

# Topical Scientific Workshop on Soil Risk Assessment

Helsinki, 7 – 8 October, 2015

Thought-starter

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## Introduction<sup>1</sup>

The Topical Scientific Workshop on Soil Risk Assessment aims for an interactive scientific dialogue between academia, regulators, industry and other stakeholders on three main topics:

- 1) problem definition and conceptual model for soil risk assessment;
- 2) environmental exposure and fate assessment; and
- 3) effect assessment.

To engage and encourage experts to actively contribute to the content development of the workshop already at the preparatory phase, the scientific committee requested the participants to reply to a set of specific questions. As a background document, the experts were given an introduction to current regulatory frameworks for industrial chemicals, biocides and plant protection products.

This thought-starter document captures the current views and opinions of the experts (participants) in the field of soil risk assessment; identifying the main challenges, the adequacy of the current approaches and any future prospects in the development of the risk assessment. It is not a consensus paper on agreed lines to take or applied policies by the scientific committee members' organisations or agencies.

The aim is to identify key elements to be discussed in more depth during the workshop, especially during the break-out groups. Some of the issues are interlinked and may be covered under more than one topic.

The thought-starter outcome consists solely of the responses collected from the participants on the following sets of questions:

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<sup>1</sup> **Disclaimer:** This thought-starter is a background document for facilitating the workshop discussions and does not represent a position of the European Chemicals Agency, European Food Safety Authority and European Medicines Agency. Readers are referred to the legal texts and guidance documents produced by the responsible European institutions (a summary of relevant guidance documents is also available as workshop background material). The views or opinions expressed herein are solely those of the author and do not necessarily represent the policy or guidance of the U.S. Environmental Protection Agency or of Environment Canada.

## **1. Problem definition and conceptual model for soil risk assessment**

### 1.1. Main challenges in soil risk assessment and protection goals harmonisation

- What are the main challenges and development needs in regulatory soil risk assessment?
- What could the relevant specific protection goals (e.g. based on the ecosystem services approach) be for maintaining the structural and functional capacity in the soil?
- Is there scope for harmonisation of these specific protection goals between different regulations?
- How can biodiversity be adequately considered as a general protection goal of the different regulations: is the ecosystem services concept a tool for that?

### 1.2. Adequacy of current soil risk assessment approaches within different frameworks

- Are the currently applied soil risk assessment approaches under the Biocidal Products Regulation (BPR) adequate and useful (e.g. the variety of soil exposure assessments provided in emission scenario documents (ESDs) for different product types (PTs)?
- Are the currently applied soil risk assessment approaches under REACH adequate and useful?
- Is protecting the structure of soil organism communities always the most appropriate approach for protecting soil functions (and services)?
- How are the results of soil risk assessment used in regulatory risk management under different jurisdictions?

### 1.3. Expanding the conceptual model for soil risk assessment: Integration of additional endpoints

- How can the soil/ground/air interphase be integrated in the conceptual model for soil risk assessment?
- How can recovery and/or recolonisation processes be taken into account after initial effects on soil organisms? Which information is available for different organism groups on recolonisation times/distances and on internal recovery capacity?
- Moving to a landscape level would be preferable to better take environmental and ecological variability into account. What sources of spatial and temporal data are currently available?

## **2. Environmental exposure and fate assessment**

### 2.1. Elements, processes and parameters driving the fate/exposure of chemical substances in the soil

- What are the key elements and processes to be considered in the environmental exposure and fate assessment?
- What are the key physico-chemical parameters to be considered in soil exposure and fate assessment including e.g. release, transfer/partitioning, aging of the different type of substances; metals, ionisable substances, surfactants etc.?

- Which processing steps/operational conditions/set of physico-chemical properties would indicate high potential for indirect exposure (e.g. deposition from air or via sludge from wastewater treatment plants (WWTPs) etc.) of the soil?
- How is exposure measured in current laboratory and field scale guideline ecotoxicity studies intended for soil risk assessment? How could the exposure aspect in these guideline studies be improved?

## 2.2. Tools and methods for the soil exposure assessment

- How are exposure modelling software tools used in soil risk assessment under different regulations today and what is their potential for the future? What are the possibilities for using modelling tools for regulatory purposes?
- What would be the available tools and tests to be used as intermediate tiers from lab to field in the exposure assessment?
- What methodology and tools are available today to carry out exposure assessments at landscape level? What data and tools are needed to make it possible in the future?

