemicals and biota types, statistical as well as modelled data can be used to produce estimates of pollution loads across Europe.

Statistical and modelled data

Statistical data refer to pollution loads estimated from different sources of information concerning the use and emissions of chemicals.

For industrial chemicals, emissions reported under the E-PRTR regulation (EC) No 166/2006 (EU, 2006) may be usable to calculate the load of chemicals released into the terrestrial environment at specific

locations. For agrochemicals, the reported national sales and the type of agricultural land where the chemicals may be used can serve as proxy for calculating predicted environmental concentrations, assuming specific application frequency and rates. Such approach is under development at the European Joint Research Centre (JRC) (Galimberti et al., 2020).

The transformation from loads to soil concentrations can be based on dispersion modelling taking into account the area of relevant land use within Member-states or the European Union. Ideally, also typical application rates per crop types should be taken into account for pesticides, to demonstrate the treatment frequency. Once typical application rates are identified, they can be transferred towards soil concentrations by using standard assumptions captured in EC (2002).

Different types of models exist for predicting the environmental fate of chemicals, based on the chemical's emission and transport pathway. For example, metals and industrial chemicals may be deposited to soils from fumes or sludge application, while pesticides are typically sprayed onto soil with water.

The Nested Exposure Model (NEM) (Breivik et al., 2021) is a temporally (dynamic) and spatially resolved integrated environmental fate and bioaccumulation model for organic contaminants that links global emissions with biotic exposure, with a user-defined spatial resolution (up to 0.5°x0.5° latitude/longitude). In this model, detailed environmental and biological data, global emissions and physicochemical properties are used to predict concentrations in both the physical environment and biota. The bioaccumulation module is currently parameterized for a food web typical of the European sub-Arctic and Arctic areas, and spatial movement of biota is not yet accounted for. In a study by Krogseth et al. (2022) the NEM model was found to reproduce well the spatial and temporal trends of PCB-153 in the Norwegian marine ecosystem, and succeeded in linking global historical emission of PCB-153 with northern ecosystem exposure, including bioaccumulation across trophic levels. NEM has the potential to be expanded to other contaminants, species and ecosystems of interest, making it an interesting tool also for the purpose of producing occurrence data for a European-wide ecosystem specific indicator.

In the context of agrichemicals, Tiktak et al. (2013) developed a methodology for selecting realistic worst-case scenarios for exposure of soil organisms to pesticides. This includes the development of a simple statistical model, the Persistence in Soil Analytical Model (PERSAM), for predicting the concentration of pesticide in European soils. Their study showed that the 95th percentile of the concentration distribution simulated with PERSAM was within a factor three of difference with the concentrations simulated with the widely used numerical models PEARL and PELMO (Tiktak et al., 2013).

The NEM and PERSAM models are given as potential usable examples. While full review of models was not performed in this study, a series of selection criteria for models was identified:

- The model has been tested or validated by several peer-reviewed references.
- The model outputs have a spatial resolution suitable for overlaying occurrence and habitat maps.
- The simulations can be run across all European countries. This implies that:
    - the necessary inputs are available
    - the simulation time is reasonable

Looking ahead, agricultural statistics may be available from 2028 as part of the regulation proposal *Statistics on Agricultural Input and Output* (SAIO, EU, 2021). This will include information on the treated crops and pesticide application rates and displays the 'golden standard' of risk demonstration as uses do not need to be estimated by assumptions of crop share within Europe or typical application rates.

Pros and Cons of monitoring vs. modelling data to feed an indicator

The advantage and drawbacks of using one approach or the other are summarized in Table 3.1.

Table 3.1: Pros and Cons of monitoring vs. modelling data to feed an indicator

	Pros	Cons
Monitoring data	More accurate in terms of: environmental concentrations and exposure pollution distribution	Lack of completeness (number of chemicals monitored, spatial and temporal coverage) Suitability depends on the sampling method (*e.g.*, soil depth, time of the year). Potentially larger lag time for updating the data
Modelled/statistical data	More complete coverage of chemicals and countries Depending on the data availability at the EU level, possibility to frequently update the loads Several models might be needed for several types of chemicals (*e.g.*, pesticides and industrial chemicals).	The estimated load may overestimate and underestimate the exposure depending on the chemicals bioavailability in connection with occurring soil types. 'Real' application scenarios are not known. Chemical loads might be underestimated due to lack of application data. Access to input parameters might be differently limited across Europe. The resolution of the outputs might be too coarse compared to the habitat maps.

3.2.4 Spatial and temporal representation of the indicator

The indicator may be calculated at a specific time and location or be developed so as to be representative of a time period and a given habitat/ecosystem/geographical region.

Temporal dimension

The development of the indicator involves:

- defining the period of time for which the indicator is built;
- if relevant, defining the way input data used to build the indicator should be aggregated within this period.

The period of time depends on the time resolution of the data that are available to describe chemical pressures (occurrence/monitoring data, modelled or statistical data) and should be in agreement with the chemical and ecological processes at stake.

A period of one year is often considered as is the case for several EEA indicators related to health and environment (*e.g.* population exposure to air pollution) or biodiversity and ecosystems (*e.g.* annual

area of drought impact on vegetation productivity). Furthermore, if pollution load is estimated from statistical data, a one-year period is generally consistent with available sources of information (*e.g.* annual reported emissions, annual sales of pesticides pesticide).

A multi-year time range, *e.g.* 3 to 5 years, may also be a suitable period to compensate for a limited number of data, to smooth the effect of specific years or to align with management and monitoring cycles as under the Water framework directive (*e.g.* Percentage of water bodies, not in good ecological status or potential, per river basic district).

A sub-annual period of time could be appropriate where the chemicals of concern and related exposure display temporal patterns (*e.g.* variability of pesticides occurrence in relation to application periods). However, the number of available data within monthly or seasonal periods is likely to be a major limitation.

Temporal aggregation consists in deriving a statistical value representative of the considered timeframe from the point or short-term data. This mainly applies to sampling data but can also concern modelled data if they are produced at a high resolution (*e.g.* daily values). Different statistics can be used for such operation: average concentrations; median concentrations; higher percentiles. The median is less sensitive to extreme values (potential outliers) than the mean. In a more protective goal, a higher percentile, such as the 90^{th} or 95^{th} percentile could be considered.

Spatial representation of the indicator

Spatial representation of the indicator depends on technical, scientific and decision factors, in particular:

- the spatial resolution of the input data;
- the approach that is considered to link the chemical component with ecosystems;
- the scale at which the indicator is intended to be used.

It may stick to the original resolution of the input data or involve spatial aggregation. Different types of representation and ways of putting together the chemical data and data on ecosystems are introduced hereafter.

Mapping at the same spatial resolution of the input data

In this representation, the indicator is calculated and mapped at the resolution of the original input data used to assess chemical concentrations: at specific monitoring locations, at grid points or by grid cell (regular monitoring network, modelled data), by administrative unit such as a region or a country (e.g. data derived from reported statistics at national or regional scale).

In the following example (Map 3.1, from Tang et al., 2021), a spatially explicit model was applied, using geographically gridded input data (in particular 5 arc-min resolution maps of estimated active substance application rates), with a view to determining risk quotients (PEC/PNEC) and an overall risk score due to pesticide pollution at the global scale. The result of this modelling is a 5 arc-min resolution map of the risk score.

Map 3.1: Example of spatially explicit map

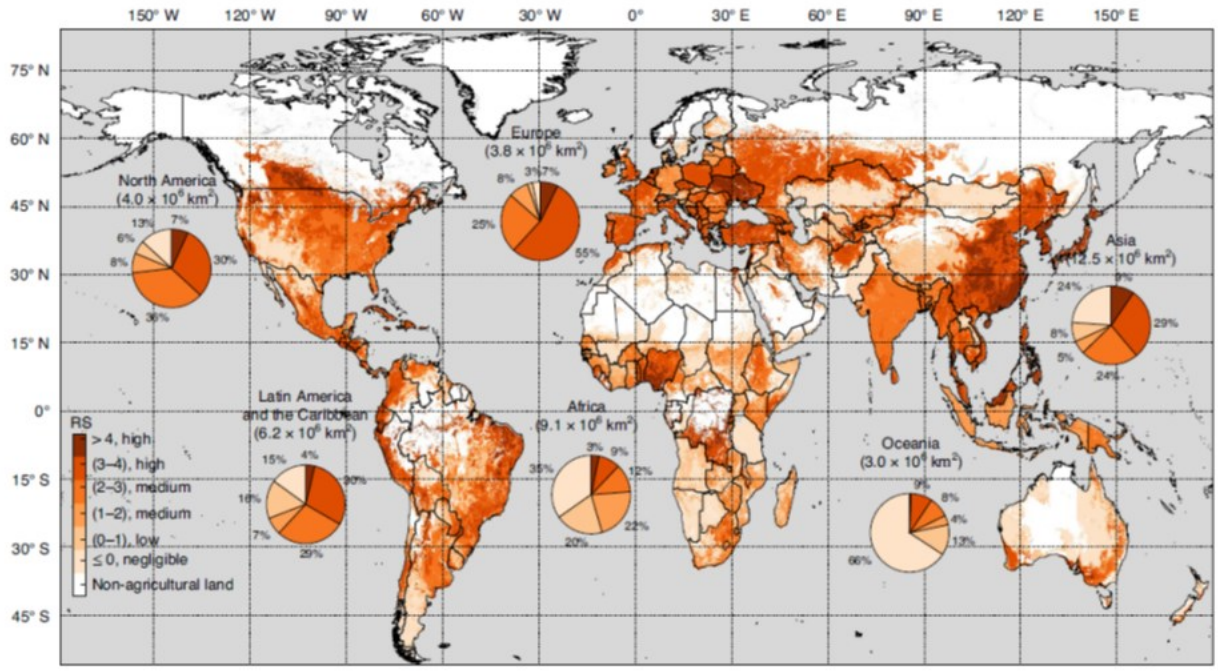


Fig. 1 | Global map of pesticide RS. The map has a spatial resolution of 5 arcmin, which is approximately 10 km × 10 km at the Equator. The pie charts represent the fraction of agricultural land classed under different RS in each region, and the values in parentheses above the pie charts denote the total agricultural land in that region.

Notes: Estimated Risk score due to pesticide pollution at the global scale.

Source: Tang et al., 2021.

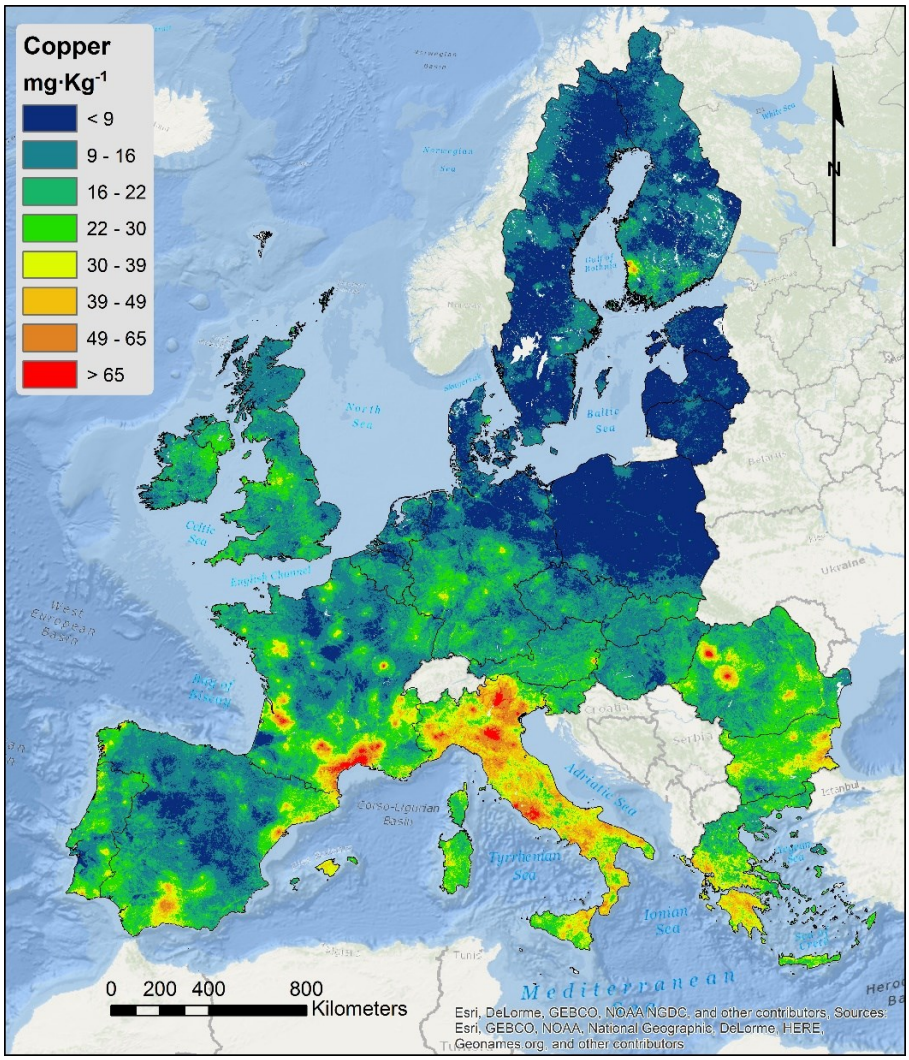
Spatial aggregation

Spatial aggregation consists in moving from raw point or fine-resolution data to coarser resolution data to derive meaningful information (Allain et al., 2018). This operation can serve different purposes like, fitting to process scale, addressing data uncertainty, increasing readability, highlighting spatial patterns, etc. It should find the best balance between scientific soundness and ease of use. This process can result in a single value for the entire zone of interest or to several values, one per aggregation unit.

The aggregation operator may be a spatial average or other statistics (like median or percentiles) based on the distribution of data within the aggregation unit. Where input data are sparse or irregularly distributed, an intermediate step of spatial interpolation may be necessary.

In the following example (Map 3.2), a regression model combined with kriging was used to map copper concentration in topsoils from LUCAS topsoil survey (21,682 samples). The geostatistical and regression models take various covariates into account: geology, land use and vegetation, climate, topography, soil properties and management covariates (as administrative units).

Map 3.2: Example of interpolation map, displaying copper concentrations in soil



Notes: Interpolated topsoil Cu concentrations (µg kg^{-1}). The assessment is based on 21682 LUCAS samples (0-20cm) from 25 European Union countries. Year: 2018.

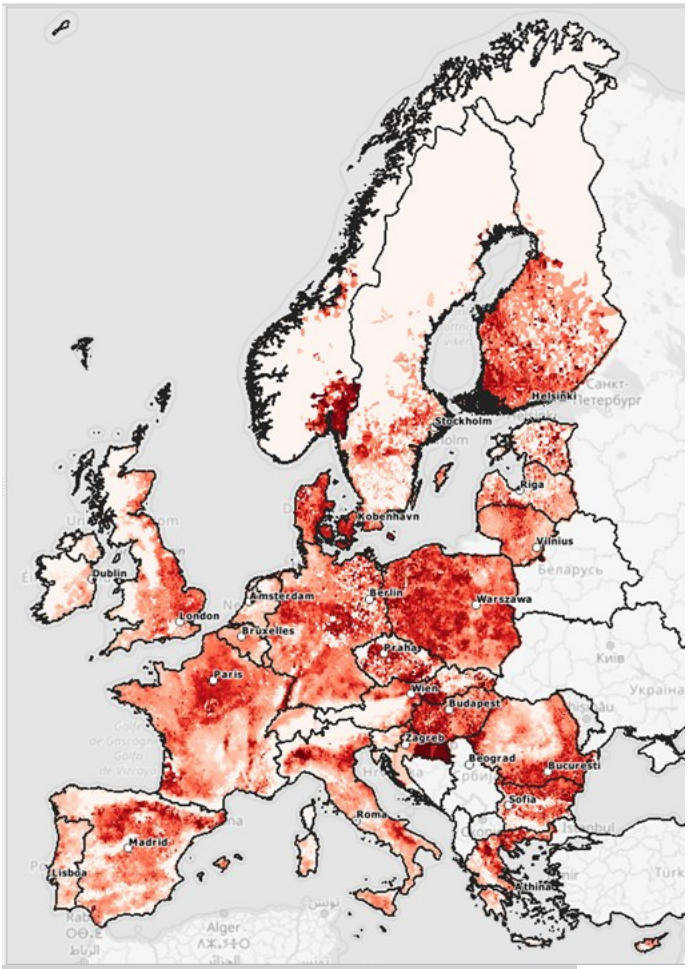
Source: https://esdac.jrc.ec.europa.eu/

Linkage with ecosystems and habitats

Map overlay

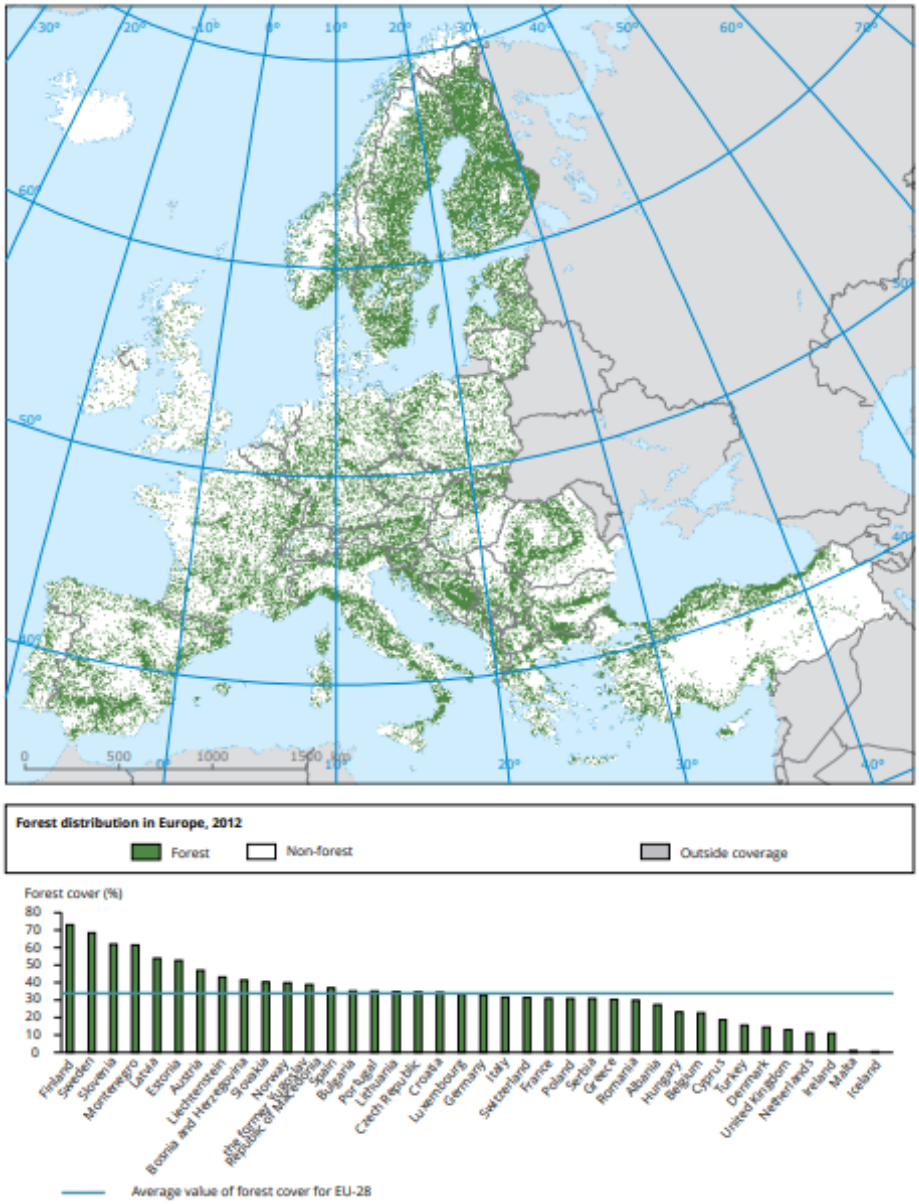
Map overlay consists in superimposing different layers of information. Analysis of the data layers and identification of potential relationships between them are left to the user of the maps. In the present context this would consist in overlaying indicator values calculated at specific locations, grid points or by administrative unit (country, region, etc.), depending on the spatial resolution of chemical pressure data, with one or several data layers describing ecosystems or habitats: *e.g.* vegetation plot data from the EVA database (http://euroveg.org/eva-database), EUNIS (European Nature Information System) habitat or Annex I habitat types (Habitats Directive) distribution data, data describing the occurrence of agricultural crop data (like cereals, see Map 3.3), forests (see Map 3.4 or broader spatial data related to Land-cover and land-use (Corine Land Cover), or on protected areas like NATURA 2000 (see Map 3.5).

Map 3.3: Distribution of arable sites, growing cereals within Europe



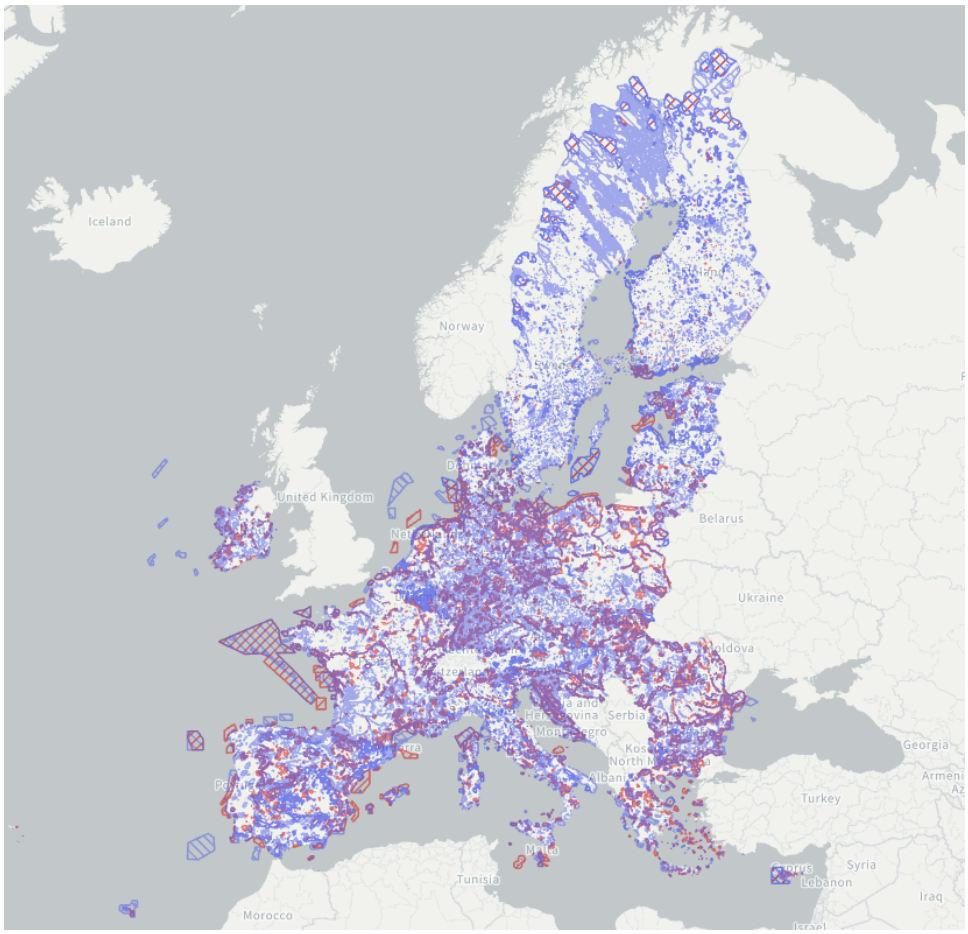
Source: Pegasus data for cereals (Eurostat-2010 FSS).

Map 3.4: Distribution of forest cover in percent related to the land cover in Europe in 2012



Source: EEA Report on European forest ecosystems (EEA, 2016).

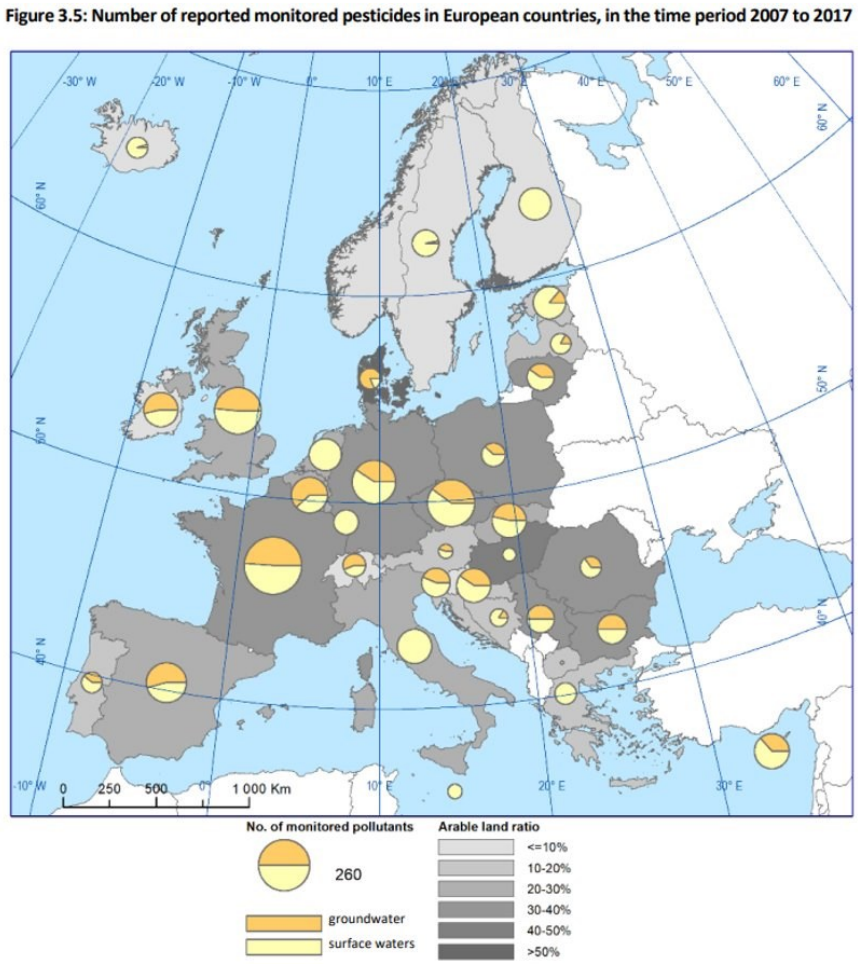
Map 3.5: Natura 2000 areas in Europe



Source: Natura 2000 Network Viewer (europa.eu).