## 2.3. Specific aspects of exposure/fate in the soil risk assessment

- What are the key aspects to be taken into account in degradation/dissipation assessment; triggers for testing degradation in soil (simulation testing), relevant temperature for assessing degradation rate, minimum level of information needed for acceptable weight of evidence (WoE)?
- Which substance specific properties would benefit the identification of the key exposure pathways to be considered in risk assessment to minimise animal testing (Intelligent Testing Strategy)?
- How is exposure- and effect assessment linked today? How could they be better linked in the future?
- How might the background concentrations (i.e. natural and/or anthropogenic 'ambient' levels) of soil contaminants be incorporated into the risk assessment process?

## 2.4. Inclusion of bioavailability and bioaccumulation in current and future soil ERA strategies

- How is the formation of bound residues currently taken into account within the different regulations as part of the soil risk assessment (trigger values for further characterisation of the non-extractable residues (NERs) and field studies)?
- How can the bioavailability in soil be taken into account in relation to the effects assessment? Does stabilisation of a substance (NER) always mean a loss of effects on non-target organisms?
- How can the bioaccumulation in soil organisms be taken into account as a part of the (regulatory) soil risk assessment?
- What are the possibilities and timescale based on state-of-science? What are the uncertainties and what kind of research work still needs to be done to overcome these? How to interpret the results of terrestrial bioaccumulation?

## 3. Effect assessment

### 3.1. Species representativeness and sensitivity

- Which taxonomic groups and species, habitats, routes of exposure, and functions should be considered in the effects assessment of different regulatory contexts?

- Are the species currently tested in the framework of approval of pesticides the most representative ones, especially with regard to some ecosystem services (e.g. soil formation)? How can interspecies variability be addressed?
- Testing of additional species is only triggered based on the persistence of a pesticide in soil. For non-persistent substances, can other species than earthworms be considered protected and sufficiently covered in the risk assessment?
- How should inter-species sensitivity be taken into account?

### 3.2. Selection of the most appropriate test method(s)/how to assure that the test method suits the purpose/ From effect (hazard) assessment to risk assessment (RA)

- In which cases would long-term soil toxicity testing be preferred and when would short-term toxicity testing be adequate or relevant?
- How can bioavailability be accounted for in the hazard characterisation (correction factor, study design)?
- What would be the alternative approaches to currently used methods to predict effects on soil microorganisms (OECD 216/217) to improve protection of the soil microbial communities and functions? Should only inhibition or also an increase in nitrification/carbon dioxide evolution be considered as a relevant effect and therefore used for the PNEC derivation?
- How is exposure measured in current laboratory and field scale guideline ecotoxicity studies intended for soil risk assessment? How could the exposure aspect in these guideline studies be improved?
- How are ecological modelling software tools used in soil risk assessment today and what is their potential for the future? What are the possibilities for using modelling tools for regulatory purposes?
- What methodology and tools are available today to carry out ecological assessments at landscape level? What data and tools are needed to make it possible in the future?
- What would be the available tools and tests to be used as intermediate tiers from lab to field in the effect assessment e.g. multispecies test, TMEs etc.?

### 3.3. Challenges for soil toxicity assessment and CLP

- How is exposure- and effect assessment linked today? How could they be better linked in the future?
- What would be adequate information to prove low toxicity to soil organisms (WoE) e.g. when no aquatic toxicity is observed and no PNEC aquatic can be derived?
- Is there a possibility to develop cut-off toxicity values for soil organisms which would be comparable with the quantitative T criteria in Annex XIII to REACH? What are the possibilities and timescales based on state-of-science? What are the uncertainties and what kind of research work still needs to be done to overcome these?
- Why would there be a need to have criteria for classification and labelling of substances as hazardous to the terrestrial environment? Would the scheme be beneficial for all substances or would it have a limited scope e.g. substances not classified for the aquatic environment or classified in a lower hazard group for aquatic toxicity or substances with some specified uses?

# 1 Problem definition and conceptual model for soil risk assessment

## 1.1 Main challenges in soil risk assessment and protection goals harmonisation

Chemical risk assessment for the soil compartment has traditionally focused on prospective and retrospective (remediation) evaluation, in general focusing on impacts of well-defined chemicals on well-defined endpoints for relatively well-defined soils. The emergence of new scientific insights and novel societal challenges has generated various challenges.

Soil risk assessment does not take the possible benefits for the public (like socio-economic aspects and ecosystem services) sufficiently into account and its impact on decision making has been mostly limited to imposing some risk mitigation measures; for example, forbidding the soil application of sewage treatment sludge as fertiliser if the lower tier triggers for a chemical are exceeded without a higher tier assessment of the actual risk.

A main challenge therefore is to define more specific protection goals in the frame of the various regulations (REACH, biocides and plant protection products).

The risk managers, with input from risk assessors, should consider what the benefits would be for society to protect a certain type of soil, at a certain time and on a certain space scale. In other words, a better link has to be created between the risk assessment results regarding potential impacts on ecosystem services (specific protection goals), the ecological requirements for the ecosystem services and the indicators to assess the potential chemical stress on the ecological requirements, to support risk management considerations such as the socio-economic benefits of soil quality.

A key challenge with regard to the latter consideration is to feed the protection goals and outputs from a risk assessment relating to soil and terrestrial organisms into a holistic assessment for the whole environment and socio-economic assessments. The challenge in holistic, risk-based decision making is to aim for 'net environmental benefits' and for implementation of realism.

The key challenges identified above translate into a number of underlying challenges and development needs, including:

- Definition of the protection goals for the risk assessment, also considering soil use patterns (e.g. agricultural soil for pesticides and fertilisers; urban/industrial environment for some biocides);
- Further clarification of the protection goals, whether structural and/or functional, and what effects over what duration are considered 'acceptable';
- Definition of baseline conditions and the use of baseline conditions for comparison in risk assessment;
- Harmonisation of the risk assessment approaches across regulations, including harmonisation of fate and effect endpoints, implementation of higher tiers in risk assessment, consistency across chemicals (most notably: organics and inorganics);
- Addressing variability among soils (soil heterogeneity) with landscape and geographical region considerations while keeping harmonised approaches;
- Increase emphasis and transparency on weight-of-evidence approaches;

- Assure ecological relevance of regulatory exposure schemes, including improved understanding of environmental recovery and general application and definition of temporal contexts;
- Development of novel tools for future holistic, risk-based decision making;
- Moving from single species (structural) to functional-, service- and resilience-based decision frameworks;
- Increasing the relevance of risk assessment to field conditions, particularly in respect of chemical mixtures, and also in terms of effects beyond the individual level, i.e. populations, communities. More field-derived ecological knowledge is required on chemical impacts on ecosystems in the face of long-term changes – it is not clear whether the current assessment approaches are sufficiently conservative to account for this;
- Appropriately addressing the proportional effects of different stressors to biodiversity in the soil ecosystem, such as agricultural practice and other land use impacts, nutrients, climate and different chemical pollutants;
- Considering scientific developments in the regulatory context (regulatory approaches should catch-up with scientific developments in soil science and terrestrial ecotoxicology) and increasing basic understanding of soil science in the context of risk assessment by practitioners.

Finally, the following challenges are to be specifically addressed:

- Developing bioaccumulation and toxicity criteria for soil;
- Further development of risk assessment of metabolites, and the consideration of non-extractable residues (NERs), ageing and reduction in bioavailability over time;
- Higher tier refinement, including use of species sensitivity distributions based on field data;
- Validation and assessment of ecological relevance of outcome of risk assessment;
- Guidance on risk assessment for fertilisers;
- Updating guidance on risk assessment for pesticides;
- Validation of correction factors, like for example correction for soil organic matter content;
- Partitioning of chemicals in the soil environment, clear understanding (for all stakeholders) of where the equilibrium partitioning model (EPM) is a suitable predictive tool for terrestrial effects;
- Development of product-specific scenarios to address REACH potential gaps;
- Read across for chemicals that are emitted in different forms than those tested, e.g. metal concentrates, mixtures of organic chemicals;
- Mixture toxicity;
- Science-based scenarios for ingestion of soil by children, uptake of pollutants by plants, ingestion of pollutants by cattle;
- Alignment of exposure modelling with effect testing in terms of taxa tested (exposure routes – including for instance ingestion by cattle and by children) and dose metrics used.

Several aspects relevant to setting specific protection goals for maintaining the structural and functional capacity of soil were recognised.

Protection goals (PGs) are seen as a social/economic/political issue as much as being a scientific issue. Hence, it makes sense that the general and specific protection goals are designed to the designated use of the soil.

Different ecosystem services may be of major importance when setting PGs for agricultural soils (e.g. production and soil fertility) when compared to natural soil. Implicitly, the scope for harmonisation between EU regulations is limited. Harmonisation



potential exists in general concepts and testing methodologies. Soil resilience is suggested as the overall target/PG.

Ecosystem services provided by soil include:

- i) food and fibre production;
- ii) soil formation;
- iii) climate regulation;
- iv) water regulation;
- v) detoxification/removal of contaminants (e.g. nutrients, pesticides, organic wastes, etc.);
- vi) erosion control; and
- vii) pest and disease regulation.

Beyond the services provided by soil, the question on what can be practically measured should lead the selection of specific protection goals.

Specific protection goals could be function-based or structural/key species related. Function-based specific protection goals would be more directly linked to the ecosystem services like soil fertility and soil functions (e.g. soil formation, nutrient cycling, and organic matter degradation). Finally, multiple soil uses over time could be considered, including a recovery principle (five years?) in protection goals for soil with a specific designed use (agricultural soils or contaminated sites).