In the following example dealing with pesticides in surface and groundwaters (Map 3.6, from Mohaupt et al., 2020), two layers of information at national scale are superimposed: the number of reported monitored substances for each country and the amount of arable land per country.

Map 3.6: Example of multi-layer information



Pesticides in European rivers, lakes and groundwaters – Data assessment 20Figure 3.5 shows the number of reported monitored pesticides for each country in the time period 2007 to 2017. The number of reported pesticide substances varies between 1 (North Macedonia and Norway) and 319 (France). Overall, there is neither correlation between the reported monitoring sites under consideration of the amount of arable land, nor the number of reported monitoring sites and reported monitored pesticide substances. Figure 3.5: Number of reported monitored pesticides in European countries, in the time period 2007 to 2017Notes: The map includes two types of information: the arable land ratio and the number of monitored pollutants. Arable land ratio represents the amount of arable land in each country. The size of the piechart represents 260 monitored pollutants in a country. Source: Waterbase – Water Quality database, version April 2019; Eurostat and Corine land cover data on arable land ratio.

Source: Mohaupt et al., 2020.

Aggregation according to ecosystems or habitats

In this case, spatial aggregation represents the last step of the indicator development. Concentration data used to build the indicator may be aggregated according to the type of ecosystem or habitat, either on European, global scale or per geographical area.

Depending on the selected aggregation criteria, aggregation zones may be either continuous areas or discontinuous sets of grid cells or polygons presenting similar characteristics in terms of ecological and geographical/climatic features. Subsequent representation of the indicator is a map displaying equal values in each aggregation zone or a chart presenting statistics per aggregation zone (Map 3.1).

Table 3.2: Pros and Cons of different approaches to link chemical pressure with ecosystems and habitats in the representation of the indicator

	Pros	Cons
Map overlay	Original resolution of data can be kept. The user has a view of two or more different data sources at the same time and can make his own analysis.	Interpretation may not be easy.
Spatial aggregation according to ecosystems or habitats	The final indicator better reflects the links between the chemical and ecological components. Easiness of use is increased.	Aggregation relies on choices that may orient or restrict the interpretation of the indicator.

3.2.5 Applying a Protection factor to different spatial entities

A protection factor (Pf) can also be applied to different spatial entities, as to modulate the sensitivity index. Indeed, this protection factor may be adjusted to reflect the different ecosystem types, according to their degree of naturality, their overall sensitivity to chemical exposure or their position in the chain of exposure (forest ecosystems are not supposed to be exposed to agro-chemicals, for example), but also according to the spatial data available, in addition to the definition of an effect level value for key species. As such, different protection factors could be applied to 1. Urban and sealed areas, 2. Agricultural areas, 3. Grasslands, 4. Small woody features, and 5. Forest ecosystems, allowing to show different risk levels for the same pesticide concentration.

But this protection factor should also vary according to the different protection levels, like for within areas classified as N2000 sites, the EU network of areas protecting the habitat types and species listed under the Nature's Directives, or for National Parks, where most of human activities are not allowed. The CDDA database of nationally designated protected areas in Europe can be used to delineate all protected areas in the EU. It also allows to use the IUCN management categories that each country should assign to their protected areas, as to adapt the protection factors according to the level of protection within each protected site (Table 3.3).

Table 3.3: Protection factors within protected sites. Source: IUCN

Ia	Strict Nature Reserve	Strictly protected areas set aside to protect biodiversity and also possibly geological/geomorphologic features, where human visitation, use and impacts are strictly controlled and limited to ensure protection of the conservation values. Such protected areas can serve as indispensable reference areas for scientific research and monitoring.
Ib	Wilderness Area	Usually large unmodified or slightly modified areas, retaining their natural character and influence without permanent or significant human habitation, which are protected and managed so as to preserve their natural condition.
II	National Park	Large natural or near natural areas set aside to protect large-scale ecological processes, along with the complement of species and ecosystems characteristic of the area, which also provide a foundation for environmentally and culturally compatible, spiritual, scientific, educational, recreational, and visitor opportunities.
III	Natural Monument or Feature	Protected areas set aside to protect a specific natural monument, which can be a landform, sea mount, submarine cavern, geological feature such as a cave, or even a living feature such as an ancient grove. They are generally quite small protected areas and often have high visitor value.
IV	Habitat/Species Management Area	Protected areas aiming to protect particular species or habitats, their management reflects this priority. Many Category IV protected areas will need regular, active interventions to address the requirements of particular species or to maintain habitats, but this is not a requirement of the category.
V	Protected Landscape/Seascape	A protected area where the interaction of people and nature over time has produced an area of distinct character with significant, ecological, biological, cultural and scenic value: and where safeguarding the integrity of this interaction is vital to protecting and sustaining the area and its associated nature conservation and other values.
VI	Protected area with sustainable use of natural resources	Protected areas that conserve ecosystems and habitats together with associated cultural values and traditional natural resource management systems. They are generally large, with most of the area in a natural condition, where a proportion is under sustainable natural resource management and where low-level non-industrial use of natural resources compatible with nature conservation is seen as one of the main aims of the area.

3.3 Equations for risk calculation

3.3.1 Foreword

As underline with Article 37 - Environmental protection of the EU Charter of Fundamental Rights "A high level of environmental protection and the improvement of the quality of the environment must be integrated into the policies of the Union and ensured in accordance with the principle of sustainable development." The objectives set out by the EU Charter acknowledge yet that countries want to protect environmental integrity but also to improve, i.e. restore the environment, if needed (if not sufficiently protected).

Whereas the approach presented hereafter is built upon the risk concept, it is reminded here that the objective of the indicator it not to display an absolute calculation of a risk. A safe criterion (such as PNEC, RAC or EQS and alike) can be considered a marker for sufficient protection (below) and insufficient protection (beyond), whereby the latter may mean no impact (if safety factor is large enough). In the following, the magnitude of the risk quotient, associated with the habitat where this exposure occurs is our main interest, with the aim to be used for both protection and restoration actions or to select areas to be looked at as a priority.

3.3.2 Generic equation – Risk quotient

The model proposed is a risk-based model that can be adapted to take into account the sensitivity of different ecosystems and/or that of individual species in this ecosystem. This can be expressed as the ecosystem-specific risk quotient (RQ): $RQ_{ecosystem\text{-}specific}$ = chemical concentration divided by an ecotoxicological threshold (RAC or PNEC) adapted to ensure an appropriate level of protection **for a specific habitat or ecosystem.** As the concentration of a chemical varies in space and time within the targeted habitat or ecosystem, this RQ is calculated at a specific location and time as:

$$RQ_{i,x_j,k,t} = \frac{C_{i,x_j,t}}{Threshold_{i,k}}$$

Equation 1

where:

- i is a specific chemical;
- x_j is the location within the specific habitat/ecosystem j where the RQ is assessed;
- k is the ecological protection goal considered in the habitat or ecosystem j, species or habitats protection for instance;
- t is the time at which the RQ is assessed;
- $C_{i,x_j,t}$ denotes the concentration of chemical i in the soil, at location x_j, in habitat or ecosystem j and time t;
- $Threshold_{i,k}$ refers to an ecotoxicity threshold such as the RAC or PNEC for chemical i and for a specific protection goal k. It includes standardised assessment factors, addressing the extrapolation from the lab to the field as well as from standard lab species towards wild-living species and the intra- and interspecies variability. Assessment factors are laid down in the regulatory areas for chemicals (*e.g.*, for PPPs, industry chemicals, biocides and pharmaceuticals). They are meant to account for extrapolation from laboratory to field.

3.3.3 Application of a protection factor

A protection factor Pf_j is applied depending on the ecosystem/habitat type j. This management factor may be adjusted to reflect different type of ecosystems or protection levels for various land uses, for example from agricultural areas to protected habitats (*e.g.*, Natura 2000 areas and nature conservation areas). Some regulatory frameworks exist for Europe (*e.g.*, Natura 2000), however Member-states and local authorities might have different instruments for nature conservation and protection. Highly sensitive areas under strict regulations (*e.g.*, Naturschutzgebiete in Germany) should be scored with the highest protection factor, whereas sealed and anthropogenic areas (for example urban areas) can be scored with lower protection factors. EFSA (2017) defined three protection goal options for agricultural sites, depending on the focused organism. However, they are not yet adopted by the European Commission.

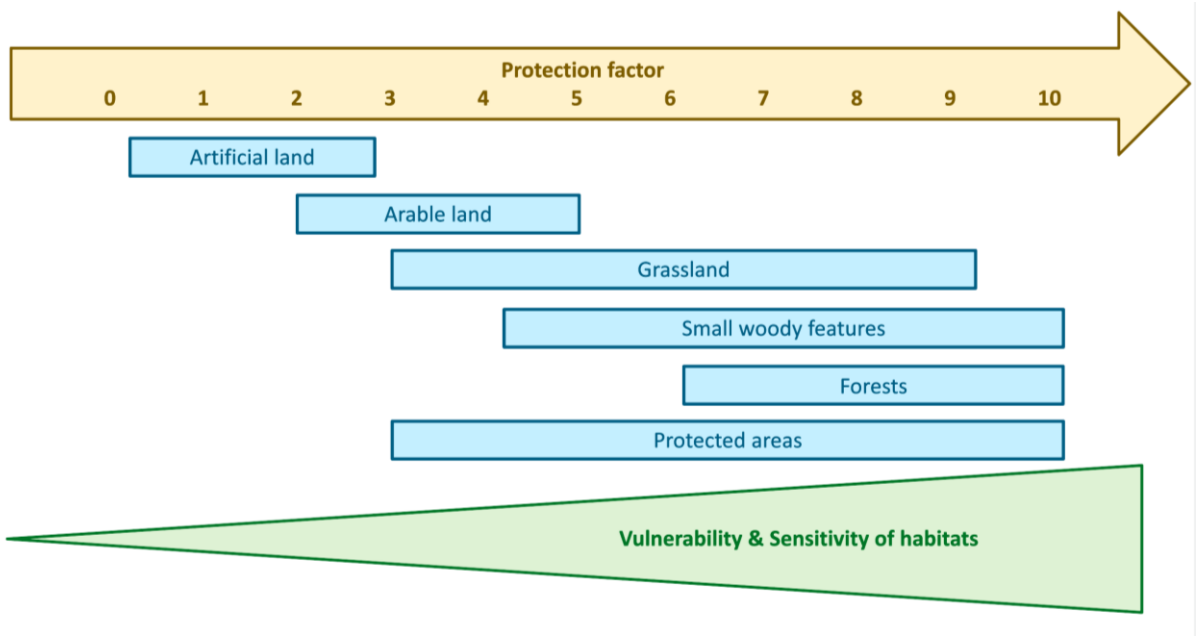
The application of protection factor Pf_j leads to the adjustment of Equation 1 as follows:

$$RQ_{x_j,k,t}^{adjusted\ \_eco} = \frac{C_{i,x_j,t}}{Threshold_{i,k}} \cdot P_{f_j}$$

Equation 2

As indicated in section 3.2 and above, the weight to be applied for the protection of a specific type of ecosystem is highly depending on the management objective. An example is provided on Figure 3.5.

Figure 3.5: Example for the choice of the protection factor reflecting vulnerability as well as sensitivity of the protected habitat



The level of biodiversity protection within protected areas varies from strict protection, like within central zones of National parks, to areas where the interaction of people and nature over time has produced an area of distinct character, and where safeguarding the integrity of this interaction is

necessary, like in most Natura 2000 sites. As a result, some protected areas allow industry, extensive agriculture or fishing to occur within their boundaries, while others prohibit all of these activities. Therefore, we propose to use the IUCN protected areas management categories system to adapt the protection factor of each ecosystem identified. On a scale from 0 – 10, urban sealed areas outside any protected area should have the lowest protection factor, while a forest habitat within a highly sensitive areas under strict protection would have the highest value possible.

In terms of the Biodiversity strategy for 2030 (EC, 2021c) in line with the legal binding nature restoration law as well as the soil strategy for 2030 (EC, 2021b), biodiversity within arable land should be enhanced as well as protected. Therefore, degradation should not be acceptable in agricultural areas, depending on the intensity of agricultural use and the occurring biodiversity (density of Landscape features, ponds, rivers, etc.). However, there is no data available on farming intensity, and only Small woody features in agricultural areas have been identified, excluding all natural elements having no woody vegetation. As such, we propose a protection factor between 2 and 5, according to the location of agricultural areas in protected areas or not. In addition, Small woody features would have a protection factor between 4 and 10, while grassland would have protection factor between 3 to 10, as they could be more subject to intensive agricultural practices outside any protected areas.

For forests, the protection factor should in theory vary according to the forestry intensity, the nature of the forest (plantation, semi-natural, natural) as well as occurring biodiversity (monospecific forest stand, mixed forests, endemic species, etc.). However, none of those data are spatially available. Therefore, we propose a protection factor between 6 and 10, only related to the level of protection.

3.3.4 Mixtures

Because environmental media contains numerous compounds, the ecotoxicity risk of a chemical mixture towards a specific ecological goal should be calculated and can be expressed according to the concentration addition principle for the risk index (RI): Risk Index$_{\text{ecosystem-specific}}$ = Sum of Risk Quotients for a number N of Chemicals. This is summarized in Equation 3:

$$RI_{x_j,k,t} = \sum_{i=1}^{N} \left(RQ_{x_j,k,t}^{adjusted\ \_eco} \right) = \sum_{i=1}^{N} \left(\frac{C_{i,x_j,t}}{Threshold_{i,k}} \right) \cdot P_{f_j}$$

Equation 3

where N is the number of different chemicals in the mixture.

$RI_{x_j,k,t}$ thus refers to the risk index for the protection goal k in habitat or ecosystem j exposed to the chemical mixture at location x_j and at time t.

The approach presented here is based on the sum of the risk quotient. It must be stressed here that this-method assumes that the aggregation of RQ's in cases of mixtures follow a linear path – which is not the case. Besides, when the aim of applying such aggregation is to assess an actual risk from the mixture, the RQ of mixtures should preferentially be calculated using the same endpoints and safety factors for the different ecotoxicity thresholds.

This approach is recommended when calculating an actual risk of a mixture, and it informs on the risk to a specific toxicity effect. For building a risk indicator however, the RQ approach combining different endpoints is nevertheless acceptable, because it can allow to draw an initial mixture risk profile (Socianu et al., 2022) in a certain location and highlight potential threats to living organisms.

Spatial and temporal aggregation

Spatial and temporal aggregation aims to move from point values of the RI to aggregated values:

- over the habitat or ecosystem j within a geographical area (which can be the entire zone of interest or sub-regions/spatial units composing this zone);
- over a given period of time.

This requires spatial and temporal aggregation of concentrations in Equation 3, leading to:

$$RI_{A_j,k,T} = \sum_{i=1}^{N} \left(\frac{C_{i,A_j,T}}{Threshold_{i,k}} \right) \cdot P_{f_j}$$

Equation 4

where:

A_j is the spatial area occupied by habitat or ecosystem j considered for aggregating concentrations;

T is the period of time considered for aggregating concentrations;

denotes the concentration of chemical i in the soil, aggregated over area Aj and period T;

$RI_{A,j,k,t}$ thus refers to the RI for the protection goal k exposed to the chemical mixture in habitat/ecosystem j over area Aj and period T.

Equations (3) and (4) can be adapted depending on the purpose of the indicator, and the specific protection goal that may be an individual species, ecosystem or habitat. This will trigger the selection of the more relevant parameters for each component. Some examples are provided in annex 4 (equations (7) to (11)).

3.3.5 Connecting the different layers of data

Exposure and hazard data

Depending on the type of occurrence information, data is linked to different units. While application data of (liquid) pesticides is usually expressed as g/ha or L/ha, monitoring data from case studies is normally expressed as soil concentration in mg/kg soil dry weight (dw). Moreover, endpoints for terrestrial organisms are expressed in different units as well. While ecotoxicity endpoints for in-soil organisms (earthworms, springtails, mites and microorganisms) are expressed as concentrations in mg/kg related to the soil dry weight, ecotoxicity endpoints for plants and non-target arthropods are expressed as rates in g/ha, endpoints for bees are expressed as µg/bee and endpoints for birds and mammals are expressed as mg/kg per body weight.

Monitoring data of soil concentrations, normally expressed as mg/kg referred to soil dry weight can easily be used for comparison of ecotoxicity data for in-soil organisms as the endpoints are also expressed in mg/kg soil dry weight. However, by using monitoring data, the sampling depth (e.g., 0 – 25 cm) should be converted to a standard penetration depth of 5 cm as sprayed chemicals typically stay in the upper soil centimeters as shown by Toschki et al. (2020) as well as cited by EFSA (2017) and EFSA (2019b).

Application data expressed in g/ha or L/ha can easily be converted to a soil concentration of mg/kg soil dry weight by using standard assumptions, described in respective guidance documents (EC, 2002), whereas modelling as a function of land use is required to move from sales data (expressed in kg/year) to application data. The comparison with ecotoxicity data on in-soil organisms as well as for terrestrial plants and non-target arthropods is therefore also possible.

For bees, birds and mammals, the comparison of monitoring data as well as application data with endpoints is more complex as the ecotoxicity endpoints are based on concentrations per bee, or mg bird / mammal. This issue remains a challenge to be met for terrestrial ecosystems. An example on how to proceed can be found in the WFD. The technical guidance for EQS (EC, 2018) provides a dedicated chapter on how ecotoxicity data expressed in e.g., the concentration in water can be back calculated from the concentration in predators tissue. This back calculation allows to estimate which concentration in water will lead to a sufficient accumulation in the first trophic levels to cause a risk for predators.

As an example for a predatory fish occupying the trophic level 4 (TL4), the QS for predator can be calculated as described in Equation 6, using the average measured bioaccumulation factors (BAF) described in Equation 5.

$$BAF\ (TL4) = BCF \cdot TMF \quad \text{Equation 5}$$

Where:

BCF refers to the bioconcentration factor
TMF refers to the trophic magnification factor

$$QS_{water,\,biota} = \frac{QS_{biota}}{BAF}$$

Equation 6

The particular case of metals

With naturally occurring substances such as metals, the consideration of the geochemical background needs a particular attention. Risk assessments performed under chemical regulation (former “existing chemicals” and REACH, ECHA, 2008, ECHA, 2017) use both as the total risk or added risk approaches. Monitoring concentrations are likely to be expressed as “total concentrations” whereas modelled exposure concentrations are more likely to be expressed as added concentrations, where C_{total} = $C_{background}$ + C_{added}. The two approaches are acceptable, but care should be taken so that effect data and exposure concentrations should be expressed using the same approach. If there is a need to connect the two types of values, an option would be to add a generic/regional background to “added concentration” (EFSA, 2021).

Connecting different types of ecotoxicity data

An approach to aggregate in a single indicator different types of ecotoxicity data (expressed in different units and durations) has been provided by Kudsk et al. (2018) for the determination of the Danish pesticide load (PL) (see also section 4.4 on indicators). This indicator was developed in Denmark as a response to the implementation of Directive 128/2009 establishing a framework for EU actions to promote a sustainable use of pesticides (EU, 2009a). The PL consists of three sub-indicators for human health, ecotoxicology and environmental fate, respectively. PL for ecotoxicology (PLECO) is calculated on the basis of the LC/LD/EC50 values of the active ingredients for acute toxicity to mammals, birds, fish, daphnia, algae, aquatic plants, earthworms and bees, and the NOEC values for chronic toxicity to fish, daphnia and earthworms. PL does not consider the actual exposure, but rather reflects the relative risks associated with the application of pesticides. For each type of endpoint, the most harmful pesticide active ingredient *i.e.* with lowest LC/LD/EC50 and NOEC values is defined as reference compound, and is allocated the maximum number of PL points per kg active ingredient. The number of PL points for all other active ingredients are expressed relative to the reference active ingredient. This standardisation of the results allows for the determination of a score, which can be aggregated for further analysis.

Aggregation can take place for a single active substance and several endpoints or to reflect the pressure due to the mixture of compounds (which can be the sum of herbicides, or the sum of all pesticides) on a single target species or taxon. The same type of scoring system is used by Bergkvist (2004) which allows for the aggregation of several endpoints in a single indicator.

4 Review of available data sources and implementation possibilities

4.1 Chemical occurrence and exposure data

Existing datasets and databases on chemical occurrence of metals and currently used pesticides (CUPs) in soil and terrestrial biota, and their associated strengths and weaknesses were assessed, especially in terms of using the data to produce an indicator on chemical impacts on ecosystems across Europe.

The relevance of data on chemical occurrence were assessed for their European-wide coverage, the uniformity in sampling procedures, analysis, quality control, and thus comparability of data, high spatial resolution, wide range of land-use categories and available soil property data available.

The detailed results of this review are provided in **Annex 1: Databases on chemical occurrence** and in a series of three **Excel files**([2]). The main findings are summarized hereafter.

From the evaluation of the various available datasets, The Land Use/Cover Area frame statistical Survey Soil (**LUCAS soil**) database appears to be the best option; however, the occurrence data of pesticides and metals are not necessarily easily accessible and contain relatively old data for the metals. LUCAS Soil is an extensive survey of soil properties and occurrence of chemical contaminants in soil across the European Union. For metals, sampling has been conducted in 2009 to 2012, 2015, and 2018 (Orgiazzi et al., 2018). However, for CUPs, analysis is currently still ongoing, and the data are thus not yet available. Other databases including metals are **GEMAS, BIOSOIL** and **FOREGS** but these have limitations either when it comes to geographical coverage, land-use coverage, old data or soil property data are not available.

Data and databases on CUPs in soil from larger surveys are still largely lacking, but several case studies on CUPs in soil have been conducted. One example is the **monitoring in Czechia** as published by Kosubová et al. (2020). During a period from 2014-2017 a large amount of soil samples at different sites were analysed. Altogether, 136 soil samples have been taken, 60 pesticides as well as four transformation products were analysed. Results showed the frequent presence of conazole fungicides as well as some herbicides and one insecticide in more than 20 % of analysed soils in at least one sampling point. A maximum residue of 14 pesticides were found, typically 2 – 7 pesticides occurred in soil samples. All together, 116 different mixtures were analysed. Residue data is available for the analysed years, sampling occasions took place between February and October in a soil depth of 0 – 25 cm, within the seasonal application of pesticides in the field.

The use of case studies and national monitoring data have limited usefulness for a European-wide indicator, given the inherent limitations on geographical coverage, but the dataset may be useful in a potential case study.

At the moment, the usefulness of the existing monitoring data from single countries for a chemical indicator is limited by the data being single measurements at certain locations and displays a certain sampling depth (*e.g.*, soil cores of 0 – 25 cm). Especially, the extrapolation from a single monitoring site to the larger spatial unit is challenging and needs to be addressed. Seasonal variations in CUPs concentrations in soil is neither accounted for as larger residues are expected just after application of PPPs within the growing season compared to smaller amounts outside the application period (November – February). Moreover, Toschki et al. (2020) as well as EFSA (2017) pointed out, that a large part of sprayed residues remains in the upper soil layers of 0 – 1 cm as well as 0 – 2,5 cm due to adsorption processes. However, soil core measurements are conducted for deeper soil layers of 0 – 10 cm or 0 –25 cm (Example from Czechia) in the most cases. Expressing the measured residues of actives within a soil layer of 0 – 25 cm towards mg/kg soil dry weight dilutes the actual concentration, which remains in upper soil layers. Therefore, 'real' concentrations are underestimated.

([2]) 'ETC_HE_3.2.8.1_2_data_search_Monitoring_occurrence.xlsx',
'ETC_HE_3.2.8.1_2_data_search_Models_occurrence.xlsx' and 'ETC_HE_3.2.8.1_2_data_search_Biota.xlsx'.

However, based on the European Goals within the United Nations Sustainable Development Goals (EEA, 2019) as well as the Green Deal, explicitly based on the European Soil Strategy for 2030, a narrow monitoring net for soils will be established within the European Union (EEA, 2019, EC, 2019, EC, 2021b). For future reporting of chemical risks towards the terrestrial environment, monitoring data has high relevance as only measured data reflects occurring concentrations of chemicals in soils.

For chemical occurrence in terrestrial biota, the NORMAN Empodat database and the ESB-UBA database were evaluated to illustrate what data is currently available (Excel file deliverable([3])). There are large gaps when it comes to using chemical occurrence data from biota for a European-wide ecosystem specific indicator. Optimally, chemical occurrence data should be available for the targeted specie. Multimedia modelling may be one alternative to fill this gap.