Biodiversity may not be a good candidate for a general protection goal under different regulations, since it is complex and difficult to measure. The main question posed is how to determine biodiversity and what is the reference situation. Functional redundancy is an important characteristic for soil fauna, and hence should be considered when assessing biodiversity.

Not being an ecosystem service *per se*, biodiversity could be used at different levels of the ecosystem services approach, and not (only) as a general protection goal. Soil biodiversity varies largely with designated soil use, and hence a protection goal related to biodiversity should be discussed with a spatial aspect, e.g. "where to protect what".

Applying the ecosystem services approach would help determine the habitats for which biodiversity is important in terms of providing a specific service. For example, biodiversity of plant communities may not be critical in terms of the "food provisioning" service for a cropland habitat, but may be much more important in terms of cultural services provided by woodlands and forests. Trade-offs may need to be found, and biodiversity targets could be compensated by specific measurements in other areas.

Soil biodiversity can be considered as an indicator for the soil functions and processes, or as an ecological requirement/specific protection goal to deliver soil ecosystem services (e.g. soil functional biodiversity necessary for the fertility of soil), or as a final ecosystem service or a good (e.g. biodiversity can have a cultural value). Alternatively, biodiversity could be a protection goal by itself (good ecological status), beyond its value in terms of ecosystem services.

## 1.2 Adequacy of current soil risk assessment approaches within different frameworks

Opinions are divided on whether protecting the structure of soil organism communities is always the most appropriate approach for protecting soil functions and services. It is argued that the relationship between the structure of the soil community, its ecological functions, and ecosystem services is complex and has not been sufficiently elucidated by the research community for full integration within regulatory programmes. More field experiments and assessments under local conditions are needed to clarify this relationship. Functional redundancy in soil ecosystems will require threshold values for structural endpoints to be set.

A 'standard' soil community structure is hard to define, and soil ecological functions are more important drivers for ecosystem services. Some argue that measuring structural elements (in terms of impact on species) is a conservative approach. Directly measuring soil functions would be more relevant, and the resilience of soils is best assessed using soil functional tests. However, focusing on structure alone may be destined to failure, and a more appropriate question might be "regardless of the community structure, are ecosystem functions preserved?". It is likely that the diversity of functions is more important for the sustainability of ecosystem services than species diversity *per se*. Thus, the complex interplay between structure and function has resulted in settling for a combination of structural and functional endpoints in effects assessment.

The general goals and principles of the soil risk assessment within the biocides (BPR), plant protection products (PPP) and industrial chemicals (REACH) regulations are the same. Nevertheless, some particular aspects and requirements on the effect and the exposure assessment of biocides, PPPs and industrial chemicals are different (table 1). Results of soil risk assessment of biocides, PPPs or industrial chemicals are evaluated at different time and spatial levels.

	Industrial chemicals	PPPs	Biocides
Emission	Assessed throughout the entire life cycle of the substance; tonnage-based approach	Mostly focused on emissions during intended use (application and service life; consumption-based approach)	Mostly focused on emissions during intended use (application and service life; consumption-based approach)
Exposure	Direct or indirect	Direct	Direct or indirect, depending on the product type
Effect and risk characterisation	PEC/PNEC approach; effects on indicator organisms and expected environmental exposures for defined environmental compartments are assessed; persistence and the potential for accumulation up the food chain are taken into account	TER (Toxicity Exposure Ratio), calculated for each standard species in the terrestrial compartment and for a given time period, which allows to identify specific areas of concern for further refinement in a tiered approach	PEC/PNEC approach; effects on indicator organisms and expected environmental exposures for defined environmental compartments are assessed; persistence and the potential for accumulation up the food chain are taken into account

**Table 1. Some aspects of the effect and the exposure assessment of biocides, PPPs and industrial chemicals**

Depending on the outcome of the risk assessment, mitigation measures may be applied for PPPs and biocides. These include: reducing the application rate, reducing the number of applications, changing the frequency of applications, applying at an earlier or later stage.

If a risk of industrial chemicals is predicted within REACH, the registrants may be asked to refine their assessment (of exposure or hazard or uncertainties/assessment factor) and/or manage the risk somehow, e.g. through emission controls. There are few circumstances where higher tier soil/terrestrial testing, such as field or semi-field studies, has thus far been required under REACH. It is unclear that the predicted risk alone would instigate formal restriction measures, but it could contribute to an impression that restriction was appropriate.

There is a distinction between risk assessment for avoiding risks to soil (e.g. prospective assessments under REACH, BPR, PPP) and for management of existing soil contaminations (retrospective assessments for screening and assessments including predictions for checking risk management options). In the latter case, a certain degree of effects to some groups of terrestrial organisms is generally accepted before it is decided that the contamination poses an unacceptable risk to the environment or human

health and hence must be removed. However, the same toxicity data can be used for both risk assessment types, with different derivations of soil quality standards depending on the protection goals (e.g. by varying assessment factors, using different effect levels ( $EC_x$ ), etc.).

Risk management, assessment tools and decision making appear more advanced, flexible and confident in the retrospective risk assessment (use of protection goals, conceptual models, soil-based screening values, soil and groundwater modelling, ecological surveys). There could be lessons to be learned here, where the emphasis is on 'breaking' the exposure pathway and land that is 'fit for purpose'.

Several approaches are taken into account in different ways by various jurisdictions regarding the assessment of contaminated soil. Some examples were provided in the responses to the questions, such as US eco-SSL (soil screening levels) approach for triggering the consideration of contaminants as contaminants of potential concern at remediation sites; European approaches to calculate risk-based screening levels for contaminated sites, including flexible approaches that account for metal bioavailability and the ageing and leaching of metals; or the Australian soil ecological investigation levels. Nevertheless, this is not an exhaustive list of available methodologies and tools. Risk assessment should aim to quickly exclude pathways where exposure is unlikely and adopt a step-wise process to refining assessment. Where residual risks remain, management approaches could be developed. Socio-economic analysis could help to refine and quantify risk management options.

In the absence of toxicity data for soil organisms, REACH allows the use of the equilibrium partitioning method (EPM) to assess the hazard to soil organisms. From a scientific point of view, there seems to be a consensus that the EPM should be applied only where there is no alternative methodology, and that it should never be regarded as a substitute for having an adequate amount of terrestrial toxicity data on the substance in question. Different arguments against the application of EPM are in place:

- For metals, the EPM is not defensible as the impact of differences in (pore)water composition need to be explicitly considered (terrestrial biotic ligand model (BLM) corrections);
- For organics, PNEC levels derived by means of EPM may lead to completely different risk estimates than  $PNEC_{soil}$  derived by soil testing;
- EPM is not applicable for substances with high volatility, unless the toxicity data are properly corrected for the volatile fraction and exposure of soil organisms from the soil pore air is accounted for;
- EPM might be inadequate for hydrophobic chemicals (such as black carbon) that interact much more strongly with specific soil components than predicted by conventional partitioning models based on  $K_{oc}$ . In addition, specific interactions for polar and ionic chemicals may make  $K_{oc}$  inappropriate for these chemicals;
- Soil microorganisms are to be considered a specific taxonomic group for which the EPM does not function properly;
- EPM is expected to work properly only for soil organisms where exposure occurs directly soil pore water, e.g. via the dermis. Dietary exposure and secondary poisoning with exposure is mostly due to ingestion of contaminated food, aquatic waterborne toxicity data are expected to be poor predictors of soil toxicity.

On the other hand, some publications demonstrate that the EPM approach does work, e.g. Redman et al. 2014.<sup>2</sup>

It has been recognised that the use of additional assessment factors may be a pragmatic approach, but that a more scientifically-based model would be preferable. The additional assessment factor should be decided on a case-by-case basis considering all lines of evidence. On the one hand, it is in this respect argued that given the assessment factors already applied and the conservativeness of the exposure assessment, the use of a factor of 10 is not justified for soils. On the other hand, it is to be recognised that in the absence of information on exposure via different exposure routes (like food ingestion), an assessment factor is appropriate until information on the exposure becomes available. Hence, without any further supporting evidence on the toxicity of a substance to terrestrial organisms, an additional assessment factor should indeed be used to account for different exposure routes.

Opinions are divided on whether the currently applied soil risk assessment approaches under the Biocidal Products Regulation (BPR) are adequate and useful. On the one hand, experts from the pesticides area find the approach chosen for biocides not detailed enough e.g. with regard to soil characteristics. Further criticism was made on the inconsistent/non-harmonised approaches in-between different product types and the missing definition of protection goals. On the other hand, there seems to be a consensus that the currently applied soil risk assessment approaches under the BPR give a reliable estimation of the rate of degradation and the products of degradation. The fate and behaviour of major metabolites is assessed, and a reliable estimation of potential accumulation in soil is possible.