4.2 Effect level data on non-target organisms

Existing publicly available databases on effects on ecotoxicological data of chemicals on non-target organisms as well as their associated strengths and weaknesses in terms of using the data to produce an indicator on chemical impacts on ecosystems across Europe, have been assessed.

The detailed results of this review are provided in **Annex 2: Databases on ecotoxicological effect data** and in an Excel file([4]). The main findings are summarized below.

In general, the use of publicly available ecotoxicity data is preferable in terms of traceability. Moreover, clear information about used guidelines, acceptability within regulatory processes as well as test conditions (*e.g.* used soil types) is necessary to assess reliability of the data set. Chemicals in Europe are regulated by different Authorities and for the time being, data for different regulating areas is distributed to different databases or -sources. However, the OECD eChemPortal can be classified as overarching collecting point for several databases containing ecotoxicological information about chemical substances.

For PPPs – which are the best studied chemicals regarding their impacts on the environment due to their intended direct use in natural systems and therefore corresponding rather broad data requirements - the EFSA OpenFoodTox database would be the best choice in terms of reliability of the data as the included data is peer-reviewed by European Member states as well as the European Food Safety Authority. Unfortunately, the included datasets display just a subset of authorized active substance up to know. Assessed data sets are also captured in UBA ETOX database, it holds a broader dataset than EFSA OpenFoodTox but still just a subset of active substances.

French authorities are hosting the AGRITOX database, which provides a large dataset on ecotoxicological endpoints for aquatic organisms, classification and labeling as well as physico-chemical properties proved by authorities for the regulation of chemicals as well as information from scientific reports. A large dataset for terrestrial and aquatic ecotoxicity values is included in US EPA ECOTOX, which is hosted by the Environmental Protection Agency of the United States of America, contains a huge dataset of ecotoxicity data. However, it also includes lots of open literature data which is not assessed by authorities. The Pesticides Properties database (PPDB) is hosted by the Agriculture & Environment Research Unit (AERU) at the University of Hertfordshire and includes ecotoxicity as well as fate data for pesticides, which is public available and aims to include data used by EFSA at a first step. If EFSA data is not available, other sources like open literature or safety data sheets are used to fill up data gaps. Therefore, it is not restricted to assessed data by authorities, only.

([3]) 'ETC_HE_3.2.8.1_2_data search_Biota.xlsx'.
([4]) 'ETC_HE_3.2.8.1_2_data_search_Toxicity_data.xlsx'.

The ECHA IUCLID contains mainly data required under the REACH regulation, collected under the registration process. As such, these dossiers have been provided by Industry and may or may not have been verified by ECHA or Member State authorities depending of the dossier status.

The ECHA dissemination portal also contains data on biocides assessed under BPR (add ref) by regulating authorities. The European Chemicals Agency (ECHA) developed and maintained this database in cooperation with the Organisation for Economic Co-operation and Development (OECD) and the European Commission.

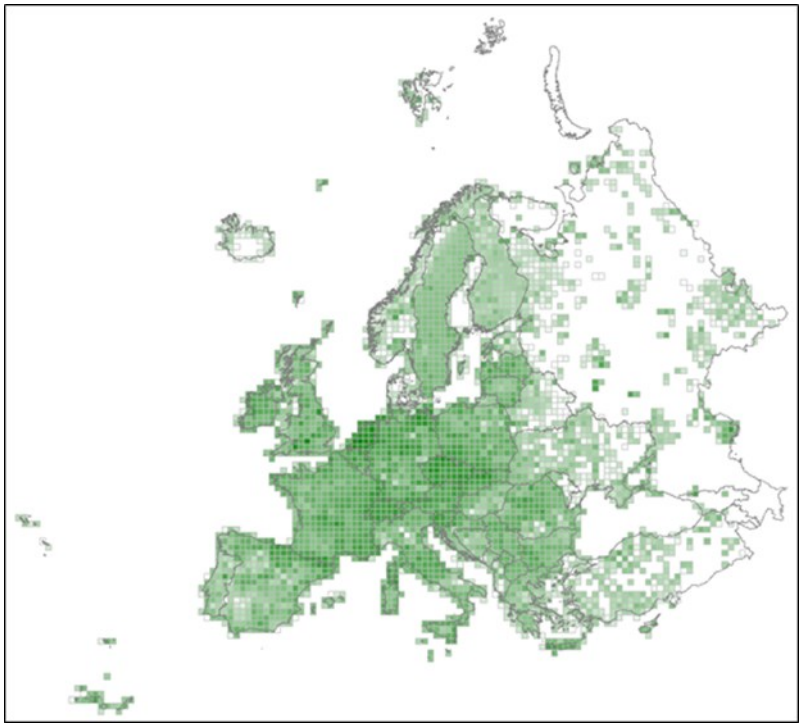
The NORMAN database could also be used for entering ecotoxicity data for terrestrial organisms, independently from regulatory assessment. NORMAN has an ambition to become the primary data source and global one-stop-shop for all issues regarding emerging substances, contributing to the creation of the early-warning system for emerging pollutants and subsequent policy actions. The database contains very few data on terrestrial organisms, so far.

4.3 Biodiversity data

4.3.1 Terrestrial plant data

The EVA database is the database of the International Association for Vegetation Science (IAVS), available upon request (http://euroveg.org/eva-database). It contains phytosociological data all over Europe (Map 4.1). The main available data are plots of vegetation relevés, including records of plant taxon co-occurrence at particular sites. The classification of those vegetation relevés is based on the Vegetation of Europe: a hierarchical floristic classification system of vascular plants, bryophytes, lichens, and algal communities. Based on their occurrence and abundance, species can be assigned to different categories, i.e. dominant species, characteristic species.

Map 4.1: Density distribution of the total of 1,612.287 georeferenced plots in EVA and other plots provided for this project in 50 x 50 km grid cells (accessed on 28 November 2019)



4.3.2 Terrestrial Habitats

The Habitats Directive and related Annex I Habitat types

The EU Habitats Directive aims to achieve a favourable conservation status for all habitat types listed in its Annex I, grouped along 9 groups (Coastal habitats, Dunes habitats, Freshwater habitats, Heath & scrub, Sclerophyllous scrubs, Grasslands, Bogs, mires & fens, Rocky habitats, Forests). This Annex I is now listing 233 European natural habitat types, including 71 priority habitats (i.e. habitat types in danger of disappearance and whose natural range mainly falls within the territory of the European Union). This list was initially based on the hierarchical classification of European habitats developed by the CORINE Biotopes project 2, the only existing classification at European level at the time.

The Article 17 web tool for "Habitat assessments at EU biogeographical level" (https://nature-art17.eionet.europa.eu/article17/habitat/summary/) provides an access to EU biogeographical and Member States' assessments of the conservation status of the habitat types of Community interest, compiled as part of the Habitats Directive (Article 17) reporting process. These assessments have been carried out in EU25 for the period 2001-2006, in EU 27 for the period 2007-2012 and in EU28 for the period 2013-2018. A distribution map can be extracted for each individual habitat type, at the EU level or for individual Biogeographical regions.

The EUNIS habitat classification

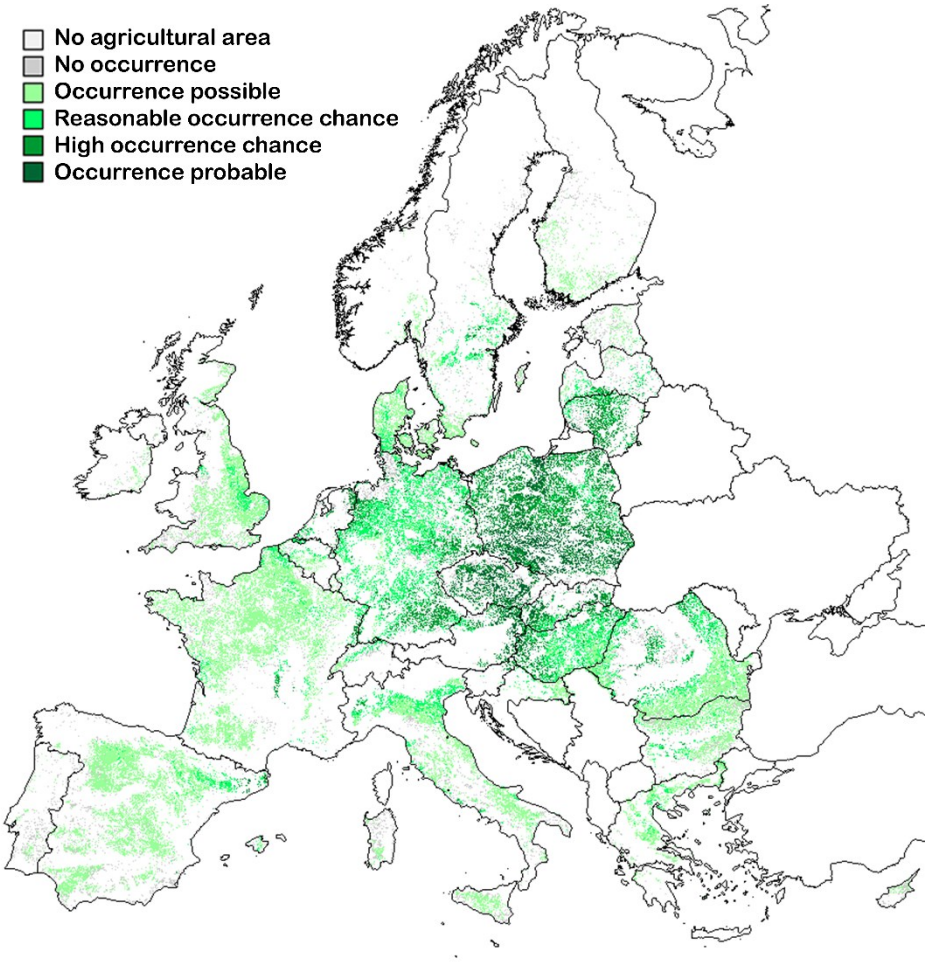
The EUNIS (European Nature Information System) habitat classification expert system can be used to link terrestrial plant data and other biological data to habitats. EUNIS is indeed the reference framework for European habitats (https://eunis.eea.europa.eu), designed to give a common pan-European reference set of natural and semi-natural habitat, with a shared description of all those units through a common hierarchical classification.

Terrestrial habitats in EUNIS are often based on phytosociological vegetation types, such as those defined in EuroVegChecklist and present in the EVA database, based on species composition and vegetation structure. But habitats also emphasize the abiotic environment and their geographic location, as classification criteria. EUNIS also includes habitats in which plants are nearly or entirely absent.

Still, most of the terrestrial habitats of EUNIS can be successfully defined using methods of vegetation science (Chytry et al., 2020). As such, a new online database called FloraVeg (https://floraveg.eu/) is now able to link those vegetation plots with the EUNIS classification system as to give a brief description of each habitat type, as well as the details of the main characteristic species combinations (e.g. diagnostic, constant, dominant), and a distribution maps based on the location of vegetation plots assigned to the habitat type. This expert system was applied to classify 1,261,373 vegetation plots from the European Vegetation Archive (EVA) and other databases, and assigned to EUNIS habitats (level 3) by calculating species-to-habitat fidelity and constancy (occurrence frequency) in the classified data set. Each EUNIS habitat is characterized by all the species occurring in this specific EUNIS type with a frequency > 5 %.

Another initiative led by ETC/BD over the past years intended to predict (modelisation) where a vegetation type or a reference community for EUNIS habitats could potentially occur, combining data from on the ground vegetation relevés (EVA database) with ecological drivers like climate, soil, topography and remote sensed Essential Biodiversity Variables (RS-EBV's). (NB. A complete list of predictors can be added in an appendix). The result of such prediction is a series of suitability and probability maps (Hennekens, 2018, Hennekens, 2019, Hennekens, 2020, Hennekens, 2020a). These maps have currently a resolution of 1 x 1 km (Map 4.2).

Map 4.2: Potential occurrence of one of the EUNIS habitats (V11, I.e. Intensive unmixed crops (Cereal and other non-woody crops grown on large, unbroken surfaces in open field landscapes) in agricultural land surrounding wheat crops. The higher the potential occurrence, the more intense the green colour (Arts et al., 2021a, Arts et al., 2021b)



4.3.3 Terrestrial Ecosystem types under the EU-wide ecosystem assessment

The EUNIS classification and the Habitats Directive do not define ecosystems but natural habitats, meaning terrestrial or aquatic areas distinguished by geographic, abiotic and biotic features, whether entirely natural or semi-natural. In contrast, ecosystem mapping is the spatial delineation of ecological units, following an agreed ecosystem typology of ecosystem types which strongly depends on mapping purpose and scale.

The ecosystem types of the MAES classification have been identified because of their distinct natural properties, which are reflected by their abiotic characteristics, biodiversity, vegetation structure, and their ecosystem functions (Maes, 2020). A practical approach to the spatial delimitation of an ecosystem is to build up a series of overlays of significant factors, mapping the location of discontinuities, such as in the distribution of organisms, the biophysical environment (soil types, drainage basins, depth in a water body), and spatial interactions (home ranges, migration patterns, fluxes of matter). A useful ecosystem boundary is the place where a number of these relative

discontinuities coincide. Ecosystems within each category share a suite of biological, climatic, and social factors that tend to differ across categories.

More specifically, there generally is greater similarity within than between each ecosystem type in:

- Climatic conditions;
- Geophysical conditions;
- Dominant use by humans;
- Surface cover (based on type of vegetative cover in terrestrial ecosystems or on fresh water, brackish water, or salt water in aquatic ecosystems);
- Species composition;
- Resource management systems and institutions

For practical purposes, mainly triggered by data availability, and because of the strong links to the emerging Copernicus land monitoring services, the proposed method of ecosystem mapping for the EU Ecosystem assessment implies that CORINE Land Cover (CLC) classes monitored in Copernicus are aggregated into ecosystem types, in the most meaningful way possible to represent broad-scale ecosystems, and combined with ecosystem-relevant information. This aggregation is based on detailed expert analysis of the relationships between land cover classes and habitat classification systems (i.e. EUNIS) to ensure consistency between these approaches.

The present typology separates at level 1 three major ecosystems: terrestrial systems, freshwater and the marine environment. It also anticipates the different reporting schemes of the environmental directives (HD, WFD, MSFD) and the implemented typologies. There are seven terrestrial ecosystem types at level 2: urban ecosystems, cropland, grassland, forests, wetlands, heathland and shrubs, sparsely vegetated land.

4.3.4 Protected areas

The CDDA database, managed by the EEA, is the official source of protected area information from the 38 EEA European countries to the World Database of Protected Areas (WDPA). Following the United Kingdom's withdrawal from the EU on 31 January 2020, it ceased to be part of the EEA's institutional networks and governance. The CDDA data can be queried online in the European Nature Information System (EUNIS). The latest version 20 covers data reported until May 2022 (https://www.eea.europa.eu/data-and-maps/data/nationally-designated-areas-national-cdda-17), including all individual protected areas in national legislation and their assigned IUCN Management Category, when available.

With the assistance of the European Environment Agency, the European Commission has developed a public Natura 2000 viewer (https://natura2000.eea.europa.eu/#), which makes it possible to explore Natura 2000 sites in every part of the EU. Built on state of the art GIS (Geographical Information System) technology, the public viewer is an interactive and user-friendly tool that allows the user to travel seamlessly through the Natura 2000 sites (further designated as N2000 sites) over different types of backgrounds (street maps, satellite imagery, bio-geographical regions, Corine Land Cover, etc.) and to quickly locate sites and related information on species and habitats of interest.

In 2020, the ETC/BD produced a map of the physical Green Infrastructure (GI) network of the EU, regrouping all N2000 sites (hubs), together with the contiguous patches of natural and semi-natural areas which connect two or more of those sites (links). Natural and semi-natural areas are based on the CORINE land cover (CLC) map of 2012, and exclude all Urban and Peri-urban areas, Arable land and Permanent crops that are not classified as High Nature value (HNV) farmland. Other land cover types, such as those included in the 2012 Imperviousness HRL layer, as well as isolated patches of natural and

semi-natural areas not connecting protected sites, and patches of natural and semi-natural areas smaller than 25ha or with a minimum mapping width less than 100m, are also not included in the physical GI networks. The GI Network layer is available at ETC/BD.

4.3.5 High Resolution Layers from COPERNICUS LAND MONITORING SERVICE

Pan-European High Resolution Layers (HRL) provide information on specific land cover characteristics, and are complementary to land cover / land use mapping such as in the CORINE land cover (CLC) datasets (https://land.copernicus.eu/pan-european/high-resolution-layers). The HRLs are produced from satellite imagery through a combination of automatic processing and interactive rule based classification. The main sources are now (since the 2018 reference year) the Sentinel Satellites (in particular Sentinel-2 and Sentinel-1). In addition to high resolution (HR) data, since 2015, COPERNICUS also use very high resolution (VHR) imagery for some of the products. Since 2018, the products have increased in resolution to 10 meters, thus following the source resolution of the Sentinel-2 imagery.

Five themes have been identified so far, corresponding with the main themes from CLC,

- The level of sealed soil (imperviousness),
- Tree cover density and forest type,
- Grasslands,
- Wetness and water, and
- Small woody features (linear structures such as hedgerows, as well as patches (200 m² ≤ area ≤ 5000 m²) of woody features across)

All of these five products are continuing existing products, some with longer time series existing (Imperviousness and tree-cover/forest), and three products that have only one previous reference year (2015) (grassland, the water & wetness products and Small Woody Features). All products are mapping the features under consideration for the whole of the EEA-39 area.

4.3.6 Agricultural area Mask

The estimates for Utilized Agricultural Areas in the EU was until 2020 only based on estimates reported by Member-States, and no EU-wide geospatial data on UAA existed. Therefore, the EEA proposed to create a spatial reference layer for "**agricultural area mask**", aiming at achieving the best possible coverage today, based on available European spatial data.

This spatial (GIS compatible) is using Corine Land Cover as a basic geographical skeleton (i.e. the 1 hectare CLC2018 accounting layer([5])), in addition to other Copernicus data for the refinement of the reference area. The approach follows the same basic concept as already applied for the development of HNV Farmland layer in 2019, starting from the spatial extent provided by CLC and successively subtracting, respectively adding areas (patches) which were included, respectively excluded in the original CLC due to the 25 ha minimum mapping unit. From the CLC agriculture classes (CLC 2xx) and CLC class natural grassland (CLC 321), non-agricultural patches which had originally been included in CLC due to the generalisation to the 25 ha minimum mapping unit, were subtracted using different Copernicus High Resolution Layer (HRL):

- Woody vegetation (on the basis of FTY 100m layer)
- Sealed surfaces (on the basis of IMD 100m density layer)
- Permanent water surfaces (on the basis of a 100m Permanent Water Density (PWD) layer

([5]) https://sdi.eea.europa.eu/catalogue/srv/eng/catalog.search#/metadata/5a5f43ca-1447-4ed0-b0a6-4bd2e17e4f4d

By contrast, some grassland areas (on the basis of a 100m Grassland layer, if not covered by forest or sealed areas) were added to the AA mask, as potential agricultural areas within non-agricultural CLC classes.
The output layer is created as a 100m (1 ha) raster layer and provided as a mask (class 1 = AA, rest = NODATA) in GeoTiff format.

4.3.7 Soil organisms

Edaphobase is a project to collect and publish information on the distribution and ecology of soil invertebrates. The database developed in this project records and manages literature and collection data on soil fauna. These data are linked to species levels with ecological background information of the soil fauna sites (*e.g.* geography, soil, habitat type and climate) and are available to the public (www.edaphobase.org). The database can be used to identify vulnerable sites for in-soil organisms.

4.4 Indicators

For the time being, several indicators describing trends for pesticide uses are available and also established at European (Harmonised risk indicator) or national level (e.g. Pesticide load indicator). Up until to now, no indicator has been established, linking risks of chemicals with occurring habitats or sensitive areas. Landscape based approaches based on environmental parameters like climatic conditions or soil types have been suggested from different authors such as Urionabarrenetxea et al. (2022).

A review of existing indicators related to the risk associated to chemical and their repartition in Europe has been conducted within this project, and some of the relevant examples are summarized below.

- *Methodology for calculating harmonised risk indicators for pesticides under Directive 2009/128/EC. (EU, 2019)*

  This report displays the methodology used to calculate the Harmonised Risk Indicators for pesticides (HRIs) are used by the European Commission for monitoring trends in risk reduction from pesticide use at European Union level. They can also be used at EU or at country level. Two distinct indicators are used at the moment:

  - HRI1 is calculated by combining the statistics on the quantities of pesticide active substances placed on the market and the information on active substances. Substances are classified within four groups: low risk active substances, approved substances, candidates for substitution and not approved substances. The four groups are scored with weighting factors of 1, 8 ,1 6 and 64, respectively.
  - HRI2 is calculated based on the number of emergency authorisations granted to PPP and the same categorisation and weighting as HRI 1.

  For these indicators, the reference area is by countries for their national territory (NUTS0) and for the whole EU, and thus, cannot be related to a specific habitat. The HRI's are based on the amounts of sold pesticides within the EU and can also be demonstrated on sales within one country. Within current regulatory frames, the reference period of the trend is set at a time period of 2011-2013 and the trend is reported on a yearly basis from the European Union. Active substances are grouped as categories, taking into account their regulatory status and certain properties of concern. The HRI's can demonstrate the sales of pesticide ingredient per country but they cannot display a risk of pesticides as the four categories (substances with low

risk, approved substances, hazardous substances and not approved substances) do not reflect the intrinsic toxicity potential of substances.

- *Pesticide Load—A new Danish pesticide risk indicator with multiple Applications. (Kudsk et al., 2018)*

  The Pesticide Load (PL), introduced in Denmark. Replaces the Treatment Frequency Index (TFI) as the official pesticide risk indicator. The PL consists of three sub-indicators for human health, ecotoxicology and environmental fate, respectively, each of them being expressed as the PL per unit commercial product (kg, L or tablet). The approach used to determine PL for ecotoxicology (PLECO) is explained in section 3.3, connectors). Because in Denmark, the obligation for farmers to upload their pesticide use data on an annual (and rather than sales), pesticide use data is available for each farm, and allows for the production of maps providing detailed information on pesticide use in different regions. This indicator has not been linked to ecological area, or habitat, but shows already significant geographical differences, which could be attributed to differences in crop rotations and may help to the identification of 'hot spots'.

  A similar approach has been proposed by Neumeister (2017) and is presented as an alternative to monitor the impacts pesticides may have for people and the planet beyond a "pounds on the ground" approach.

- *Rapid rise in toxic load for bees revealed by analysis of pesticide use in Great Britain (Goulson et al., 2018)*

  The authors investigated the changes in the mass of pesticides used, the area sprayed, and the total number of honey bees that could potentially be killed in Great Britain in the period covering 1990 to 2015. Pesticide usage is recorded as both the mass applied each year, and the area treated. LC50 values) are used for bee toxicity. The reference area is at country level and differences in habitats are not taken into account.

- *An assessment of acute insecticide toxicity loading (AITL) of chemical pesticides used on agricultural land in the United States (DiBartolomeis et al., 2019)*

  This paper presents a method for calculating the Acute Insecticide Toxicity Loading (AITL) on US agricultural lands and surrounding areas. The AITL method accounts for the total mass of insecticides used in the US, acute toxicity to insects using honey bee contact and oral LD50 as reference values for arthropod toxicity, and is with this respect comparable to the work done by Goulson et al. (2018). However, here the persistency is also taken into account. As stated by the authors (DiBartolomeis et al., 2019), the analysis also does not provide specific information on actual exposures experienced by insects in the environment nor on the timing and mode of pesticide application or the dissipation of the pesticide into the environment and the AITL is not a standard risk assessment method. The AITL values can be calculated by chemical class, by individual chemical for the top chemicals contributing to the loading, or by crop groups. This indicator is used to assess the trends of insecticides uses by calculating the changes in AITL from 1992 through 2014.

- *Pesticide Risk Indicators at National Level and Farm Level – A Swedish approach (Bergkvist, 2004)*

  Two Pesticide Risk Indicator are described, PRI-Nation and PRI-Farm, the reference area being at country level for the 1st one, and at local scale for the 2nd one. These two indicators are risk-based with a score determined for hazard (fate and impact on ecosystems /related to operator health) and exposure and combined with data on use intensity. The scoring systems for hazard is based on the classification and labelling. The exposure score considers among other parameters the application method, and the dose rate as being a part of the leaching index score. The "use intensity" at national level is calculated as the total number of hectare doses the annual sold amount of the substance theoretically could yield. At farm level, the actual

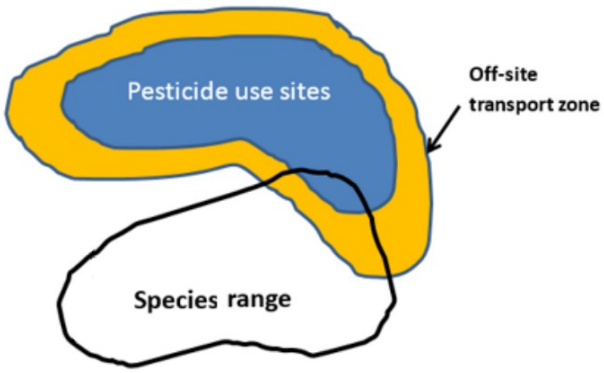
hectare dose for a particular product is used, with some modification including e-fate. The scoring system allows for the aggregation of different endpoint to a single score for each substance. The indicators does not allow for the differentiation of habitats.