Comments on the currently applied soil risk assessment approaches under the BPR can be summarised as follows:

- There is a wide variety of exposure scenarios; however, the ecological relevance of the various scenarios or the organisms that are intended to be protected has never been defined;
- The soil risk assessment needs to be integrated with food risk assessment, also accounting for inputs on soil from biosolids/compost i.e. those originating from wastewater treatment plants;
- The exposure assessment for biocides is different in-between product types (PTs) since the emission scenarios for each PT were developed independently. This leads to divergence e.g. in default values, the spatial and time scales;
- Modelling approaches are not always sufficiently detailed or clearly relevant in relation e.g. to the scale of assessment or any protection goal. In addition, some required data are very hard to obtain, e.g. the amount of leaching of active substances from different surfaces;
- There is a lack of adequate models to precisely address the diversity of soils and applications; the soil type as such is not specified in the emission scenario documents (ESDs) for different PTs;
- The assessments are based on a relatively high organic matter content in soil (ecotoxicity data are normalised to an organic matter content of 3.4%), whereas lower contents are reported in agricultural soil. This could lead to an underestimation of the predicted no effect concentration (PNEC) in soil;
- The basis for current assessment factors (AFs) is unclear and the AFs differ from those used for pesticides, leading to a lack of harmonisation in PNECs for the same substance with different uses;

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<sup>2</sup> Redman et al. 2014. Extension and validation of the target lipid model for deriving predicted no effect concentrations for soils and sediments. *Environmental Toxicology and Chemistry* 33(12): 2679–2687

- The results obtained from the effect assessment of pesticides might be more accurate and reliable since the effects are evaluated for each indicator species of the terrestrial compartment on a tiered approach, which is not the same procedure for biocides. For biocides, the tests are focused mainly on the effects on earthworms, soil-microorganisms and plants;
- There is a general impression of resistance to taking into account technical progress or non-standard (higher tier) studies for biocides.

### 1.3 Expanding the conceptual model for soil risk assessment: Integration of additional endpoints

The conceptual model for soil risk assessment may be expanded in several ways. The soil/water/air interphase could be better integrated, recovery and recolonisation processes of soil organisms could be taken into account, and environmental and ecological variability could be considered by moving to a landscape level.

By definition, a conceptual model should be an integration of soil/water/air pathways and receptors. Guidance exists for this in the contaminated land sector. In the conceptual model, the different interphases could be added one-by-one related to their relevance in the risk assessment for the soil organisms. The soil/water/air interphase should be considered for both human health and ecosystem assessments using similar approaches. Before integrating this within any conceptual model, the relevance/need should be determined. Integration is needed depending on different factors:

- The specific use and the pathway of the chemical: e.g. if aerial deposition represents a significant route of exposure;
- The chemical properties, e.g. volatilisation, ionisation;
- The protection goals: in conservation agriculture this interphase is crucial for litter decomposition – if soil functions are considered as a specific protection goal, the interphase would also be considered;
- Addressing the interphase in the effect assessment part: effects of combined exposure to soil, pore water and air phases to soil organisms are covered by standard toxicity tests where it is assumed that substances added to soil partition to the different phases within the exposure period. Differences in partition between laboratory studies and the field are considered, at least in higher tier assessments, for particles and pore water, but should be extended to pore air if needed.

To integrate the soil/air interphase into the conceptual risk assessment model, assessment of the significance of aerial deposition as a route of exposure of the soil and of biota is needed. The soil/air interphase is best integrated through fugacity modelling, and this is already incorporated in EUSES2.0 or others by means of partitioning coefficients ( $K_{OA}$ , although the underlying models for this property may still be in a rather conceptual stage). In addition to screening the relevance of the soil/air interface on the basis of  $K_{OA}$ , in a more advanced stage of assessment it is necessary to take into account wind speed, soil moisture content, texture, porosity, etc. Photodegradation could also be included in the exposure modelling.

There seems to be a consensus in the fact that recovery is an important issue in environmental risk assessment for soil organisms. The recovery times and ecological succession patterns of different species/groups of organisms could help to define acceptable effect levels (over time and space) to maintain ecosystem functions and services. While the shortage of information on recovery is evident in the scientific literature, field studies data (mainly on earthworms and macroarthropods) do exist in

companies' databases. These data could be used to better assess recovery of these groups after the use of different types of compounds.

Both internal and external recovery (where recolonisation potential of the different species plays a key role) should be considered important. Internal recovery could be tackled by performing multi-generation tests in the laboratory. Appropriate assessment factors could be determined by comparing field data with these multi-generation approaches, therefore allowing a robust extrapolation from laboratory to field situations. This implies the need for more field monitoring data. Regarding external recovery, even though the recolonisation process in soil organisms can be slow due to their general low dispersal capacity, the importance of the recolonisation process for population recovery is high. There is a need to maintain donor areas off-field from where recolonisation to in-field could take place. In this context, landscape configuration is important for the in-field recovery potential as well as the need to establish "minimum quality thresholds" for landscape configuration allowing recovery. This is connected to the need to develop good modelling approaches (e.g. individual based models) that, supported by good empirical data (data on dispersal and life cycle traits of the key driver species and on field monitoring), could be a way to properly address recovery issues.

Both modelling and monitoring are potential tools for moving to a landscape level to better take environmental and ecological variability into account. Existing soil quality databases could be utilised both by individual countries as well as EU-wide. Country specific databases exist both for soil physical/chemical parameters and soil fauna. However, harmonisation and comparability of such data is not always a given.

Besides GIS data and satellite imaging, field studies, existing ecosystem service case studies, and (US) industrial site remediation studies are deemed to provide useful data. In several projects (GEMAS, UseTox, EDAPHOBASE, etc.), such relevant data have already been collated/used.

Reservations for moving to a landscape level are driven by the perceived high efforts needed to generate the data for a complex matrix of highly variable soil types in Europe and corresponding variability in soil ecosystems. The question of scale/resolution needs to be addressed and a scenario-based approach would have to be used. Soil organisms have limited mobility and as such the need/opportunity to include larger landscape aspects in risk assessment may be reduced.

## **2 Environmental exposure and fate assessment**

### **2.1 Elements, processes and parameters driving the fate/exposure of chemical substances in the soil**

The environmental exposure of a chemical is determined by the use pattern of the product containing the chemical, the properties of the receiving environmental compartment (including climate factors) and the substance-specific characteristics. There are, therefore, numerous processes which can impact the potential fate and behaviour of the chemical in the soil matrix.

However, in terms of regulatory exposure assessments only a limited number of processes taking place in practice are considered in the modelling tools. First tier exposure modelling should normally rely only on data which can be obtained within the studies laid out within the legislative data requirements set out under the relevant regulations.

In summary, the following key issues in fate and exposure assessment are most commonly distinguished:

- Compartment specific emissions and details of application;
- Chemical properties of the substance, in particular:
  - Partitioning coefficients;
  - Degradation half-lives;
- Environmental parameterization, in particular;
  - Distribution, composition, and size of compartments;
  - Fluxes within and between compartments (including run-off);
  - Properties of the compartment (e.g. temperature within compartments, pH, solid fraction, organic matter and carbon content).

Furthermore, in the risk assessment environmental effects of exposure to the substance should be considered, in particular

- Toxicity (acute and chronic);
- PBT characteristics;
- Long-range transport behaviour.

A further subdivision may well be obtained for each of these key issues, whereas properties may be derived from these key issues (like bioavailability, bound residue formation, uptake rates, secondary poisoning). In this sense, it should be noted that the soil and substance (at least for the large tonnage substances) physico-chemical characteristics and processes relevant to soil exposure assessment are fairly well known. What is less well known is actual bioavailability and the toxicological interface with soil biota, or what might be considered sufficiently representative soils to suit representative risk assessment situations. It is also important to make sure that the exposure metrics and chemical forms should match those used in ecotoxicological testing.

Other elements to be considered in the environmental exposure and fate assessment are the impact of soil composition (including moisture content and soil decomposition/ weathering) and climate on environmental fate processes. Therefore, the factor of time as related to ageing of a chemical in the soil matrix is an important element in increasing realism in fate and exposure assessment. It is also recognised that plant uptake might affect the environmental fate of some chemicals, as is bioturbation. There is a gap in knowledge concerning ionisable chemicals which can show interactions with organic matter but also with mineral matter in soil.

In general terms, an important consideration in fate assessment is the relevance of the soils used in (laboratory) fate and effect assessment studies for the 'real' environment, whereas special attention is needed regarding the non-homogeneous nature of soil.

Substance specific physico-chemical parameters are to be considered in soil exposure and fate assessment. Before summarising key physico-chemical parameters to be considered in soil exposure and fate assessment, it is important to consider the purposes for which the parameters are to be used. Specific purposes include:

- to identify the potential for direct physical hazards posed by the chemical or material;
- to determine the environmental compartments into which the chemical will partition;
- to estimate the potential for bioconcentration and bioavailability;
- to estimate the likely routes of exposure of biota, bioavailability, and the related likelihood for toxicity;
- to estimate the potential for inducing human toxicity.



Given these purposes, a number of key parameters can be identified. These include:

- half-lives in soil due to biodegradation, hydrolysis, volatility;
- partitioning coefficients (which are driven by sorption potential, water solubility and vapour pressure);
- speciation/nature of transformation products.

These should be considered in combination with the soil parameters:

- soil type/nature and texture;
- erosion rate;
- resuspension rate;
- horizontal and vertical mass transport in soil (tilling in agricultural soil, bioturbation, cryoturbation, leaching, facilitated transport, drift).

These properties are affected by the composition of the soil as expressed by means of, for instance, cation exchange capacity (CEC), organic carbon (OC) and clay content, pH, redox potential, temperature, soil moisture content, and air content of soil pores.