❖ *DRAFT EPA Proposed Revised Method for National Level Endangered Species Risk Assessment Process for Biological Evaluations of Pesticides (US-EPA, 2019)*
The Endangered Species Act (ESA) requires to ensure that Agency actions related to pesticides registrations are not likely to jeopardize federally listed threatened or endangered species or destroy or adversely modify designated critical habitat of such species. A biological evaluation (BE) BE determines whether the pesticide's registration:

- "may affect, but is not likely to adversely affect" the species or designated critical habitat (NLAA); or
- "may affect and is likely to adversely affect" the species or designated critical habitat (LAA)

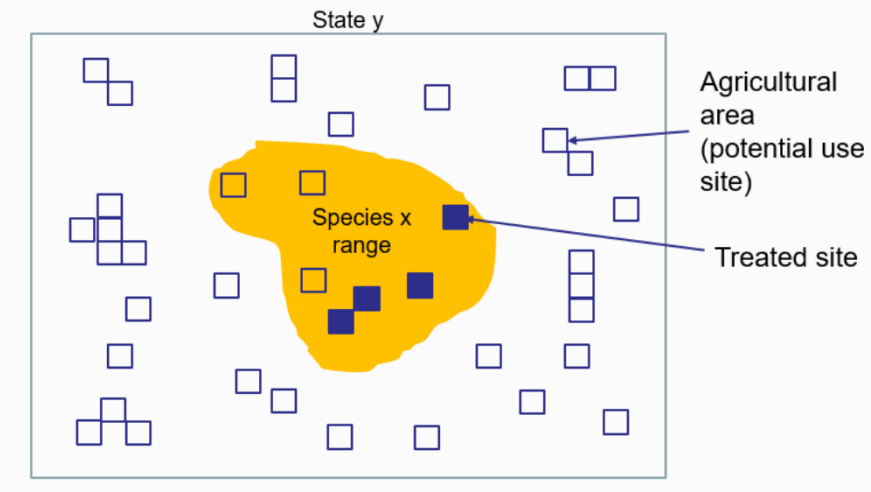
As explained in the draft method (*(US-EPA, 2019)* BE is a 3-step evaluation: Step 1 screens whether there is an overlap of areas of effect (based on where the chemical being assessed is likely to be used) with species range/critical habitat (Figure 4.1). This process is carried out one species at a time for each pesticide. The same process is carried out for the designated critical habitat. Endpoint considered for this assessment are comparable to those use in EU for PPP assessment.

Figure 4.1: Listed species range and action area (i.e. pesticide use site plus off-site transport zone. An overlap <1% will be considered as to lead to no effect. (US-EPA, 2019)



Step 2, notably uses a more refined spatial-overlap with specific chemical use sites that considers life history information and is intended to identify those species for which it is likely that an individual will be adversely impacted. Species where impacts to an individual are not measurable, observable, or likely to occur. Step 3 is the "biological opinion", which determines whether an adverse effect will jeopardize the continued existence of a species or destroy or adversely modify its designated critical habitat. The scale is no longer at an individual level and is focused on assessing risks to the species' population that is listed as endangered or threatened. The scale of Step 3 is the landscape that represents the range of a listed species (Figure 4.2).

Figure 4.2: Conceptual illustration of approach for assigning treated acres to area relative to species range. (US-EPA, 2019)

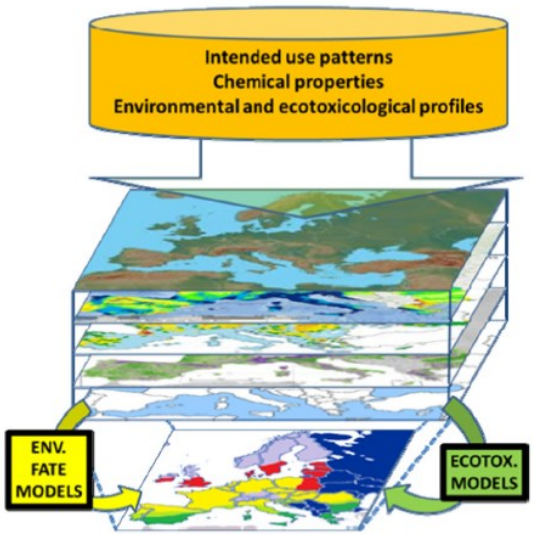


- *BS ISO 19204:2017 Soil quality. Procedure for site-specific ecological risk assessment of soil contamination (soil quality TRIAD approach)*
  The TRIAD approach is applied locally and considers 3 lines of evidence (Chemistry *e.g.* PEC/PNEC, Ecotoxicology i.e. ecotox bioassays on filed soils matrices, and Ecology expressed as biodiversity and species abundance). The indicator considers the result of these 3 approaches and most importantly, their consistency.

- *Human Biomonitoring Indicators for Chemical Exposure.*
  Buekers et al. (2018) developed indicators related to human health. Two types of indicators are proposed: '(sum) indicator(s) of internal exposure' derived directly from HBM biomarker concentrations and 'indicators for health risk', comparing HBM concentrations to HBM health-based guidance values (HBM HBGVs). The translation of this indicator for ecosystems would be to compare biota analysis to threshold in biota (both based on chemical analysis or biomarker analysis).

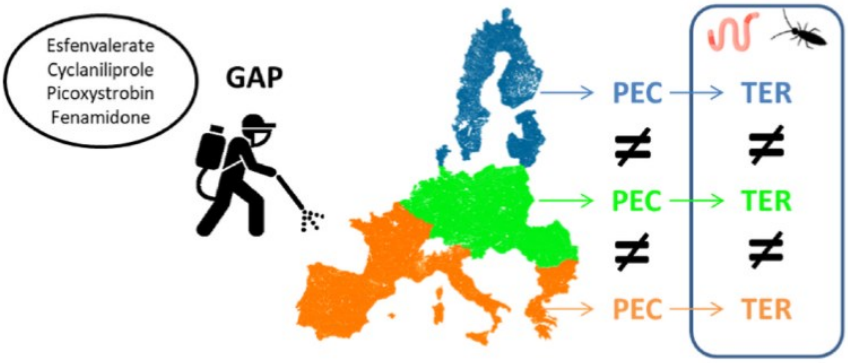
- *Landscape based approach 1 by Streissl et al. (2018):*
  Streissl et al. (2018) suggest including use patters as well as physical chemical properties in combination with eco-regions or landscape ecotypes in current risk assessment schemes of PPPs. The authors suggest refining risk, identified within the first step of the risk assessment based on lab studies with further information to refine these risks at a next step of the risk assessment. For this sake, they apply an ecosystem service approach within the risk assessment for pesticides to identify long term impact on biodiversity (Figure 4.3).

Figure 4.3: Schematic representation of the linking of different layers of spatial information to exposure and ecotox models using the spatial information to assess the risk for different areas in Europe. Source: Streissl et al., 2018



- *Landscape based approach 2 by Urionabarrenetxea et al. (2022).*
  The authors predicted environmental concentrations and the potential risk of PPPs on non-target soil organisms accounting for regional and landscape ecological variability in European soils. They suggest addressing regional variability to perform a landscape bases environmental risk assessment. Within a case study, they used biological endpoints on two soil organisms on 5 chemical substances to demonstrate the risk of pesticide application within three regulatory zones by using specific environmental parameters (temperature, pH and Organic matter content in occurring soil types). Predicted environmental concentrations ranged and therefore, also the risk quotient varied across Europe (Figure 4.4).

Figure 4.4: Risk of 5 pesticides for two soil organisms (*Eisenia Fetida* and *Folsomia candida*) in North, Central and South of Europe. Resulting Predicted Environmental concentrations and in consequence, also the risk quotient ranged. Source: Urionabarrenetxea et al. (2022)



4.5 Findability, accessibility, interoperability and reusability (FAIR) of existing data sources

Data on chemical occurrence in soil as well as biota and ecotoxicological effect levels are spread between several databases (see Annex 1: Databases on chemical occurrence and Annex 2: Databases on ecotoxicological effect data). This makes it challenging to find the data.

The structure of the databases as well as the included information of each database vary, but as a minimum, information on chemicals name and/or chemical number is available in all databases. The interoperability is however challenged by the difference between the codes, units and how the information is structured, linked to the architecture of the databases. A key challenge is that there is no common agreement on which unique identifier to use for chemicals, since CAS Numbers are not unique and legislative entry codes may cover mixtures, *e.g.* for REACH. The Norman network has proposed to use InChI keys, which gives the structure of a chemical, and which are can be linked to monitoring data reported by common instrument softwares (Schymanski and Bolton, 2021). Ideally such unique identifiers should be used for both monitoring and effect data, to make the data interoperable and traceable.

The type and detail level of information made available also vary across databases.

Data on biodiversity, habitats and species sensitivity are captured within different access points, such as OECD, EFSA and ECHA websites. A challenge here are the differences in the type of tests required, and the underlying assumptions. With the One Substance One Assessment, called for under the CSS (EC, 2020b), there is ongoing work to align hazard and other tests on chemicals intrinsic properties, that will make it easier to compare across databases, at EU level, but also at the international level.

Occurrence data on terrestrial plants, in-soil organisms or habitats like urban sites, agricultural areas, forests and nature conservation areas are to some extent publicly available from national sites and/or the EU Information Platform for Chemical Monitoring (IPCHEM, 1995).

When bringing datasets together across databases, quite substantive harmonisation and sometimes also transformation/processing of data are therefore needed. The permissions to access or to reuse data is another obstacle which may hamper the ability to use, assess and perform new queries to datasets. For effect data the permissions may be linked to Confidentiality of Business Information (CBI), while for the monitoring data, there may be safety or other concerns regarding identification of a specific farmer, facility (waterwork) polluted site, or national disinterest in disclosing 'non-compliant' data.

Altogether, this limits the ability to assess the chemical risks, which are used both in premarket lifecycle analyses (*e.g.* for SSBD), for inputs to risk assessments used in a regulatory context, or as inputs to indicator and other assessments of policy effectiveness.

To address these needs and to make better use of publicly funded data, the EU commission has pledged (*e.g.* in the CSS), to explore the options to set up a European wide database, collecting data from different sources and harmonise existing data for further analysis. This is the work referred to as the Open Data Platform on Chemicals, led by DG Environment with the contribution across the EC and EU Agencies, with reference to the INSPIRE directive and Aarhus Convention, which demands data to be made publicly available, according to FAIR principles (**F**indable, **A**ccessible, **I**nteroperable and **R**e-useable (EU, 2022a). It is still debated whether the Open Data Platform will only link to existing databases, or also host data. For the toxicity/effect data the IUCLID format is foreseen to be used, while for the monitoring data the IPCHEM is foreseen to be used in some format. With the recent agreement to make pesticide load data available from 2027 (EU, 2022b) and with initiatives to further develop the Industrial Emissions Directive on diffuse emissions into regional areas, we expect that data sources in the future will become much more available.

5 Case study

5.1 Objective

Within this case study, we are aiming to **assess and discuss the feasibility of the developed methodology** through its application to real datasets.

The indicator defined in section 3.3 (Equations for risk calculation) is successively applied to non-target/representative plant species and soil organisms in different habitats based on laboratory data in a monospecific approach in combination with occurrence data related to residues of active ingredients from PPPs. The data used originate from regular monitoring surveys conducted in Czechia (Kosubová et al., 2020) which is taken as the study area.

5.2 Input data

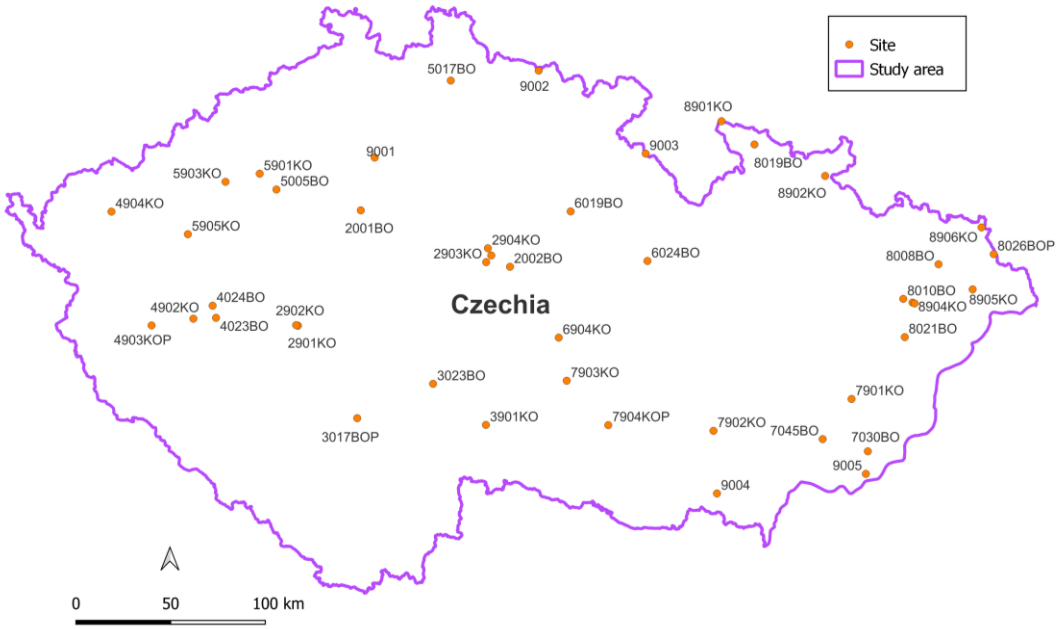
5.2.1 Chemical occurrence data

Data were provided by ÚKZÚZ, the Central Institute for Supervising and Testing in Agriculture of Czechia, Section of Agricultural Inputs. They correspond to 45 monitoring points mostly distributed in agricultural land across the country (Map 5.1).

They consist of:

- Geographical coordinates (S-JTSK- EPSG:5514 projected coordinate system) of the sampling sites;
- Land use types (arable land or grassland);
- Concentration values, if quantified (> limit of quantification), measured in topsoil (0–25 cm for arable soil, 0-10 cm for grassland) for 104 substances;
- Sampling time, covering the years 2014 to 2021. The sampling frequency was once a year except for years 2017 and 2018 during which 10 localities were sampled twice;
- Sampling period. The sampling period changed over time: initially, it extended over the whole vegetation period; a few years ago, it was restricted to early spring (15/02 – 31/03) in order to find how much pesticides would remain in soil after the last pesticide application, which were reported to occur until November.

Map 5.1: Location of the 45 soil sampling sites in Czechia for pesticide residue monitoring



Source: Monitoring data provided by ÚKZÚZ.

Remarks:

- A few particularly high concentration values have been identified in the dataset. As this case study only aims at evaluating the feasibility of the indicator, no investigation on these potential outliers has been carried out and all the data have been kept in the processing.
- From a spatial analysis, 3 points out of the 45 appear to be located outside an agricultural area as defined by Corine Land Cover data (see subsection below on biodiversity data): 9002, 9003 and 9004.

5.2.2 Effect level data

Ecotoxicological data were collected for the substances monitored under the Czech surveys described above. Databases listed in Annex 2 were searched for ecotoxicological data on soil organisms like earthworms, springtails, mites, microorganisms as well as terrestrial plants. Data were extracted and transferred to a central Excel sheet. As the focus has been set on data assessed by authorities, data from the peer review of active substances were preferred. Therefore, priority has been set on the database EFSA Open Food Tox. However, as only data on a subset of active ingredients were included in the EFSA Open Food Tox, data gathered from other databases listed in Annex 2 have been examined based on a list of endpoints for active ingredients, provided by EFSA. If no list of endpoints was available or if the list of endpoints did not include relevant toxicity data, assessment reports for active substances were screened.

For some of the active substances that have been measured in the Czech monitoring study (19 in total), no or only scarce ecotoxicity data was available in the databases nor in the list of endpoints or assessment reports. Most of these substances were either legacy or not approved pesticides and metabolites. In addition, they were all analyzed in the samples but not all of them could actually be significantly quantified (Table 5.1).

Table 5.1 Active substances for which no effect level could be retrieved from the selected databases

Active substance	Number of sampling points with quantified concentration	Total number of sampling points	% of sampling points where the substance could be quantified
2-hydroxyatrazine	44	45	98%
2-hydroxyterbuthylazine	38	45	84%
Quinoxyfen	6	45	13%
Alachlor	1	45	2%
Prometryn	1	45	2%
Desethylatrazine	0	45	0%
Desisopropylatrazine	0	45	0%
Fluazifop ;	0	45	0%
Haloxyfop-2-ethoxyethyl	0	45	0%
Haloxyfop-methyl	0	45	0%
Hexazinone	0	45	0%
Ometoate	0	45	0%
Pirimiphos	0	45	0%
Methyl propachlor	0	45	0%
Quinclorac	0	45	0%
Simazine	0	45	0%
Terbutryn	0	45	0%

Only 2 metabolites (hydroxyatrazine and 2-hydroxyterbuthylazine) and one active substance (quinoxyfen) were quantified in more than one sampling point. For these 3 compounds, considering the purpose of the case study, it was decided to make the best use of the monitoring data and to use alternative sources, namely the Pesticide Properties Database, the US EPA Database, and for Quinoxyfen the ECHA dissemination portal (all 3 are described in Annex 2). For metabolites, the data from the parent compounds were used when data were still missing for certain endpoints.

Information was extracted and centralized in a data sheet whereby effect values derived from mono-formulations have been converted to effect values based on active ingredients. If the values were expressed in g/ha, transformation to mg/kg has been done according to standard assumptions of a soil bulk density of 1.5 g/cm^3, a soil volume of 500 m^3/ha and a penetration or soil depth of 5 cm.

For each organism, standard assessment factors have been applied to calculate the regulatory acceptable concentration (RAC). For chronic endpoints expressed as NOEC or EC10 values on earthworms, springtails and mites, an assessment factor of 10 was applied. For effect values on microorganisms, no assessment factor was applied. For regulatory relevant endpoints derived from standardized ecotoxicity tests on terrestrial plants, expressed as E_RC50 values, a standard assessment factor of 10 was applied.

As described in equation 6, if more than one effect value (e.g., biomass and reproduction) for the same species was available, the lowest available endpoint was selected.

For terrestrial plants, data from the seedling emergence as well as the vegetative vigor test were available in most cases. According to equation 7, the lowest effect value from both tests was selected.

As stated by equation 8, the lowest available RAC was used, if more than one species was tested with the same chemical.

5.2.3 Biodiversity data

The following spatial data available for Czechia were considered to characterize background biodiversity and protected areas:

Background biodiversity data:

- Broad ecosystem types available from COPERNICUS High Resolution Layers (https://land.copernicus.eu/pan-european/high-resolution-layers):
    - Imperviousness density 2018
    - Forest type 2018,
    - Grasslands 2018,
    - Small woody features 2015

- Or more simplified mapping material, Corine Land Cover (CLC) 2018 Classes (https://land.copernicus.eu/pan-european/corine-land-cover/clc2018) at level 1:
    - Artificial,
    - Agricultural,
    - Forest and semi-natural,

- The Agricultural Area Mask, a spatial reference layer aiming at achieving the best possible coverage of the Utilized Agricultural Area (https://www.eea.europa.eu/data-and-maps/data/european-agricultural-areas-based-on)

At this point, it would not be useful to use the distribution maps of Annex I habitat types or protected species, or even EUNIS habitats probability maps, as there are not enough details in the effect level data to define more specific risk coefficient, like in relation with key, structural or endemic species.

Still, those background data could be combined with data on Biodiversity protection:

- The network of Nationally designated protected areas in the EU, according to their IUCN management category: CDDA database (without N2000). Such maps have been done by EEA in the past: https://www.eea.europa.eu/themes/biodiversity/protected-areas/facts-and-figures/IUCN-management-categories

- The Physical Green Infrastructure (GI) Network Layer, produced by ETC/BD in 2020:
    - GI network Hubs: N2000 network (generally equal to IUCN management category V)
    - GI network Links: most natural and semi-natural elements in between them

The physical GI network is regrouping all N2000 sites (hubs), together with the contiguous patches of natural and semi-natural areas which connect two or more of those sites (links). Natural and semi-natural areas are based on the CORINE land cover (CLC) map of 2012, and exclude all Urban and Peri-urban areas, Arable land and Permanent crops that are not classified as High Nature value (HNV) farmland.

5.3 Methodology and results

A data processing chain using the GIS tool QGIS was developed to apply equations 3 and 4 to a specific year, in this case 2020 (the most recent year for which data were available at the start of the study).

It was implemented distinctly for plants and soil organisms.

5.3.1 Calculation of the risk quotient per site

For each sampling site, measured concentrations of PPP residues for the considered year are divided by the corresponding ecotoxicological thresholds and summed over the substances.

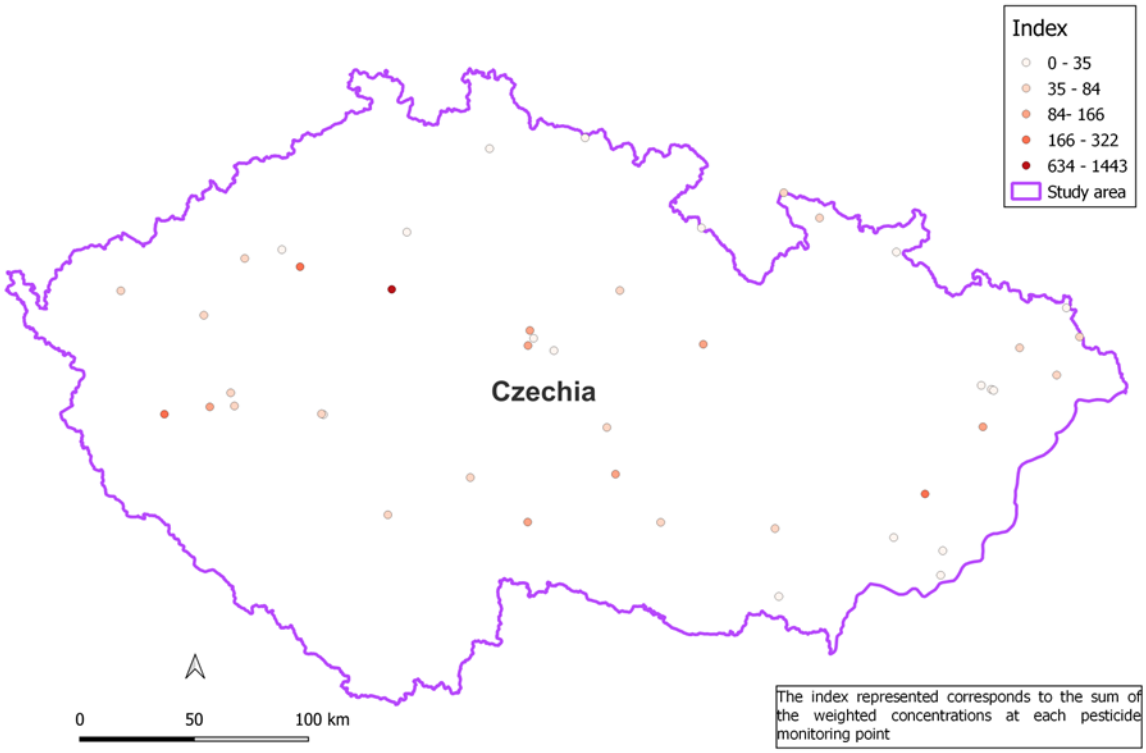
The result at each point corresponds to the left factor (in blue) of equation (3):

$$RI_{x_j,k,2020} = \sum_{i=1}^{N} \left(\frac{C_{i,x_j,2020}}{Threshold_{i,k}} \right) \cdot P_{f_j}$$

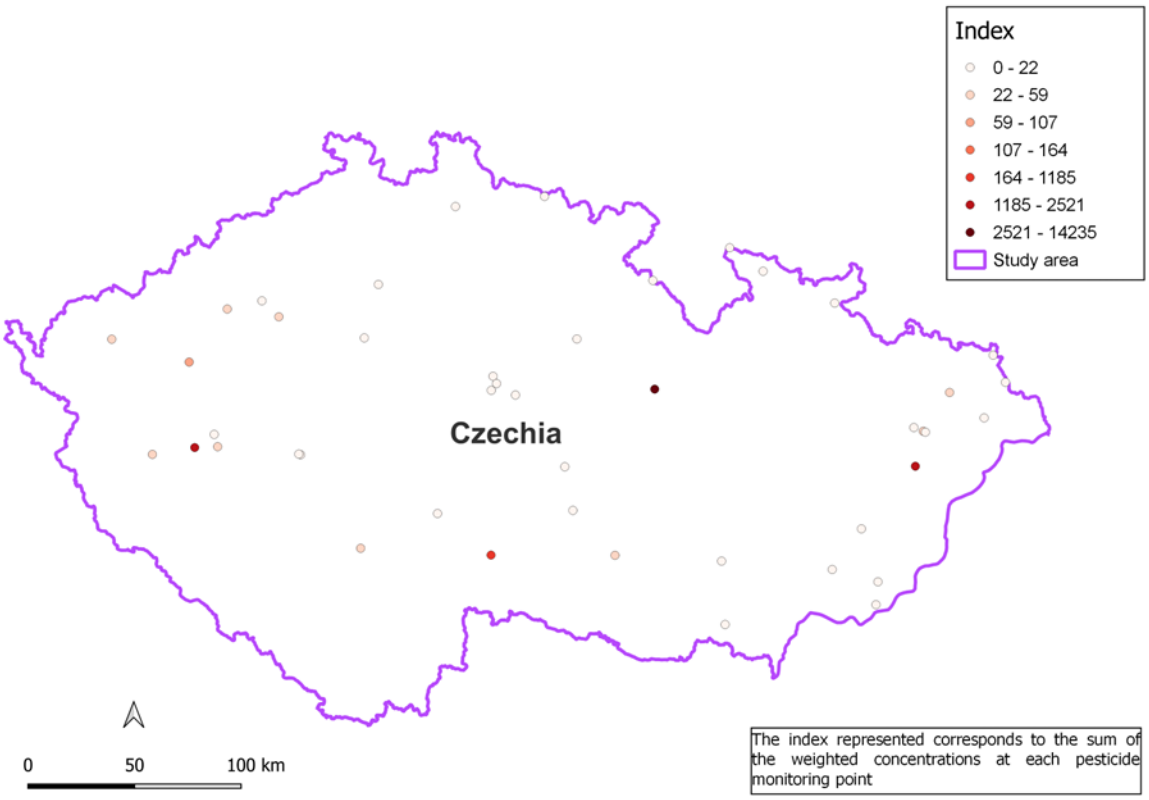
Since there is only one sample per site for the year considered, no prior temporal aggregation is needed.

This sum is then cross-referenced with the geolocated measurement points in order to map the results (Map 5.2, Map 5.3) and allow further weighting according to the type of ecosystem.

Map 5.2: Multi-substance risk quotient for plants (before application of a protection factor) at each monitoring site



Map 5.3: Multi-substance risk quotient for soil organisms (before application of a protection factor) at each monitoring site



5.3.2 Weighting by a protection factor

Application of equation (3) requires the definition of a protection factor Pf_j function of habitat or ecosystem *j*. It is proposed to define a protection factor for each ecosystem identified and adapt it according to the presence and the type of a protected area (see section 3.3). We suggest using the IUCN protected areas management categories as it appears from the CDDA database that Czechia has assigned an IUCN category to all its protected areas.

The values proposed for the protection factor Pf_j range from 0 to 10, as presented below.

Urban and sealed areas

The lowest protection factor will be chosen for urban sites and sealed areas. According to the imperviousness value (1-100%), different protection factors could be chosen:

- 0: >80%
- 1: 50-80%
- 2: 30-50%
- 3: 0-30%

If only the Artificial areas CLC class are used, then:

- 1: all artificial areas
- 3: sub-class 1.4 “Artificial, non-agricultural vegetated areas”

Cropland or arable areas

- 2: generic Agricultural area
- 3: Agricultural area in Protected area of category VI
- 4: Agricultural area in Protected area of category V and N2000 areas
- 5: Agricultural area in Protected area of category IV

Grasslands

- 3: generic Grassland area
- 4: Grassland area in Protected area of category VI
- 5: Grassland area in Protected area of category V and N2000 areas
- 6: Grassland area in Protected area of category IV
- 7: Grassland area in Protected area of category III
- 8: Grassland area in Protected area of category II
- 9: Grassland area in Protected area of category I

Small woody features

- 4: Small woody features within Agricultural area
- 5: Small woody features outside Agricultural area
- 6: Small woody features in Protected area of category VI
- 7: Small woody features in Protected area of category V and N2000 areas
- 8: Small woody features in Protected area of category IV
- 9: Small woody features in Protected area of category III
- 10: Small woody features in Protected area of category II & I

Forest ecosystems

- 6: generic Forest ecosystems
- 7: Forest ecosystems in Protected area of category VI
- 8: Forest ecosystems in Protected area of category V and N2000 areas
- 9: Forest ecosystems in Protected area of category IV
- 10: Forest ecosystems in Protected area of category III, II and I

In the end, only the Corine Land Cover (CLC) 2018([6]) "Agricultural" class is selected for this case study, in combination with all nationally designed Protected areas according to their IUCN management category. Indeed, all of the concentration points available for the study except for three appear to be only present in agricultural areas.

This involves extracting agricultural areas from CLC via an attribute selection and cross-referencing these areas with the CDDA database containing the different categories of protected areas (Map 5.4).

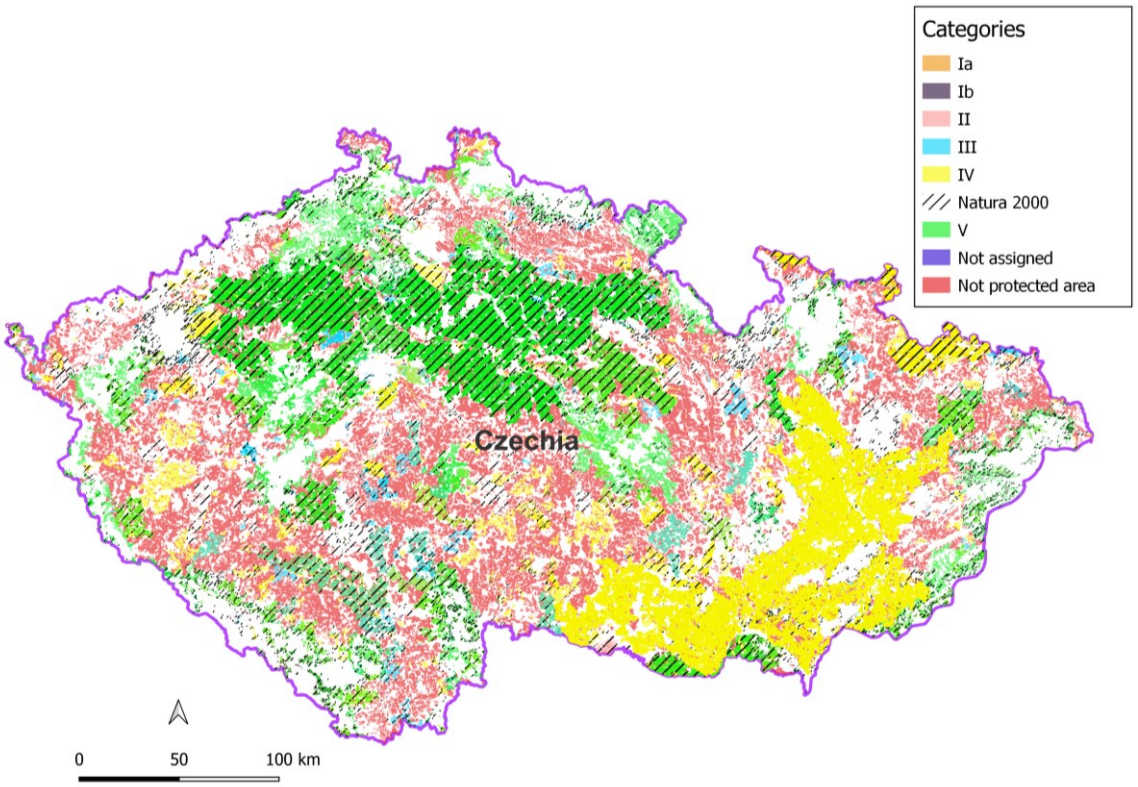
Remarks:

- The Agricultural mask could have been used instead of CLC data to characterize the agricultural areas in a more precise way (see 4.3). On the other hand, should other types of ecosystems be considered later on, the use of CLC data would make it easier to extend the processing to other land cover classes. The choice of one or another dataset according to the targeted precision and technical feasibility could be investigated in future developments of the indicator.

([6]) https://land.copernicus.eu/pan-european/corine-land-cover/clc2018.

- Overlapping of different categories of protected areas was noticed during the processing, leading to several possible values of the protection factor at the same place. The highest values of the protection factor were selected in such cases.

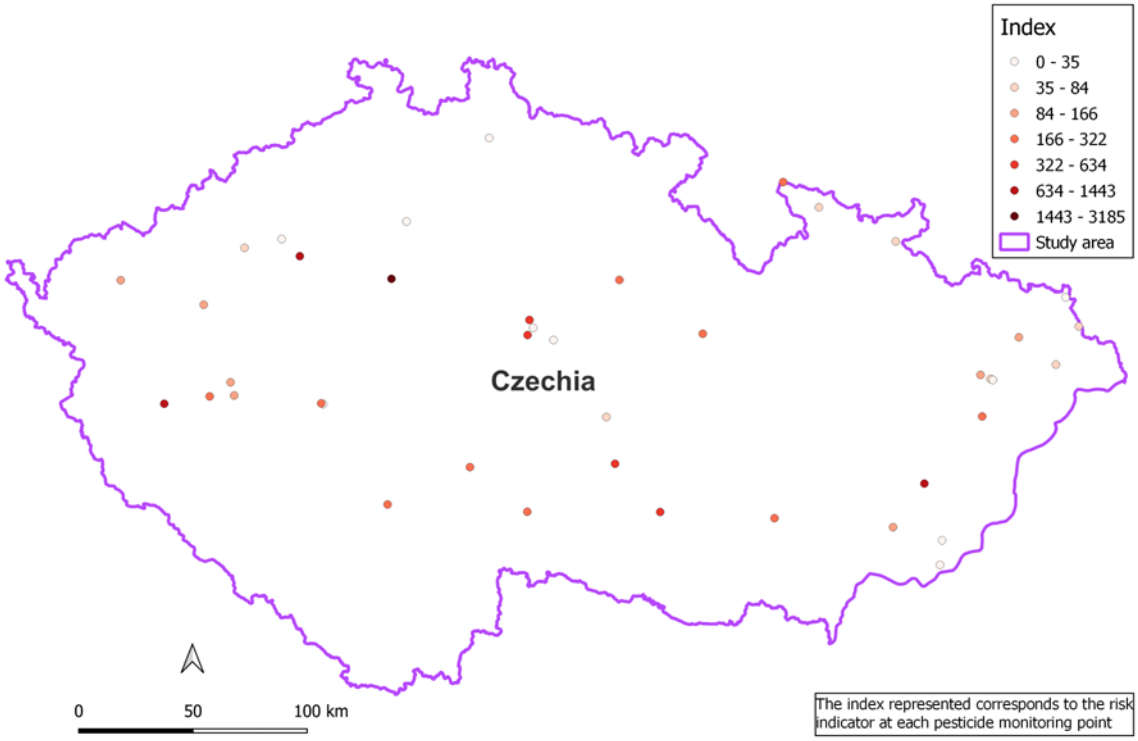
Map 5.4: Agricultural areas coloured as a function of the category of protected areas



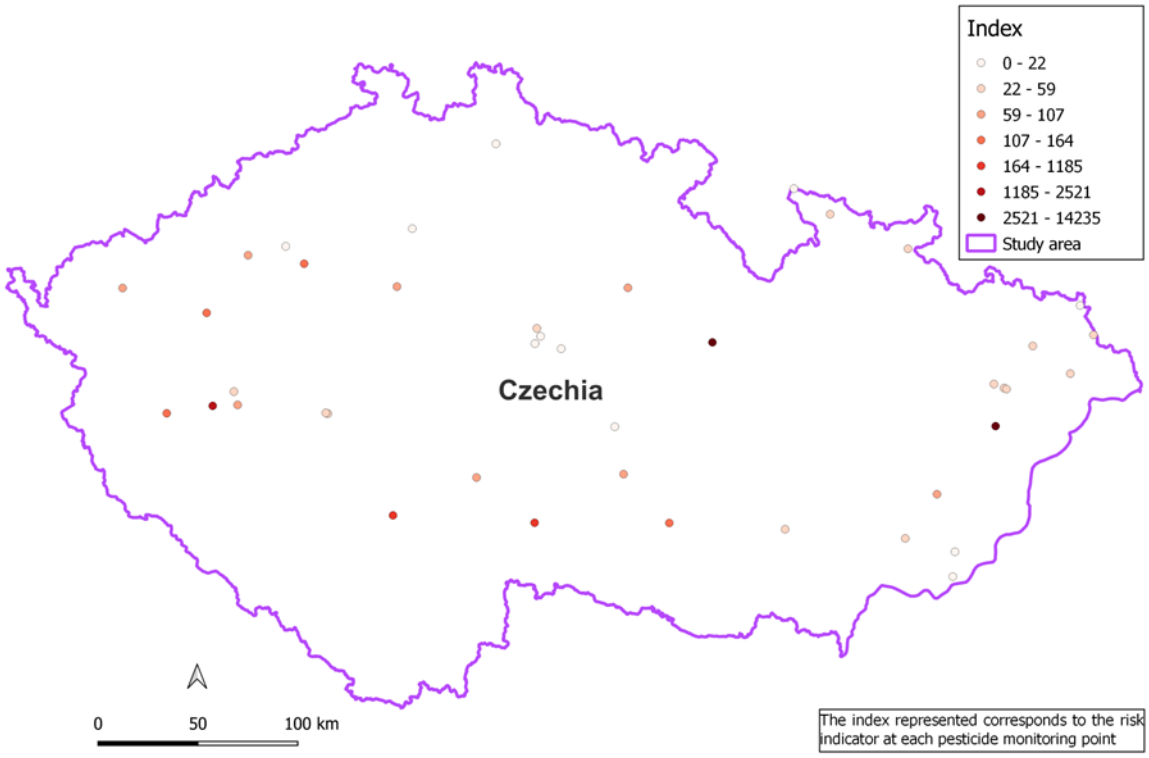
At each monitoring site:

- the value of the protection factor can be obtained from Map 5.4;
- the multi-substance risk quotient is then multiplied by this factor to get the value of the indicator (Map 5.5, Map 5.6).

Map 5.5: Point value of the indicator for plants (i.e. multi-substance risk quotient for plants after application of a protection factor) at each monitoring site



Map 5.6: Point value of the indicator for soil organisms (i.e. multi-substance risk quotient for soil organisms after application of a protection factor) at each monitoring site



5.3.3 Spatial representation of the indicator

The previous maps give only point information on the indicator. In this section, several methods are tested to provide a spatial representation of this indicator. Given equation (3), this involves estimating concentrations outside measurement points x_j.

Note that these tests are limited by:

- the spatial density of measurement sites: **these tests are not intended to provide precise maps of the indicator in the Czechia, as mentioned only feasibility of the methods is assessed**;
- the representativeness of the monitoring sites with regard to the ecosystems: given the location of these sites, **the mapping is limited to agricultural areas** as delimited by Corine Land Cover. No extrapolation to other types of ecosystems is performed.

Different approaches are considered:

One consists in interpolating concentrations from the point values by e.g. geostatistical modelling and kriging estimation. Auxiliary variables may be introduced in the interpolation to obtain more precise maps as was performed by JRC for metals (see Map 3.2). In this case study, the application of such an approach comes up against several issues: the limited number of sampling points and the difficulty to find appropriate auxiliary variables (land cover or other relevant factors for stratification) likely to describe the variations of pesticide concentrations in soils. These limitations do not enable the definition of a proper geostatistical model and consequently this approach is not further considered.

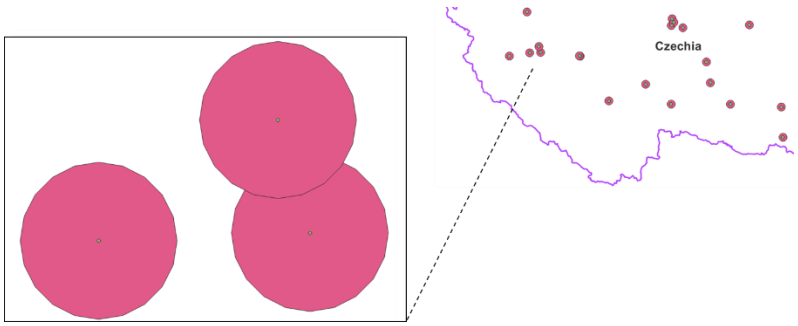
Another approach consists in assuming that the point data are representative of chemical exposure within a given area around the point. Under this assumption, three methods are investigated.

Method 1

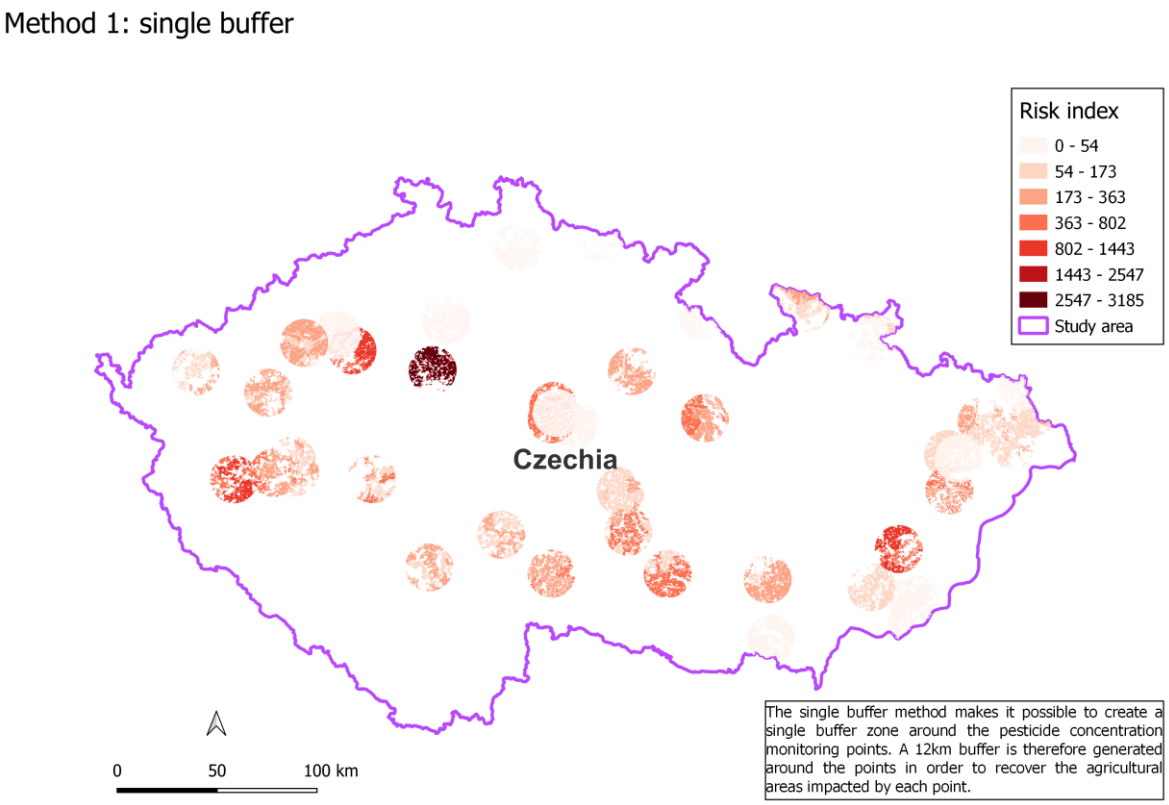
Let be considered a circular buffer centered on the sampling point. In a first stage, the agricultural area located within this buffer is attributed the concentration value measured at this point.

To be in agreement with the physico-chemical processes at stake, the size of the buffer should be defined according to the substance properties, characteristics of the environment and land use. Such an analysis falls out of the scope of the present case study. Here, for practical and visual reasons (to make the resulting maps easier to distinguish from the previous point representation of the indicator), a common rather large radius of 12 km has been defined for all substances (Map 5.7). Where two or more sampling points are located close to each other, the corresponding buffers may intersect (Figure 5.1). Different ways of aggregating concentrations in these overlapping zones could be tested. For the present calculations, the maximum concentration value is retained.

Figure 5.1: Example of overlapping buffers



Map 5.7: Spatial indicator for plants. Method 1: concentrations in the agricultural area are assumed constant within a buffer around each monitoring site

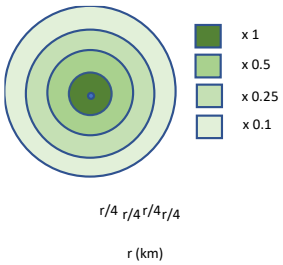


In this method, the spatial variations of the indicator within each buffer are only due to the presence of protected areas and subsequent variations of the protection factor.

Method 2

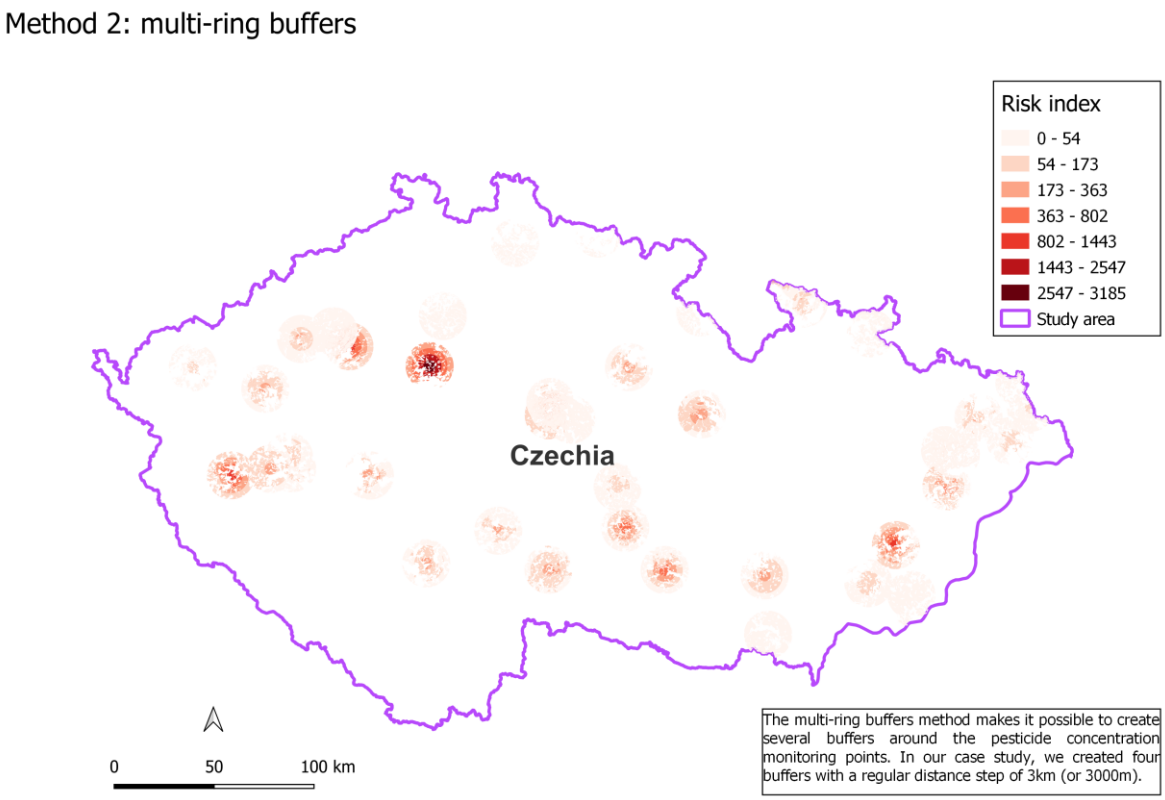
Concentrations are assumed to be constant in the treated parcel(s) represented by the sampling point and to decrease when one moves away from the parcel. For testing purpose, and since the search for and inclusion of data on agricultural parcels would have taken too much time in the scope of this case study, a simplification is applied: the buffer centred on the monitoring point is divided in rings and inside each ring a reduction factor is applied to the measured concentrations (Figure 5.2). As in method 1, the reduction factor should in principle be defined according to the substance properties, characteristics of the environment and land use. Here as well, the maximum concentration value is kept where several buffers intersect each other.

Figure 5.2: Multi-ring buffer and application of a reduction factor



The resulting indicator is presented below for plants (Map 5.8).

Map 5.8: Spatial indicator for plants. Method 2: concentrations decrease with distance from the treated parcel (from the monitoring point in these simplified calculations) within a buffer around each monitoring site



In this method, the spatial variations of the indicator within each buffer are due to both variations of the protection factor and assumed variations of pesticide concentrations.

Method 3

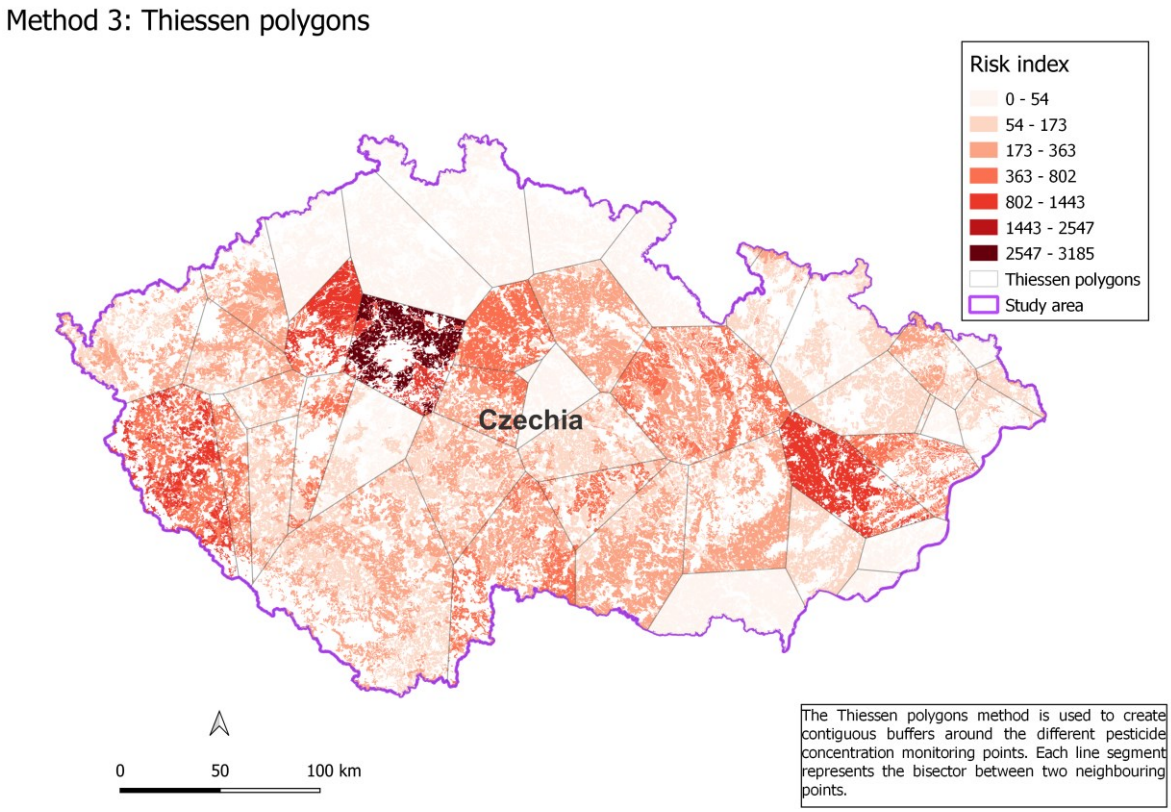
In the maps obtained from methods 1 and 2, the representation of the indicator remains scattered. Since kriging could not be properly applied, a simpler method is tested to get a more continuous view of the indicator: the Thiessen (or Voronoï) polygon method. This spatial method consists in dividing a given area into convex polygons from randomly distributed points so that 1) each polygon contains

exactly one generating point and 2) every point in a given polygon is closer to its generating point than to any other (Map 5.9).

It is assumed that the measured concentrations of pesticide residues at each monitoring site are representative of the concentrations in agricultural soils in the whole polygon generated by this site. In the present case, considering the relatively low density of measurement points and the large dimensions of some polygons, this assumption does not appear realistic. The objective is only to give an idea of the type of map resulting from this method (Map 5.10).

Map 5.9: Division of the study area into Thiessen polygons

Map 5.10: Spatial indicator for plants. Method 3: Partition of the study area into Thyssen polygons



Maps of the spatialized indicator obtained for soil organisms with the three tested methods are provided in Annex 5.

6 Discussion

This work is a scoping study where the objective is to develop an indicator that would be able to link the risk of chemical exposure to ecosystems (see chapter 2 for the risk definition). When building the conceptual scheme, it was made clear that the project should not be limited by data availability and technical feasibility.

Several issues, shared with any risk assessment work, were thoroughly considered such as mixture and bioavailability. However, the two main innovative questions brought by the project were about moving from top-down EU policies, regulating the placing on the market of chemicals, to bottom-up "field" information, in particular the terrestrial environment. This entailed questions on:

- Species sensitivity: how do we link knowledge on laboratory species to wild species, and species to ecosystems;
- The geographical scale at which the indicator should be defined: whereas the current risk assessment is made at EU level using generic scenario considering an agricultural field and a default field edge, how can we consider the specificities of local habitats?

The conceptual scheme was translated into generic equations presented in section 3.3, with an adaptation to specific protection goals as presented in Annex 4. The developed case study intended to test the feasibility of applying those equations to real data sets displaying chemical occurrence in natural soils.

6.1 Case study for the development of a risk indicator

The data set used for the case study had the following characteristics:

- National level (Czechia);
- 45 monitoring points distributed in agricultural land across the country;
- 104 substances, used as PPPs;
- Data available from 2014 to 2021 with year 2020 considered in the test.

The case study was successful in the way that it was technically feasible to calculate a value for the indicator in agricultural areas, based on ecotoxicological effect values for indicator species.

Experience learned from the case study with regards to effect information underlines that even by focusing on pesticides, which are considered as data rich chemicals due to strong regulatory data requirements, and the effort from EFSA to make these data publicly available int the database EFSA Open Food Tox, it was not always possible to calculate easily and consistently the ecotoxicity component of the indicator.

The main difficulties faced during the process were:

- The lack of information for certain legacy/not approved chemicals, which are nevertheless quantified in field;
- The lack of information for certain metabolites/degradation products which have been quantified in field;
- Some species/endpoints data were not available, preventing the meaningful application of certain scenarios/equations initially foreseen from a methodological point of view;
- Some data needed to be transformed, in order to be normalized and be compared with soil concentrations, introducing uncertainty via the conversion process.

It was possible to overcome most of the difficulties listed above, the main remaining issue being the data missing for some species/endpoints, which has an impact on the mixture calculation. The approach followed here is based on the sum of the risk quotients, which should preferentially be calculated using the same endpoints and safety factors for the different ecotoxicity thresholds, as this allows to draw conclusions on the risk of a mixture with regards to a specific toxicity effect. For building a risk indicator however, combining different endpoints can allow to draw an initial mixture risk profile (Socianu et al., 2022) in a certain location and highlight potential threats to living organisms. With such, mixtures or individual chemicals driving the risk may be identified and allow for further investigations and/or prioritization of governance actions.

For example, Socianu et al. (2022) estimated the health risk posed by a chemical mixture based on the concentration addition principle of risk quotients. Human biomonitoring concentrations collected under the HBM4EU project were compared to health-based guidance values which represent human toxicity thresholds for internal concentrations and which are derived from different toxicological endpoints.

Overall, the biggest challenge was the production of a spatial indicator from a limited number of monitoring sites, namely an indicator not limited to point values. Rather simple methods were tested like the use of buffers and the division of the domain into Thiessen (Voronoï) polygons. The resulting maps should be considered as highly uncertain with regard to the spatial distribution of the indicator but they illustrate how this indicator could look like according to the method applied and assumptions made. Other approaches have not been investigated due to the limited number of data available (application of geostatistical methods) or because it was out of the scope of the study (use of a fate model).

The question of temporal aggregation was not addressed since only one sample was collected at each site during the considered year (2020). However, this could become a subject for study where several samples per year are collected.

As the monitoring data set focussed on the analysis of active substances, used for plant protection, other chemicals like biocides, pharmaceuticals or industry chemicals have not been included in the scoping study. In this context, it is necessary to i) define relevant substances for monitoring surveys across all regulated areas as it might not be possible to monitor all substances placed on the market and ii) to set up a European wide soil monitoring program.

The indicator could in principle be applied to larger (EU) or smaller (regional, local) scale, and cover a greater diversity of ecosystems. This intermediate scale was deemed appropriate to demonstrate the applicability of the indicator. It could, in principle, also be applied to other types of ecosystems than agricultural area, should additional monitoring data be available in other types of land, in order to reflect other type of pollution such as industrial emissions.

The location of the monitoring sites allows for the discussion of several scenarios and calculations:

- **Sampling points were all located in agricultural fields, but some of them were within or in direct connection with a protected area or conversely in connection with an urban area, questioning the protection factor to be applied**.
- The 45 sampling sites provided a good coverage of the entire country. Their number was however overall insufficient, and the distance between the different sites too high to allow for a meaningful interpolation/extrapolation of data. It was however feasible, for the purpose of testing the indicator, to perform calculations and provide a map which represents an example of the goal that the project aims to achieve.

- Working at a lowest scale (local) provided interesting insight of the indicator possibility, and also the needs for further methodological developments. For example, some of the sampling points were close to each other, which involved dealing with the superposition of the areas surrounding the sampling points. Different calculations were explored to aggregate data for the spatial definition of the indicator.
- Temporal analysis over 2014 to 2021 is not presented in this scoping study, although the indicator is in principle able to show temporal trends. Samples were taken once a year and the sampling period changed over time: it was restricted to early spring (15. 2 – 31. 3.) in order to find how much pesticides would remain in soil after the last seasonal pesticide application of the previous year, which can occur until November. This approach does not reflect the highest exposure period, but this integrative measure is somehow less sensitive to sampling time, which could otherwise be highly dependent on agricultural practice.

The indicator is proven to be flexible to adapt to the context of the analysis:

- The indicator is risk-based in its construction but should not be interpreted as a risk, rather as a toxic pressure to certain habitat. The higher values of the indicator should be interpreted together with their spatial distribution for setting priorities, within protected areas.
- The indicator has been calculated for plants or invertebrates, or both, and is therefore suitable to provide information on different communities.
- The indicator can be calculated for individual pesticides, for a sum of chemicals with a common use (e.g. herbicides), or for the sum of pesticides analyzed.
- The protection factor applied allows to discriminate different area according to certain habitats.
- Because the indicator can be applied to mixtures, it is highly dependent on the number of substances monitored and on how concentration lying between the limits of detection and quantification are included in the overall contamination pressure. This question was outside of the scope of the study but should be addressed for further development.

6.2 Conceptual considerations

Although the species sensitivity issue could be addressed as a variability problem, the meaning of an indicator based on different organisms has to be defined as a fit for purpose parameter. During the construction phase of the indicator, the purpose of the indicator was questioned, including with the consultation of the advisory board supporting the project. The expectations and needs were largely stretched from EU to local points. Pesticides in the terrestrial environment were chosen as example for developing the project because these are data-rich chemicals, but consequently this raised several issues, described thereafter.

Starting from the information available as monitoring data, a conceptually correct approach using measured data on fine grid for all compounds and their mixtures would permit the concurrent application of bioavailability models. The study has underlined the scarcity of the data and such indicator would require an important and costly monitoring effort. The terrestrial environment as such is not only less studied and regulated than the water compartments, it should be treated (at least) as a 2D environment whereas rivers are mostly treated as unidirectional system (in terms of fluxes of contamination also).

Some conceptual difficulties related to the scale were raised specifically as a consequence of using pesticides as a case study. The questions were of different nature: on the protection goals first, under the current regulation for pesticides, risk is assessed in field, off-field and/or at the edge of the field depending on the target species. With regards to exposure data, the pattern of use implies that the

concentration should be constant over the field area but it is not possible to extrapolate it to the adjacent field and other types of habitat.

On the other hand, a top-down indicator based for instance on sales volume could be re-calculated to be area-specific and be used for whole-of-Europe, but it would also require the availability of these sales data with a spatial resolution that could allow for comparison with a specific habitat. Statistics on pesticide sales by country and type of pesticide are provided by Eurostat. Country surveys would be necessary to collect data at finer scale and by substance.

Instead of sales statistics, data on the actual use of pesticides would provide more accurate input for building such an indicator. However, with the exception of Denmark, this kind of information is not currently required by EU or other MS policy, but shall be available for all European Member States by 2028 (EU, 2021). It would however be useful to test the applicability of the method using the Danish data, which appear to take place at a spatial scale relevant to make a link with ecosystems/habitats.

7 Conclusions, outlook and options for future improvements

This conceptual study has investigated potential methodologies and datasets that could feed indicators on risks from chemicals to different ecosystems, which could be used to assess EU policy aims to decrease the harm of chemicals on ecosystems.

As discussed in the introduction, indicators have to fulfil multiple criteria, such as relevance in terms of the policy aims/targets that the indicators should shed light on and ease of communication towards the target audience. It is key to understand that imprecisions are inherent and acceptable characteristics of indicators in general, since the purpose of indicators is to indicate a direction which is sufficiently good to support policy assessment and decisions, rather than being an exact scientific measure of some quantity.

The study explored methodologies and datasets to produce spatial risk maps for chemicals on ecosystems that could be applied to various ecosystems. Terrestrial ecosystems were taken as an example, due to its policy relevance (CSS, ZP, F2F and BDS, and link to planetary boundaries), and because indicators on chemical risk to soil and terrestrial ecosystems are scarce and less developed than for *e.g.* aquatic ecosystems.

Spatial layers included information on ecosystems/habitats, on species, and on chemical occurrences in soil or biota. Urban sites, agricultural lands (covering a large area, high load of chemicals), forests and protected habitats (rich in biodiversity) were chosen as examples. Key species were chosen based on a combination of their importance to the ecology (*e.g.* plants feeding higher tropic levels, soil invertebrates for several ecosystem services within soils, microbiota assisting nutrient cycles) and availability of data (*e.g.* ecotoxicity data on non-target plants, earthworms etc.). Chemicals included pesticides, some veterinary drugs and metals, which all are known to be bioactive and used/present across Europe, and which have relevance to policy ambitions. Industrial chemicals emitted from urban areas or spread with fertilisers were in this limited study not included, though they also could have been assessed.

The spatial layers were linked by 'connectors' such as effect level data, factors and some other not yet implemented such as bioavailability that could link occurrence data with potential chemical exposure to biota and potential protection factors for different habitats.

A review of effect-level data was produced, see Annex 2. The review highlights the high variability of data availability reflecting the differences in the data requirement set up by the various regulatory frameworks.

Terrestrial effect data on different species are very scarce and limit the possibility to use Species Sensitivity Distribution (SSDs) for ecosystems. Instead, a single most sensitive species approach was used, based on regulatory datasets. Likewise the variety of toxicological endpoints tested for each species was very limited.

Consequently, it is currently impossible to use a concentration addition approach for sub-groups of chemicals based on similar toxicological endpoints/AOPs/disease outcomes, to calculate the risk of chemical mixtures. Instead, it is proposed to calculate a hazard index based on the sum of risk quotients (i.e. concentration divided by an effect threshold) for the most vulnerable species, for the most sensitive toxicological endpoint, and for each chemical.

There is an urgent need to expand assessments for terrestrial micro and mesobiota, plant and animal species relevant to specific ecosystems/habitats**. As a start, effect data can be harvested from different sources like *e.g.* the pesticides properties database, the US EPA as well as from OECD and EFSA FoodTox Database. The main goal within the next years should be to harmonise data from different sources and make it publicly available *e.g.* via planned EU Open Chemicals Data Platform**.

In addition, production of more effect data is needed, either by modelling (*e.g.* Toxicokinetic/Toxicodynamic (TKTD) effect models) and/or by testing in-vitro, in-vivo or in the

environment. However, in a first step, environmental monitoring of effects in actual habitats must serve to validate models. National and EU surveys and research studies would be needed to do so.

With regards to exposure data, the two main approaches using either monitored chemical occurrence data, or statistical/modelled use data were considered. While monitored data may give the most accurate exposure data, such data is very scarce and lack completeness of chemicals, spatial coverage and time trends. They are also difficult to compare with effect level data (based on *in vitro* or *in vivo* laboratory studies), because the concentrations (doses) are sometimes reported as load doses, and not monitored/bioavailable concentrations. Statistical/modelled load data may offer more completeness in chemical, spatial and temporal coverage, and it would be possible to calculate soil accumulation for different soil types and weather scenarios. Models may need to be further improved to take into account drifts such as dust and soil run-off from farmed and urban lands, into protected lands, provided that they can be validated based on actual chemical monitoring.

Further investigation on existing models and their need for improvements is needed, potentially as part of EU research programs. Load statistics for pesticide uses across countries has been politically agreed and will become available by 2028 (EU, 2021, EU, 2022b).

Information of high quality on ecosystems and habitats exists at European scale and is available via different information systems like the EVA database on vegetation, the EUNIS habitat classification or the Corine Land Cover Inventory. Expert systems aiming to combine different layers of information, e.g. to assign vegetation plots to habitats, are also developed.

The extent to which different types of lands should be protected and the safety level applied to account for methodological uncertainties, is a political decision. **There is a need for both studies and policy discussions on the ambitions to protect species diversity and population size in *e.g.* farmed land. This can provide a basis to decide, in the future, on the value of protection factors applied onto the effect levels.**

Several dimensions were not addressed in this limited scoping study, including the effects of multiple stressors, and the assessment of exact exposure of the biota related to soil pH, soil type, bioavailability, weather patterns, multiple exposure times and routes, and application methods of chemicals on land.

These uncertainties could however be dealt with by the introduction of factors which can be scaled (or made into functions) in case new information becomes available. The temporal aspect was not presented in the result section but the indicator would in principle be sensitive to a change in chemical use. These and other inherent uncertainties (*e.g.* representativeness of sampling, or annual variations in sales vs. use data of pesticides) were however estimated not to fundamentally affect the direction of trend, and hence not to hamper the indicator.

Two case studies were originally intended to be included, but permissions were not cleared for the LUCAS soil data which has EU coverage and data for pesticides, some veterinary drugs and metals. We therefore illustrated the concept of the monitoring methodology on a Czech dataset on pesticides. Although it is regrettable that these data were not accessible, it was also plausible regarding the analysis (see annex 1) of the current content of this monitoring data, that it would have been difficult to provide a meaningful map at EU level, because of the very limited coverage in time and space that would have allowed for interpolation of exposure data. In the course of the project, it became clear that load statistics/modelling may be a very good future approach to build the indicator. It was however not possible within the time frame to get access to (pesticides) load and use statistics which exist at country level, *e.g.* in Denmark, but we recommend to include such as case study in a follow-up study.

While this study was challenging in bringing information and expertise together from different disciplines, the study has also been successful in identifying potential methodologies and datasets, which in the future could help assess the progress on environmental policy aiming to reduce harm of chemicals on ecosystems. Eventually, the methodology could be used to assess if human use of

chemicals is exceeding the carrying capacity of ecosystems and thereby our ability to stay within planetary boundaries for healthy ecosystems. This would however require both research on what sustainable carrying capacities are for chemicals on various ecosystems, and politically set targets for what an acceptable harm is for the use and emissions of chemicals.

List of abbreviations and definitions

Abbreviation	Name	Reference
AF	Assessment Factor	
AOP	Adverse Outcome Pathways	
BCF	Bioconcentration Factor	
CAS	Chemical Abstracts Service	
CBD	Convention on Biological Diversity	
CDDA	Common Database on Designated Areas	
CLC	Corine Land Cover	
CSS	Chemicals Strategy for Sustainability Towards a Toxic-Free Environment	
ECx	Concentration where x % effect was observed/calculated	
Ecosystem	A dynamic complex of plant, animal and micro-organism communities and their non-living environment interacting as a functional unit"	Convention on Biological Diversity (United Nations, 1992)
EEA	European Environment Agency	www.eea.europa.eu
EFSA	European Food Safety Authority	https://www.efsa.europa.eu/en
EQS	Environmental Quality Standard	
ERA	Ecological Risk Assessment	
ERO	Ecological Recovery Option	
ETO	Ecological Threshold Option	
FSS	Farm Structure Surveys	
GI	Green Infrastructure	
Habitat	In the EUNIS habitat classification, a 'habitat' is defined as: 'a place where plants or animals normally live, characterized primarily by its physical features (topography, plant or animal physiognomy, soil characteristics, climate, water quality etc.) and secondarily by the species of plants and animals that live there' Habitats are necessarily defined at a given scale. Most but not all EUNIS habitats are in effect 'biotopes', i.e. 'areas with particular environmental conditions that are sufficiently	Davies et al., 2004

Abbreviation	Name	Reference
	uniform to support a characteristic assemblage of organisms'.	
HC5	Hazard Concentration for 5 % of the species	
LC50	Lethal Concentration for 50 % of the species	
LOEC	Lowest Observed Effect Concentration	
N2000	Natura 2000	
NOEC	No-Observed Effect Concentration	
OECD	Organisation for Economic Co-operation and Development	
PX (*e.g.* P95)	X^{th} (*e.g.* 95^{th}) percentile	
PEC	Predicted Environmental Concentration	
PNEC	Predicted No-Effect Concentration	
PPP	Plant Protection Product	
QS	Quality Standard	
RA	Risk Assessment	
RAC	Regulatory Acceptable Concentration	
RI	Risk Index	
RQ	Risk Quotient	
SPG	Specific Protection Goal	
SSD	Species Sensitivity Distribution	
TME	Terrestrial Model Ecosystem	
TMF	Trophic Magnification Factor	
WFD	Water Framework Directive	

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Annex 1: Databases on chemical occurrence

The production of an ecosystem specific indicator of risk associated with chemical pollution at the European scale rely on the availability of good quality data on the levels of chemicals in various terrestrial ecosystems across Europe. Here we briefly describe existing datasets and databases on chemical occurrence of metals and currently used pesticides (CUPs) in soil and terrestrial biota and their associated strengths and weaknesses in terms of usefulness within an ecosystem specific indicator.

Databases and datasets on chemical occurrence from European-wide soil surveys:

The use of data on chemical occurrence from European-wide surveys is beneficial, given uniformity in sampling procedures, analysis, and quality control, and thus comparability of data.

LUCAS soil

The Land Use/Cover Area frame statistical Survey Soil (LUCAS Soil) is an extensive survey of soil properties and occurrence of chemical contaminants in soil across the European Union. Sampling has been conducted in 2009 to 2012, 2015, and 2018 Orgiazzi et al., 2018.

Metals in LUCAS soil: Data from the 2009 campaign (~22 000 locations) for Hg and Cu data are available on request in the form of maps, based on the studies from Ballabio et al. (2021) and Ballabio et al. (2018), respectively (ESDAC - European Commission (europa.eu)). Raw data are not publicly available. Data for other metals analysed in the LUCAS Soil survey, As, Cd, Cr, Pb, Mn, Sb, Co, and Ni, are reported in Tóth et al. (2016) in the form of maps, but raw data are not publicly available.

The LUCAS survey has wide geographical coverage (one sample per 200 km^2) and covers a wide range of nature types/land-use categories (artificial land, cropland, woodland, shrubland, grassland, bare land, and wetlands). The survey has also collected data on a wide range of factors which are relevant for toxicity and bioavailability of metals in soil, including pH, grain size, cation exchange capacity, and organic carbon content. These factors make the data collected by the LUCAS survey highly relevant for the creation of an ecosystem specific indicator on a European-wide scale. However, limited accessibility of raw data is a crucial drawback.

CUPs in LUCAS soil: For the 2018 LUCAS Soil campaign, samples were collected for analysis for 113 pesticides at approximately 3500 locations across Europe. Analysis is currently still ongoing, and the data are thus not yet available. In future, this dataset may be a valuable resource for producing an indicator for CUPs if made available. The usefulness is however limited by the data being single measurement. Seasonal variations in CUPs concentrations in soil is thus not accounted for. Data from a subset of the soil samples (~300) from agricultural soil has been analysed for 76 pesticides and reported by Silva et al. (2019).

GEMAS

Metals in GEMAS: The Geochemical Mapping of Agricultural and Grazing Land Soil in Europe (GEMAS) project collected 2108 samples from agricultural soil and 2024 samples from grazing land soil in 2008-2009. The sampling took place in 33 European Countries with one sample per 2500 km^2, and samples were analysed for 53 chemical elements Reimann et al., 2018. Raw data is publicly available in ESRI shapefile format (https://data.gov.ie/dataset/gsi-gemas-european-geochemical-data).

The wide geographical coverage and wide range of elements included, in addition to raw data being publicly available are strengths of this dataset. However, the singular focus on agricultural soil makes

it less suitable for an ecosystem specific indicator for European terrestrial environments. In addition, information on soil physicochemical properties was not found.

BIOSOIL

Metals in BIOSOIL: For the BIOSOIL project, which ran from 2006 to 2009, samples were collected from topsoil from European forests. The main purpose of the BIOSOIL project was to gather harmonized data on soil in terms of carbon content and quality and biodiversity data Hiederer et al., 2011. Soil samples were also analysed for 17 elements (https://ipchem.jrc.ec.europa.eu/).
A strength of this dataset for an ecosystem specific indicator is the additional information on biodiversity from the same locations where chemical occurrence is reported. However, the data is not publicly available. In addition, focus only on forest soil limits the applicability of the BIOSOIL data for an ecosystem specific indicator.

FOREGS

Metals in FOREGS: The Forum of European Geological Surveys (FOREGS) database contains data on more than 50 elements in topsoil and subsoil from ~900 locations in 26 European Countries. Because of gridded sampling (one sample per ~5000 km^2) different types of landuse are most likely covered. The dataset also contains information on soil properties. Sampling was conducted between 1997 and 2001 Lado et al., 2008. The data is available to the public in the form of downloadable excel files (http://www.gtk.fi/publ/foregsatlas/). Weaknesses of this dataset in terms of an ecosystem specific indicator include the age of the data (> 20 years since sampling), in addition to relatively low spatial coverage.

NORMAN

Data in the NORMAN Empodat database are freely available, and downloadable as CSV files (NORMAN EMPODAT Database - Chemical Occurrence Data (norman-network.com)). The NORMAN database currently only contains limited data on chemical occurrence of metals and CUPs in soil, and is thus not currently suitable to use for a ecosystem specific indicator. There is however ongoing work within the NORMAN network to expand the soil data in the database.
Metals in NORMAN: Data on Cu exist for 15 locations in Sweden.
CUPs in NORMAN: Data on two CUPs (Permethrin and Dichlofluanid) can be found for three locations in Sweden.

Databases and datasets on chemical occurrence from national surveys and case studies on soil:

The use of national surveys and smaller-scale case studies have limited usefulness for a European-wide indicator, given the inherent limitations on geographical coverage. Combinations of multiple national surveys to achieve broader coverage is possible but require evaluations of comparability in terms of quality control measures and applied analytical methods (*e.g.*, total vs. aqua regia extraction for metals).

ESB-UBA

The ESB-UBA data reviewed here have been accessed through the Information Platform for Chemical Monitoring (IPCHEM) (https://ipchem.jrc.ec.europa.eu/), but data can also be accessed from https://www.umweltbundesamt.de/en/topics/health/assessing-environmentally-related-health-risks/environmental-specimen-bank. The geographical coverage is limited to Germany.
Metals in ESB-UBA: The ESB-UBA database contain data on Hg, Cu, Zn, Cd, Pb, Co, As, Cr, Fe, and Ni in topsoil, subsoil, and soil organic layer/root network from 10-12 locations. A strength of this dataset is

that sampling has been conducted at each location over multiple years (every 4 years from 2002-2010). A weakness in the context of this report is the limited geographical coverage (Germany).

RMQS-INRAE

The RMQS network is based on 2,240 monitoring sites evenly distributed over the French territory (mainland and overseas). Soil samples are taken every fifteen years at the centre of each 16kmx16km mesh. The first sampling campaign in mainland France (RMQS1) took place from 2000 to 2009 and enabled the establishment of 2170 sites. The second metropolitan campaign (RMQS2) will take place from 2016 to 2027, also including 70 sites spread in overseas territories.

Metals in RMQS: The RMQS database include data on aluminium, arsenic, cadmium, cobalt, chrome, copper, molybdene, nickel, lead, mercury, thallium, tin, titane, zinc in topsoil and subsoil. The strength of this dataset is the regular distribution of sites within the covered domain and availability of soil parameters measurements. A weakness in the context of this report is the limited geographical coverage (France) and reduced measurement frequency.

CUPs in RMQS: In 2019 and 2020, pesticides were measured at 50 sites mainly located in field crops and vineyard areas. 110 molecules were analysed. Results will be available in 2022.

BDTEM-INRAE

Metals in BDTEM: BDTEM database contain data on Cd, Cr, Cu, Hg, Ni, Pb, from two monitoring surveys carried out in 1998 and 2009. Soil samples were taken from the surface (plowed horizons) of agricultural land likely to receive sludge spreading from urban wastewater treatment plants. The dataset mainly includes agricultural soils and soils located in flat positions.

Project research

CUPs: Data on CUPs in soil from larger surveys are still largely lacking, but several case-studies on CUPs in soil have been conducted recently in European countries, *e.g.,* Hiederer et al., 2011, Humann-Guilleminot et al., 2019, Kosubová et al., 2020, Geissen et al., 2021, Pelosi et al., 2021, Riedo et al., 2021. These studies cover from 34 to 351 locations in France, the Czechia, Switzerland, Netherlands, Portugal, and Spain. All case-studies represent agricultural soil only.

Databases and datasets on chemical occurrence in terrestrial biota:

The data review conducted here have mainly focused on chemical occurrence in soil, given the better availability of data covering Europe on a larger scale, and added complexity of using biota as an indicator. However, we reviewed the NORMAN Empodat database and the ESB-UBA database for chemical occurrence in terrestrial biota, for the purpose of illustrating what data is currently available, and which gaps need to be filled in order to use chemical occurrence data from biota for a European-wide ecosystem specific indicator.

NORMAN

The search function of the NORMAN Empodat database allows for the selection of terrestrial biota as a category, but the resulting data needs to be downloaded and filtered manually to gather data for a specific terrestrial species.

Metals in terrestrial biota in NORMAN: The database contain data on Hg in terrestrial biota from 40 locations from 17 European countries. Data from the different locations are from between 2014 and 2021, and in general datapoints are single measurement.

CUPs in terrestrial biota in NORMAN: The database contains data on at least 36 CUPs in terrestrial biota from between 12 and 54 locations in between 3 and 13 European countries, but almost all data are below detection limit. Time of sampling are between 2015 and 2021, and most datapoints are single measurements.

ESB-UBA

Metals in terrestrial biota in ESB-UBA: The ESB-UBA database contain data on up-to 19 metals and elements in some plants and other terrestrial biota. The plants covered are leaves and shoots from Beech, Common spruce, Lombardy poplar, and Pine, while the animals covered are Earthworm and Roe deer. Sampling has been conducted at between 1 and 10 locations, only in Germany. Although geographical coverage is limited, the temporal coverage of this data is good, with sampling having been conducted annually or biennially from the 1980s or 1990s till current time.

Databases and dataset on soil properties

For the creation of an indicator describing the risk of chemicals for in-soil organism, soil properties as well as chemical properties of substances should be included in the considerations.
The European Agency for Food Safety (EFSA) holds a database with soil properties (Hiederer, 2012). The database has been developed in cooperation with the European Joint Research Centre (JRC). Probability densities of Organic Carbon contents as well as pH distributions have been published in EFSA (2021):

Figure A1.1: Probability density distribution of organic carbon in agricultural soils in Europe (database PERSAM/JRC;EFSA, 2012 EFSA PPR Panel, 2012; Hiederer, 2012. Visualisation © darwinstatistics)

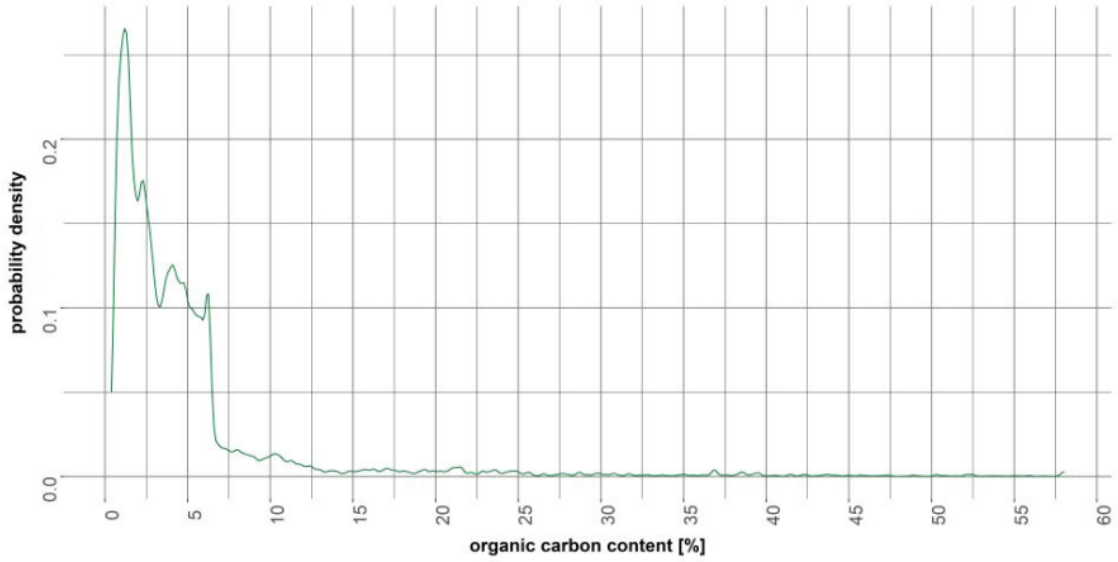
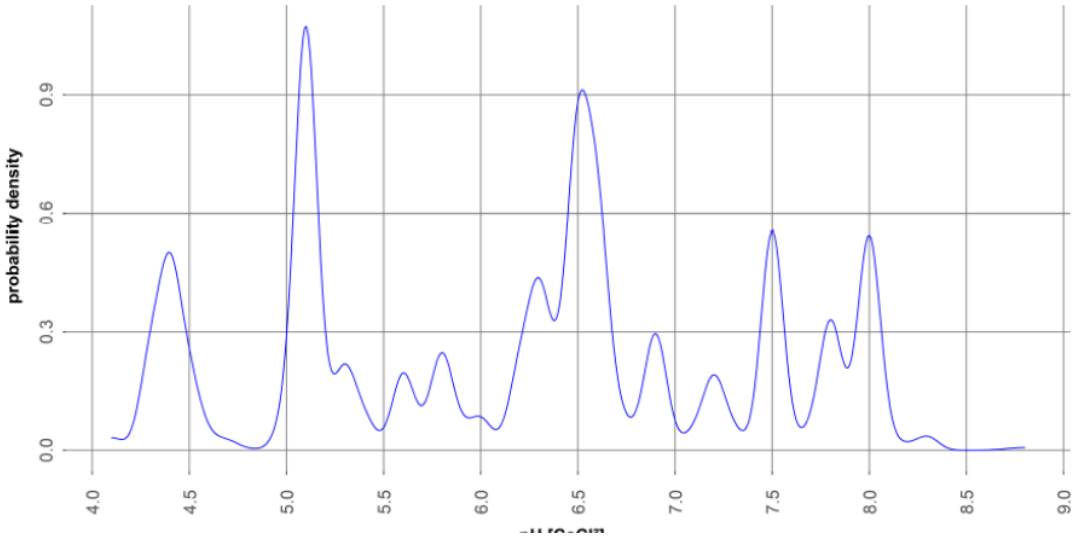


Figure A1.2: Probability density distribution of pH values in agricultural soils in Europe (database PERSAM/JRC; EFSA, 2012; Hiederer, 2012. Visualisation © darwinstatistics)



For habitat suitability modelling, a number of predictors were used including climate, topography, soil, phenological data and anthropogenic data. For soil, the following properties were used a predictors (Hennekens, 2020, Chytrý et al., 2020):

Soil

- Bulk density of the soil (kg/m³)
  Hengl et al. 2014
  https://soilgrids.org/
- Cation Exchange Capacity of the soil
  Hengl et al. 2014
  https://soilgrids.org/
- Weight in % of clay particles (<0.0002 mm)
  Hengl et al. 2014
  https://soilgrids.org/
- Volume % of coarse fragments (> 2 mm)
  Hengl et al. 2014
  https://soilgrids.org/
- Soil organic carbon content (‰)
  Hengl et al. 2014
  https://soilgrids.org/
- Soil pH (water)
  Hengl et al. 2014
  https://soilgrids.org/
- Weight in % of silt particles (0.0002-0.05 mm)
  Hengl et al. 2014
  https://soilgrids.org/
- Weight in % of sand particles (0.05-2 mm)
  Hengl et al. 2014
  https://soilgrids.org/

Annex 2: Databases on ecotoxicological effect data

Ecotoxicological effect data are mandatory for the creation of an indicator, displaying the risks of chemicals. Scholz-Starke B. (in press:) includes a short overview about some existing databases for ecotoxicity. Here we amend the list and briefly describe existing datasets and databases on ecotoxicological effect values for surrogate species and their associated strengths and weaknesses in terms of usefulness within an ecosystem specific indicator.

The use of public available Ecotox data is preferable in terms of traceability. Moreover, clear information about used guidelines, acceptability within regulatory processes, tested substances (Chemical Abstract Service (CAS) Number and Substance name) as well as organisms (Common name as well as scientific name), tested doses (incl. Units), effects levels (including operators and unites), test duration (incl. Unit), and test conditions (*e.g.* used soil types incl. Reference *e.g.* soil dry weight), temperature, pH, Application method and reference (Author, year, title) is necessary to assess reliability of the data set.

Up to now, the several databases hold ecotoxicological data. However, a central data base with an uniform structure would be ideal and necessary for future analysis.

OECD eChemPortal

This platform is an overarching portal, connecting existing databases. There are currently 35 databases connected to the eChemPortal resulting from government chemical review programmes at national, regional, and international levels. eChemPortal provides free public access to information on properties of chemicals regarding their:

- Physical Chemical Properties
- Ecotoxicity
- Toxicity
- Environmental Fate and Behaviour
- Classification and labelling
- Exposure and use

eChemPortal allows simultaneous searching of reports and datasets by chemical name and number, by chemical property, and by GHS classification. Direct links to collections of chemical hazard and risk information prepared for government chemical programmes at national, regional and international levels are obtained. Classification results according to national/regional hazard classification schemes or to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) are provided when available. In addition, eChemPortal provides also exposure and use information on chemicals. EChemPortal does not host all data itself but shares a link to respective databases. EChemPortal is an overarching collection point for several databases. However, for the evaluation of big datasets (*e.g.* > 100 Substances) it is not suitable as the data is not listed in a database itself.

Available at: eChemPortal provides free public access to information on properties of chemicals:

EFSA: OpenFoodTox

The database OpenFoodTox is hosted by the European Food Safety Authority (EFSA) and is a structured database summarising the outcomes of hazard identification and characterisation for the human health (all regulated products and contaminants), the animal health (feed additives, pesticides and contaminants) and the environment (feed additives and pesticides).

OpenFoodTox provides information on the substance characterisation, the links to EFSA's related output, background European legislation, and a summary of the critical toxicological endpoints and reference values.

The data model of OpenFoodTox has been designed using OECD Harmonised Template (OHTs) as a basis to collect and structure the data in a harmonised manner. OpenFoodTox provides open source data for the substance characterisation, EFSA outputs, reference points, reference values and genotoxicity.

In addition, OpenFoodTox has been submitted to the OECD's Global Portal to Information on Chemical Substances (eChemPortal) so that individual substances can be searched as part of the national and international databases. Further description and associated references are described in the EFSA journal editorial (Dorne et al., 2017). By May 2022, the database contains only a subset of authorized substances and is therefore not complete. The big advantage of this database is the in-depth assessment by authorities.

Available at https://zenodo.org/record/3693783#.YjH8fXpKhaR

UBA ETOX

The database of the German Environment Agency (UBA) called "Information System Ecotoxicology and Environmental Quality Targets (ETOX)" contains only validated data from ecotoxicological tests, assessed and proofed by authorities. It is public available and holds approximately 55.000 datasets on the effects of chemicals on aquatic organisms, 5.000 datasets for terrestrial organisms, and 4.500 datasets on environmental quality standards for water and soil. The database includes detailed information about the test conditions in terms of *e.g.* properties of test soils and is therefore of high relevance. Unfortunately, the database does not include information about all authorized substances.

Available at https://webetox.uba.de/webETOX/index.do

AGRITOX Database

The Agritox database has been created by the French National research Institute for Agriculture, Food and Environment (INRA) in 1986. Included data has been proven by French or European authorities and is based on submitted dossiers for the authorization of substances. Open public files include data on identity, physico-chemical properties, acute toxicity, toxicological reference value, classification as well as ecotoxicity data for aquatic organisms. As no data for terrestrial soil related organisms is included, it cannot be used for a chemical indicator for the terrestrial environment.

Available at AGRITOX Database - data.gouv.fr

US EPA ECOTOX

The database US EPA ECOTOX is hosted by the Environmental Protection Agency of the United States of America and displays ecotoxicological data of aquatic organisms, terrestrial plants, and other terrestrial species. The database is public available and includes predominantly data from peer-reviewed literature. Therefore, the data input is heterogeneous but includes a great variety of test species and experimental designs and numbers of entries compared to databases used for regulatory purposes. However, data is not assessed in-depth by regulating authorities which a major shortcoming.

Available at https://cfpub.epa.gov/ecotox/

Pesticides properties database: PPDB

The Pesticides Properties Database (PPDB) is a comprehensive relational database of pesticide chemical identity, physicochemical, human health and ecotoxicological data. It has been developed by the Agriculture & Environment Research Unit (AERU) at the University of Hertfordshire for a variety of end users to support risk assessments and risk management. The PPDB covers around 2000 records and includes data on all active substances used as plant protection products within the European Union. Data has been collected across many sources and aims to bring together information in one database. It is updated on a regular basis. The collection of peer reviewed data, published by EFSA is in the main focus of the PPDB. If EFSA documents are not available, alternative sources are used, including public domain databases from national government departments, peer reviewed scientific publications, manufactures safety datasheets and technical information. The major advantage of the PPDB is the large dataset, the shortcoming is the inclusion of not assessed data from open literature.

Available at: http://sitem.herts.ac.uk/aeru/ppdb/

ECHA IUCLID

The International Uniform Chemical Information Database – IUCLID is maintained by the European Chemicals Agency (ECHA) in Cooperation with the Organization for Economic Co-operation and Development (OECD) and the European Commission. ECHA IUCLID contains mainly data from the REACH regulation, but also data of the Biocide regulation is included in this database. ECHA IUCLID records, stores, maintains and exchanges data on hazard and intrinsic properties, classification and ecotoxicological effects of chemical substances. For data storage, "OECD Harmonized Templates" have been implemented by IUCLID, bearing the big advantage of a harmonized data set and structure. Another big advantage is the assessment of data by authorities. ECHA IUCLID contains data of a large amount of REACH chemicals, assessed by regulating authorities.

Available at https://iuclid6.echa.europa.EU/REACH-study-results

NORMAN database

The NORMAN databases are being developed and integrated with the primary aims of:

- Bringing together existing knowledge on emerging substances and,
- Setting up a framework for the systematic collection, elaboration and scientifically sound evaluation of future data.

NORMAN has an ambition to become the primary data source and global one-stop-shop for all issues regarding emerging substances, contributing to the creation of the early-warning system for emerging pollutants and subsequent policy actions. The database contains very few data on terrestrial organisms, so far.

Available at: NORMAN Database System (norman-network.com)

Annex 3: Extract of the concept paper for "Developing a framework of indicators to monitor the drivers and impacts of chemical pollution under the Chemicals Strategy for Sustainability"

European Environment Agency

1. Goal and Scope of the Framework

On 14 October 2020, the European Commission adopted its *Chemicals Strategy for Sustainability Towards a Toxic-Free Environment* (CSS) together with an accompanying Annex of actions containing more than 60 activities with respective timelines. The CSS was welcomed, and its importance emphasized, by the Council in their Conclusions of 15 March 2021. To implement the CSS, the Commission has established a series of Working Groups (WG). WG8 is supporting the implementation of the CSS action:

'Develop a framework of indicators to monitor the drivers and impacts of chemical pollution and to measure the effectiveness of chemicals legislation' (by 2024)'.

The *goal of the indicator framework* is to provide a fact base to support the assessment of progress on the CSS policy objectives. While individual indicators may not be able to "measure" progress on reducing unwanted risks/impacts of chemicals, they should, as a whole, *indicate* the effectiveness in achieving the overall aims of the CSS.

The two overarching policy objectives of the CSS are:

1. Avoid harm to people and the planet from hazardous chemicals
2. Step up the industrial transition towards the production and use of safe and sustainable chemicals

The first objective relates to the concern that the continuous and projected growth in emissions of chemicals, into an already polluted environment, may exceed the 'self-cleaning' capacity of ecosystems and thereby act as a stressor. Accumulation of chemicals result in increased exposures which are likely to exceed one or several effect levels, and thereby the risk to exceed planetary boundaries for chemicals or so-called 'novel entities'. The second objective highlights the path to obtain the first objective, by changing the focus from downstream efforts to upstream prevention of pollution in the industrial design stages, and may put Europe in a leading position on innovation that delivers on the multiple objectives of the European Green Deal. The shift in the focus from mitigation and control, towards measures to prevent pollution and harm in the first place, is a key element of the CSS.
Chapter 2.1 offers a further breakdown of the two overarching policy objectives mentioned above.

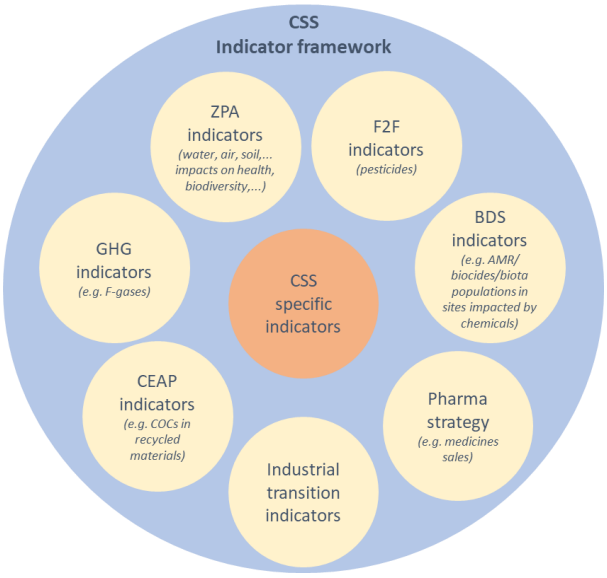
Regarding the *scope* of the framework, the indicators framework aims to monitor progress towards the goals of the CSS, including:

- The *drivers* of human and environmental exposure to chemicals, namely the production and use of chemicals, regulation of these activities and progress with the industrial transition to safe and sustainable chemicals..

- The *impacts* of chemicals, in terms of emissions and occurrence in environmental matrices and in humans compared against effect levels, and—where possible—their impacts on human health and the environment.
- The effectiveness of the *chemicals legislation* in achieving its goals in terms of health, environmental and socio-economic goals, as proposed by CSS.

The need to monitor both drivers and impacts (as well as effectiveness of legislation) poses a challenge in specifying the scope of the framework. The challenge is illustrated in Figure A3.1; while the monitoring of drivers can focus on the specific policy areas covered by the CSS, the monitoring of impacts needs to consider the pressures and states induced by multiple sources (such as industrial chemicals, pesticides, biocides, pharmaceuticals).
The proposed architecture of the framework has been designed to accommodate these differences in approach, when moving from drivers (D, *e.g.* related to chemical production and use), through pressures (P, *e.g.* related to emissions, use of resources), and states (S, *e.g.* related to concentrations in media) towards impacts (I, *e.g.* related to risks/effects due to chemicals), and responses (R, *e.g.* related to legislation, enforcement, risk governance, research policies) (cf. the DPSIR framework)[7]. As further described in Chapter 2 (and exemplified in Annex 4), this is done by mapping the indicator domains/areas along the chemical and product lifecycles (see Figure 3), while maintaining the DPSIR perspective.

Figure A3.1: Overview of the anticipated Chemicals indicator framework



Abbreviations: Chemical Sustainability Strategy (CSS), Farm to Fork (F2F), Biocide Delivery Systems (BDS), Circular Economy Action Plan (CEAP), Chain of Custody (COC), Greenhouse Gas (GHG[YB3]), Fluorinated Greenhouse Gases (F-gases), Zero Pollution Ambition (ZPA).

It is also important to note that the work on CSS indicators has links to the development of the **Key Performance Indicators (KPIs)**; KPIs will measure the industrial transition towards the production of safe and sustainable chemicals. This task is currently scoped as a separate action of the CSS and is being conducted in close cooperation with stakeholders. The two parts of the strategy are clearly connected and it is envisaged to merge them in due time.
Finally, the CSS indicator framework should also provide a good basis for future improvements, based on the experience gained in using the framework and the opportunity to develop and include new

[7] Some of the indicators in the framework may not fit into the DPSIR framework (*e.g.* those on industrial transition).

indicators. Key concepts such as “safe and sustainable by design”, “transition pathway for chemicals”, ”Key performance indicators” are still under development, therefore at this stage the availability of indicators on industrial transition is relatively limited. With the progresses in the implementation of the Chemicals Strategy, it is expected that the balance will improve. Further longer term considerations include emerging and disruptive technologies in the chemical and downstream industries that are expected over the next 5-15 years and ensuring that the indicators remain ‘fit-for-purpose’.

2. Architecture of the indicator framework

Developing the architecture of the indicator framework involves considering:

- How the indicators inform the relevant CSS policy objectives
- Which type of information can be used to develop indicators
- How the different indicators relate to each other

There may be different ways of (sub)grouping the indicators in the framework. Further methodological considerations and principles in choosing indicators are available in Annex 3. The proposal is to map the indicators according to the relevant **policy objectives** they serve and according to the part of the DPSIR and/or the **chemical/product lifecycle** they cover. Finally, specific indicators will also need to support the assessment of the **effectiveness of chemicals legislation**.

3. Frame for policy objectives

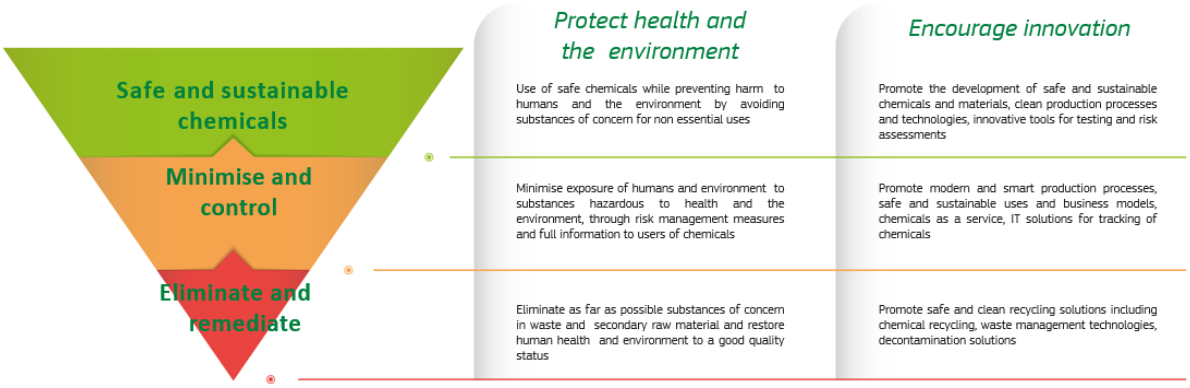
An overview of which specific CSS policy objectives (See chapter 1) to assess was made, to help prioritise which indicators to include in the framework.

The specific objectives of the CSS, in relation to the different categories of chemicals, are the following:

- ensuring the industrial transition towards ***safe and sustainable chemicals***,
- promoting that chemicals having a chronic effect for human health and the environment - ***substances of concern*** – are substituted as far as possible and otherwise minimised and tracked,
- phasing out the ***most harmful chemicals*** for non-essential societal use, in particular in consumer and professional products.

The CSS further breaks down the general objectives into specific policy objectives and focus areas. The framework can be structured according to the toxic-free hierarchy and sub-objectives of the CSS:

Figure A3.2: Overview of the Chemicals Strategy objectives



1. Safe and sustainable chemicals:
    a. Promote safe-and-sustainable-by-design chemicals, materials and products and clean production processes;
    b. Substitute substances of concern as much as possible
    c. Avoid most harmful substances in consumer products and professional uses unless they are essential for society (c.f. the ongoing development of criteria for essentiality)
    d. Reduce consumption of resources
    e. Promote innovative tools for testing (*e.g.* non-animal test) and risk assessment
2. Minimise and control the risks:
    a. Develop modern business models and smart solutions for safe and sustainable use of chemicals
    b. Ensure the development of digital solutions for tracking of chemicals and to ensure full information to users of chemicals
    c. Step up risk management measures for hazardous chemicals on the EU market (incl. from imports)
3. Eliminate and remediate:
    a. Eliminate as far as possible substances of concern from waste and secondary raw materials
    b. Restore health and environment to a good quality status
    c. Promote safe and clean recycling and waste management solutions
    d. Step up decontamination techniques

Additionally, the CSS contains more detailed actions[8] including relating to (see also Annex 4):

Mixtures and combination effects of chemicals

Endocrine Disruptors

Chemicals with intrinsic properties of concern (substances of concern, most harmful chemicals including PFAS and SVHCs)

Vulnerable populations (*e.g.* pregnant women, young children, elderly, workers, specific socioeconomic groups,...); that are focus areas of the chemicals strategy when it comes to *e.g.* specific products (toys) or categories (protection of pregnant women at work)

[8] See the Action Plan published in the Annex to the CSS: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=COM%3A2020%3A667%3AFIN#document2

4. Type of information

Indicators on drivers and impacts of chemical pollution could be constructed using a combination of metrics, such as:

- Number of structures and unique substances and mixtures on the EU market.

  Intrinsic properties: Number of hazardous (harmonised and self-classified) substances per endpoint, substances of very high concern, substances of concern. PBTs, vPvBs, PMTs, vPvMs, LRTAPs etc. (See Annex 1)

  Market volumes: production, export, import and use volumes for groups/specific chemicals measured in *e.g.* kg or sales, or per some unit (*e.g.* area, capita, annum etc).

  Regulatory status of substances in the EU: *e.g.* whether the substance is restricted or subject to authorisation under REACH, whether the substance is subject to harmonised classification under CLP, has an OEL under OSH. Other sector specific regulations may also be relevant to include, *e.g.* for pesticides, biocides, detergents, cosmetics, consumer products etc. This should support measuring the scope and impact of regulatory actions.

  Content: The presence of a substance in materials, articles, products or waste. Currently there is a gap in providing information on mass flows of hazardous substances ending up in virgin/secondary materials, articles/products, but over time this may become available, *e.g.* via the reporting or monitoring of substances of concern in articles, which may provide both data streams and ability to assess typical volumes used.

  Use(s): information on for which purposes articles/products/mixtures are used, across policy domains.

  Occurrence / (bio)monitoring: monitoring data is increasing but is still focused on a few hundred known substances of concern. Measured data may be complemented by modelled data to predict the distribution of occurrences in humans, the environment and their fate in air, water, soil, biota and/or articles.

  Exposure(s): information on the potential exposure of humans or living organisms (biota) in the environment

  Risks: risk-based (including, but not limited to, ex-ante, predictive) type of indicators have been used in the past and could be further investigated. Risk indicators compare occurrences or exposures with human and environmental effect levels, examples being indicators of specific chemicals in marine and surface waters and in biota. These may be complemented by other effect-based indicators, such as in-vivo or in-vitro tests for specific biological effects.

- Environment and health impacts: information robustly linking production and exposure to impacts tends to be limited to a very small number of substances and based on case studies rather than large-scale datasets.
- Other metrics: may become relevant as the work proceeds, such as related to circular economy, waste and reuse/recycling of chemicals and articles/products or greenhouse gas emissions.

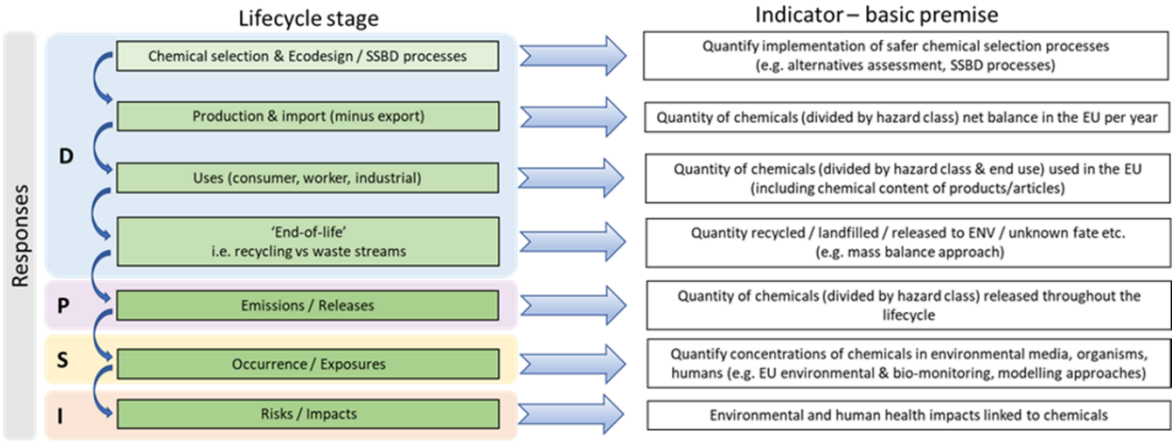
By combining the metrics, we aim to develop indicators on both the upstream drivers of chemical pollution and downstream impacts.
In addition, the use of *case studies* could be considered as a means of exemplifying how we have achieved specific objectives under the CSS. In some cases, the deep dive into a case study may be the best option to present a meaningful and reliable fact base.

5. Framework based on the lifecycles of chemicals and products including articles

Figure 3 below contains a proposal for mapping of chemical indicators according to key stages of the 'chemical lifecycle', by which is meant the whole lifecycle from substances into materials and products, including end-of-life and recycling aspects.

The framework has also been mapped to the stages of the DPSIR model (as illustrated by the coloured DPSIR boxes in Figure 3). This combined 'chemical lifecycle/DPSIR' approach will be further elaborated particularly in regard to providing more detail on the stages of the DPSIR model relevant to impacts on health and environment. Further information around the DPSIR framework is provided in Annex 2.

Figure A3.3: Simplified framework of indicators based on the lifecycle of chemicals and products including articles



Note: The impacts of risk management (RM) actions (or other relevant responses) would be expected to flow through the lifecycle stages. Measurable impacts will vary depending on the indicator level and the exact nature of the actions taken. Having indicators throughout the lifecycle allows us to build a coherent picture of the relative impacts of actions taken, and the resulting trends over time should allow assessment of the effectiveness in achieving the policy goals. In this context, and referencing the DPSIR approach, the primary *Drivers* of chemical pollution in the EU are the lifecycle stages of production, import, uses and 'end-of-life'. The *Pressures* on the environment are for example represented by the emissions/releases of chemicals throughout the lifecycle and use pf resources. *State* can be mapped to occurrence/exposure, and *Impact* within the DPSIR can be mapped to the risks/impacts indicator shown in the above diagram. 'Quantities' here refer to the most relevant metric, *e.g.* annual production volumes, or concentrations in environmental media.

Annex 4: Adaptations to specific protection goals

Individual protected/representative species

Equation 3 or 4 in section 3.3 can be used for a simple approach where, for each ecosystem/habitat type, one species is selected as particularly vulnerable or because it is the most representative of the ecosystem/habitat.

The RI could then be calculated using the same ecotoxicological threshold and toxic effect for all the chemicals in the mixture, or with the lowest threshold for different toxic effects, as described by case 1 and case 2 in the following.

Case 1 – same toxic effect for all the chemicals

		Chemical		
		1	…	n
Species	**Variable**	**Effect value 1**	**…**	**Effect value n**
Plant (*e.g.*: *Lycopersicon esculentum*)	Shoot length	**NOEC = 25**		**NOEC = 50**
	Biomass	NOEC = 45		NOEC = 30

E.g. RI for plants, one species (*e.g. Lycopersicon esculentum*), one toxic effect (*e.g.* effect on shoot length):

$$RI_{x_j,plant,t} = \sum_{i=1}^{N} \left(\frac{C_{i,x_j,t}}{Threshold_{plant\,1\_shoot\_length(NOEC)_i}} \right) \cdot P_{f_j}$$

Equation 7

$$= \left(\frac{C_{1,x_j,t}}{25} + \cdots + \frac{C_{n,x_j,t}}{50} \right) \cdot P_{f_j}$$

Case 2 – toxic effect with the lowest threshold for each chemical

		Chemical		
		1	**…**	**n**
Species	**Variable**	**Effect value 1**	**…**	**Effect value n**
Plant (*e.g.*: *Lycopersicon esculentum*)	Shoot length	**NOEC = 25**		NOEC = 50
	Biomass	NOEC = 45		**NOEC = 30**

E.g. RI for plants, one species (*e.g. Lycopersicon esculentum*), different toxic effects:

$$RI_{x_j,plant,t} = \left(\frac{C_{1,x_j,t}}{Threshold_{plant\,1\_shoot\_length(NOEC)_1}} + \cdots + \frac{C_{n,x_j,t}}{Threshold_{plant\,1\_biomass(NOEC)_n}} \right) \cdot P_{f_j}$$

$$= \left(\frac{C_{1,x_j,t}}{25} + \cdots + \frac{C_{n,x_j,t}}{30} \right) \cdot P_{f_j}$$

Equation 8

From a scientific perspective of mixture assessment, it seems more appropriate to add effects related to the same endpoint (in favor of case 1) but from a risk assessment perspective, the most sensitive endpoint / most sensitive species is usually selected.

It is to be noted that wild (endangered) species are unlikely to have been subject to laboratory testing. Thresholds obtained in standardised assay may cover several individual laboratory species belonging to the same taxonomic group.

As an example, tests on plant are usually performed on 4 to 6 non-target plant species, and the choice of a representative species for a specific ecosystem (*e.g.*, *Lycopersicon esculentum* in case 1) may require an expert judgement. In this case the most sensitive species can be used.

The approaches as described relying on a single species as in case 1 and 2 can be questionable:

- If no ecotoxicity data are available for the endangered/representative species;
- If the representativeness of a single species, valid from an ecological point of view, may not be demonstrated in terms of ecotoxic sensitivity.

Taxonomic group (multispecies and multitaxon)

However, different chemicals affect different species differently. A second approach could be to select, for each ecosystem/habitat, the species of highest sensitivity towards each of the considered chemicals. Depending on the protection goal *e.g.*, protection of several species within the same taxon or single species within several taxa, the RI could then be calculated using the same ecotoxicological threshold and toxic effect for all the chemicals in the mixture for a given taxon, or with the lowest threshold for different toxic effects and taxa, as shown in cases 3 and 4.

Case 3 - same toxic effect for all the chemicals – most sensitive species for each chemical within a taxon

		Chemical		
		1	**…**	**n**
Species	**Variable**	**Effect value 1**	**…**	**Effect value n**
Plant 1 (*e.g. Lycopersicon esculentum*)	Shoot length	**NOEC = 25**		NOEC = 50
	Biomass	NOEC = 45		NOEC = 30
Plant 2 (*e.g. Avena sativa*)	Shoot length	NOEC = 45		**NOEC = 20**
	Biomass	NOEC = 25		NOEC = 30
Earthworm (*e.g. Eisenia fetida)*	Reproduction	NOEC = 10		NOEC = 60
	Mortality	NOEC = 45		NOEC = 35

E.g. RI for plants, different species, one toxic effect (*e.g.* effect on shoot length):

$$RI_{x_j,plant,t} = \left(\frac{C_{1,x_j,t}}{Threshold_{plant1\_shoot\_length(NOEC)_1}} + \cdots + \frac{C_{n,x_j,t}}{Threshold_{plant2\_shoot\_length(NOEC)_n}} \right) \cdot P_{f_j}$$

$$= \left(\frac{C_{1,x_j,t}}{25} + \cdots + \frac{C_{n,x_j,t}}{20} \right) \cdot P_{f_j}$$

Equation 9

Case 4 - toxic effect with the lowest threshold for each chemical – most sensitive taxon for each chemical

		Chemical		
Species	**Variable**	**X1**	**…**	**Xn**
Plant 1 (*e.g. Lycopersicon esculentum*)	Shoot length	NOEC = 25		NOEC = 50
	Biomass	NOEC = 45		**NOEC = 30**
Plant 2 (*e.g. Avena sativa*)	Shoot length	NOEC = 45		NOEC = 20
	Biomass	NOEC = 25		NOEC = 30
Earthworm (*e.g. Eisenia fetida)*	Reproduction	**NOEC = 10**		NOEC = 60
	Mortality	NOEC = 45		NOEC = 35

E.g. RI for different taxa (plants and earthworm), different species, different toxic effects:

$$RI_{x_j,k,t} = \left(\frac{C_{1,x_j,t}}{Threshold_{earthworm\_reproduction(NOEC)_1}} + \cdots + \frac{C_{n,x_j,t}}{Threshold_{plant1\_biomass(NOEC)_n}} \right) \cdot P_{f_j}$$

$$= \left(\frac{C_{1,x_j,t}}{10} + \cdots + \frac{C_{n,x_j,t}}{30} \right) \cdot P_{f_j}$$

Equation 10

Whether the same ecotoxicological threshold and toxic effect are considered may ultimately depend on the data availability for the different habitats and species.

Equation 10 will typically apply when the indicator is based on regulatory thresholds such as PNEC or EQS. As described in section 3.2, PNEC are derived from the lowest experimental NOEC based on a monospecies ecotoxicity testing or from SSDs by applying assessment factors on ecotoxicological data. This assessment factor account for basal uncertainties including intra- and extra-species variabilities and extrapolation from lab to field. This factor is different from the protection factor described above which reflect the sensibility and vulnerability of a specific ecosystem. Equation 8 can be used if the chosen thresholds cover different protections goals, following the same principles than EAS for water.

In all the previous equations, C_i is derived from the estimated or measured chemical occurrence at a specific location and time or at several locations and times in case of spatio-temporal aggregation. The choice of the ecotoxicity thresholds will also depend on whether the chemical occurrence is measured internally in tissues or in the soil.

For the estimated occurrence, the load of chemical reaching the soil should be corrected for chemical, physical and biological processes affecting the bioavailability of the chemical in the soil and thus the exposure concentration, as described in Equation 9.

$$C_i = C_0\left(1 - f_{interception}\right)(1 - f_{ads})\left[1 - f_{leaching} - f_{degradation} - f_{uptake} - f_{volatilization} + f_{influx}\right] + C_{accumulation}$$

Equation 11

The different factors (interception, adsorption, leaching, degradation, uptake, volatilization and influx) are meant to describe the different processes chemicals in soils are subjected to, which influence their long-term concentration in soils. For the estimation of long-term exposure, they should be set to 0 a and could be adjusted for detailed analyses. For further detailed analysis, comprehensive information about the time of application, the habitat or culture, occurring soil types as well as physical / chemical properties of substances would be necessary.

Initial contamination of soils with chemicals is not influenced by the described parameters like leaching, degradation, uptake, volatilization and influx and should be used in a first step for the demonstration of risks from chemicals towards the terrestrial environment.

Equation 11 is mostly valid for estimating a soil concentration to which in-soil living organisms may be exposed. In the case of plants, the intercepted load should be taken into account to estimate foliage exposure to chemicals.

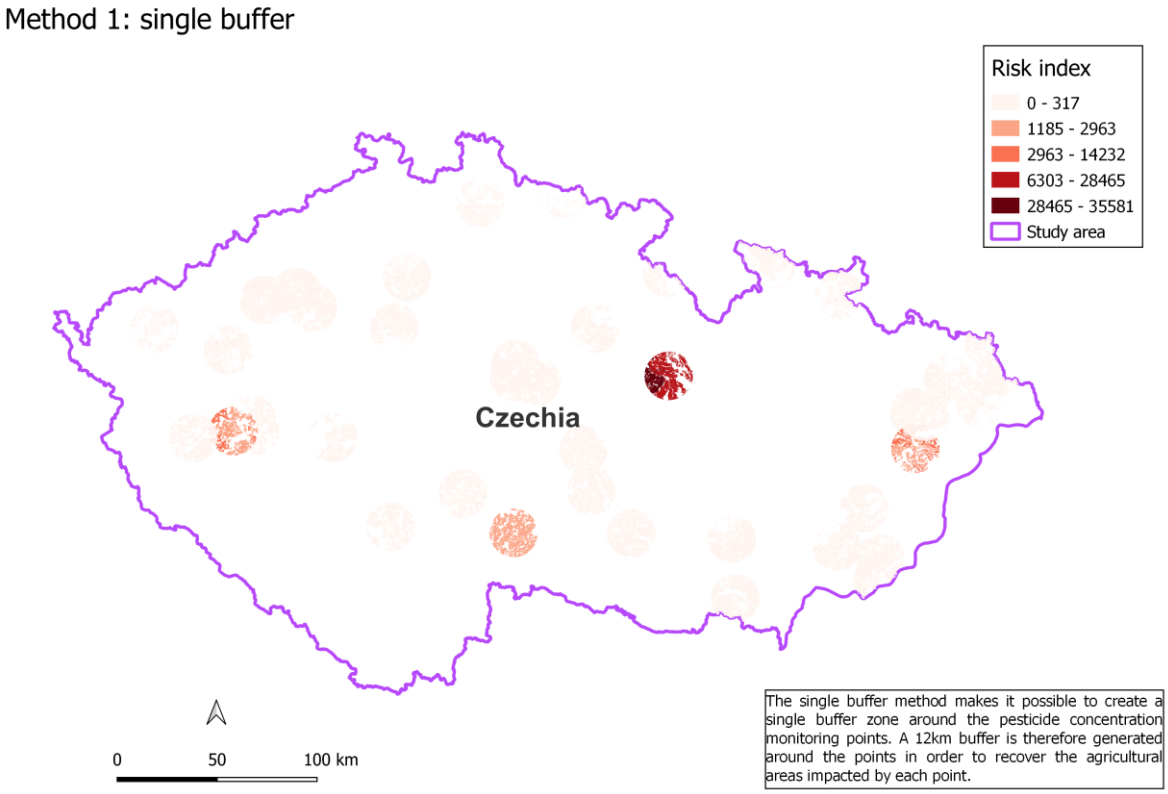
Overview and comparison of the methodological approaches usable for calculating the risk index (RI)

Table A4.1: Comparative table for methodological approaches to calculate the risk index (RI)

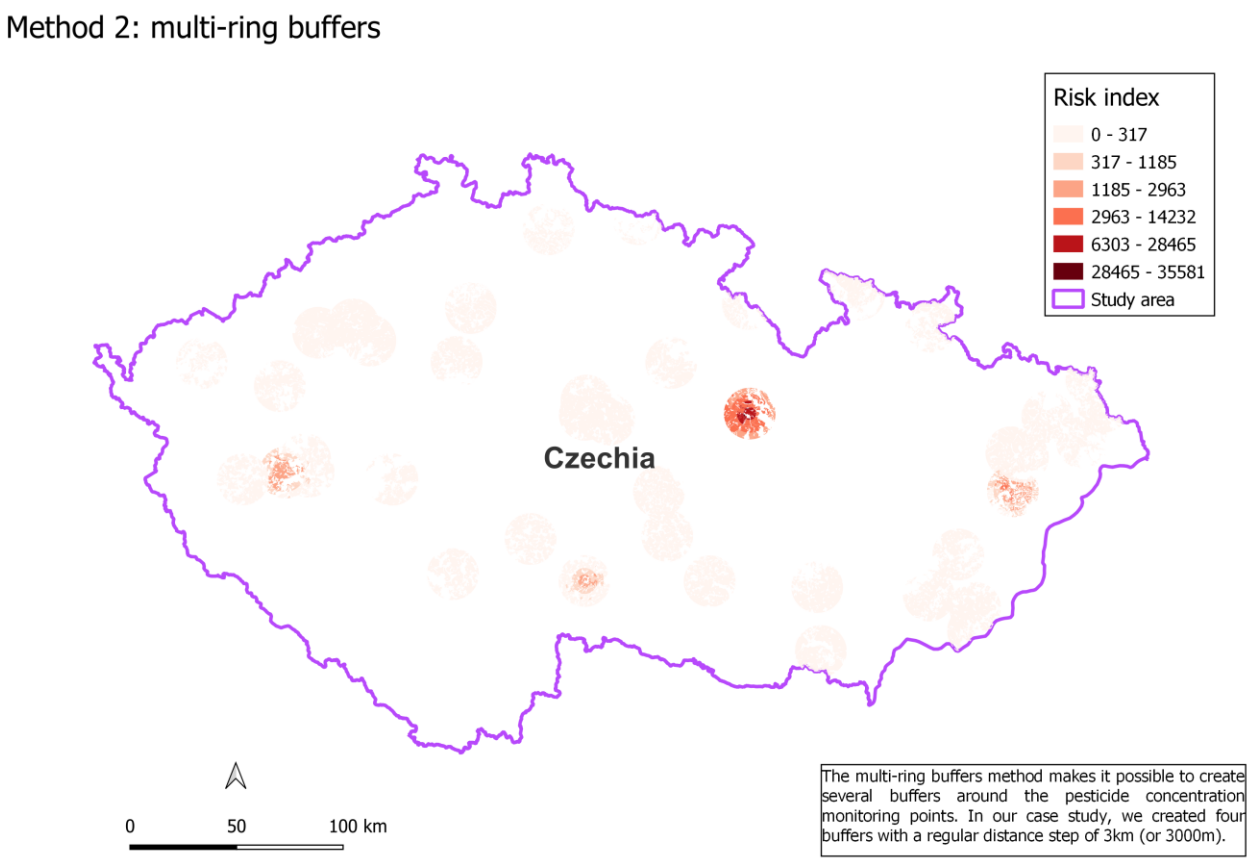
	Pros	Cons	Comment
For each habitat, the RI is calculated for one endangered or representative species	Can be related to a specific protected / representative species. Is relevant for mixture toxicity when adding effects for the same species.	The most sensitive species depend on chemical toxicity Ecotoxicity data may not be available for the considered endangered or representative species The selection of the representative species requires expert knowledge	For each species, it is possible to assess different chemicals for different toxicological endpoints.
For each habitat, the RI is calculated for a given protection goal (e.g. Plants in nature conservation areas)	Can be linked to a specific habitat. Is relevant for mixture toxicity when adding effects affecting the same taxonomic group. Integrates the interspecies variability.	A RI will have to be calculated for each habitat protection goal.	For each species, it is possible to assess different chemicals for different toxicological endpoints.
For each habitat, the SSD is calculated	Statistical multiple-species approach	Need for extensive ecotoxicity data	
For each habitat, the RI is calculated for multiple species / habitats	Integrates the food chain and different functions of the ecosystems. Calculation of a single RI.	Mixture assessment may be overprotective. Different ecotoxicological endpoints are used.	

Annex 5: Case study: maps of the spatialized indicator for soil organisms

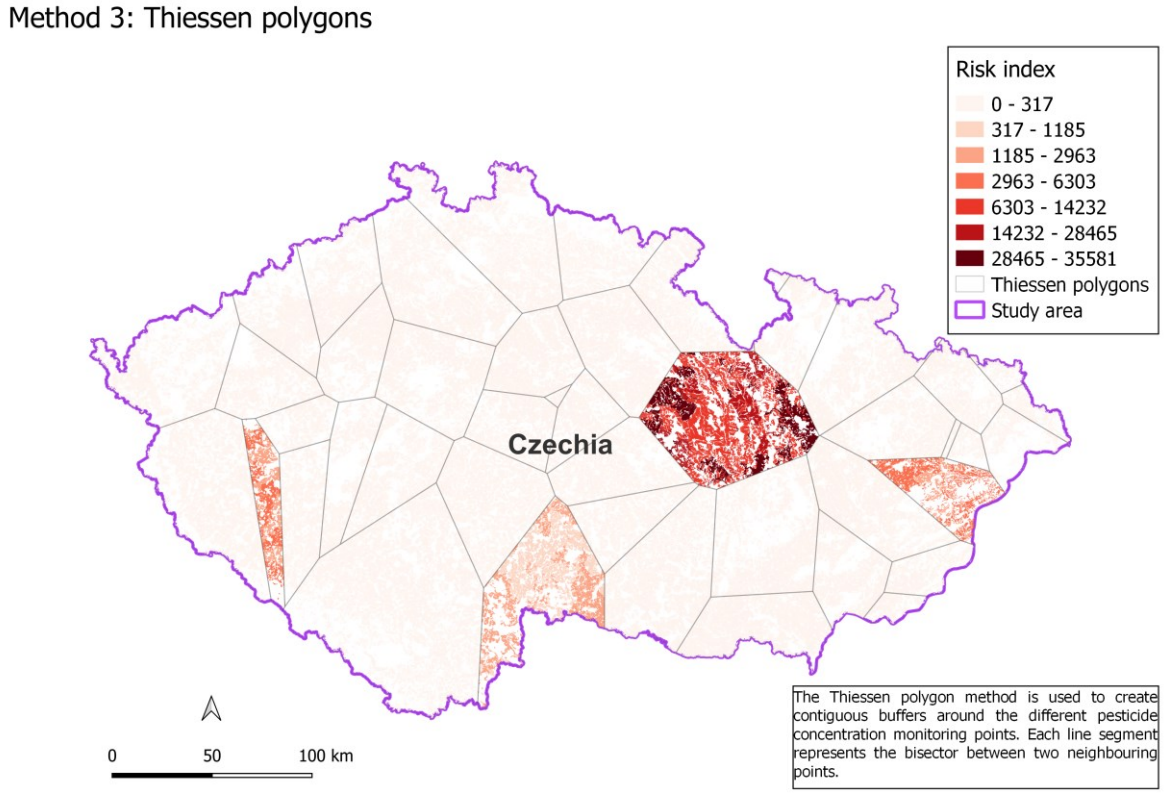
Map A5.1: Spatial indicator for soil organisms. Method 1: concentrations in the agricultural area are assumed constant within a buffer around each monitoring site



Map A5.2: Spatial indicator for soil organisms. Method 2: concentrations decrease with distance from the treated parcel (from the monitoring point in these simplified calculations) within a buffer around each monitoring site



Map A5.3: Spatial indicator for soil organisms. Method 3: Partition of the study area into Thyssen polygons



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