Key parameters of the chemicals of interest include: water solubility, solubility in other solvents, vapour pressure - Henry's law constant,  $K_{ow}/K_{oc}/K_d$  (partitioning), degradation, water dissociation constant (pKa), diffusivity in air, diffusivity in water, skin permeability constant, dermal absorption factor, gastrointestinal absorption factor, beef transfer coefficient, soil-to-dry plant uptake factor, bioconcentration factor, milk transfer coefficient. The number of parameters relevant in specific cases will depend on the required level of detail of the fate and exposure assessment.

Various substance properties and environmental conditions may induce high potential for indirect exposure. In some cases, the combination of properties and conditions may also reduce indirect exposure, like in the case of volatility giving rise to potential off site exposure: volatility will be reduced for chemicals with high aqueous solubility or with high  $K_{ow}/K_{oc}$  (high adsorption potential in general).

Important indirect exposure routes include:

- Long-distance transport and deposition for persistent chemicals with high volatility;
- Deposition from air particles and wet deposition;
- Exposure via sewage sludge following sludge application on soil;
- Exposure via manure/slurry application on agricultural soil;
- Run off;
- Leaching from treated surfaces.

Some of the most common conditions and properties to take into account include:

- Poor agricultural practices when applying fertilisers and plant protection products (PPPs) (causing excess spray drift and run off);
- Change of soil pH, in turn altering availability of chemicals;
- Weathering (mainly for treated leaching surfaces);
- Precipitation;
- Atmospheric particle content;
- Soil OC content;
- $K_d/K_{oc}/K_d$  of the substance;
- Volatility of a chemical – high Henry's law constant;
- Degradability, including biodegradation in a sewage treatment plant;
- Persistency in general.

In the current laboratory and field scale guideline ecotoxicity studies exposure is commonly measured as total concentrations of a chemical in the soil matrix. It is noted that concentration of the chemical in the pore water of the soil, concentration of the

chemical bound to solid particles and soil air concentration may be better metrics of actual exposure. Generally speaking, the distribution of exposure between the pore water pathway and the particles ingestion pathway is an important issue.

There is a broad recognition that actually measured concentrations are to be preferred over nominally applied concentrations. It is, however, also recognised that in both field studies (including mesocosms) and laboratory studies, concentrations of contaminants are not always routinely measured. This implies that in many cases correct spray deposition rates and metabolite formation are not monitored. Options to include chemical analyses in guidelines are available, including the SETAC EPFES (2003) litter bag and PERAS (2010) TME guidelines, and should be included in any developing or revised OECD/ISO earthworm field test guideline.

Improvement of exposure assessment is obtained by proper analytical verification of chemical concentrations, as in general initiated by extraction of the soil. A large range of extractions of various strengths are available, ranging from mild extraction with water up to *aqua regia* (for metals) digestion of the soil. More use needs to be made of methods that enable us to distinguish different fractions in these media as this will give a better insight into the bioavailability of the chemical. Further improvement in assessing actually available concentrations may be obtained by deploying newly developed approaches like passive sampling techniques for both organics and metals.

## 2.2 Tools and methods for the soil exposure assessment

Modelling helps to extrapolate from a (limited) number of studies/data to a wide range of circumstances (release scenarios, exposure scenarios, effect scenarios and landscapes) for which exposure and risk assessment is warranted. Once the protection goal and the area of interest are defined, specifically modelling is a versatile tool for exposure and risk assessment. The possibilities of regulatory use of the results of exposure/risk assessments (also based on modelling) are high (e.g. contaminated soil remediation in the Netherlands).

Two main features of models used for the environmental exposure assessment are release/emission estimation under specific exposure scenarios/uses and assessment of the subsequent distribution process modelled for the environmental compartments. Exposure modelling software tools intend to capture the different and diverse application/release pattern towards the receptor compartment resulting from the different uses. Once the chemical is released into the predefined environmental compartments, the environmental behaviour is calculated in a quite similar manner within the different exposure model systems currently used under various regulatory schemes in Europe.

For regulatory risk assessment purposes, computations are done by means of multimedia fate models based on the fugacity concept (e.g. EUSES is used for environmental safety assessment under REACH, while the FOCUS models and scenarios are used for plant protection products). Models have been described by Mackay et al. (1992), Van de Meent (1993) and Brandes et al. (1996) (SimpleBox). These models are box models, consisting of a number of compartments which are considered homogeneous and well mixed.

A substance released into the model scenario is distributed between the compartments according to the properties of both the substance and the model environment. Sometimes, one or the other process is explicitly considered or not in the model (e.g. the methodology applied in the EUSES model considers the following processes for removal of the chemical from the soil: biodegradation, volatilisation from soil and leaching to deeper soil layers).

In the models described above, for example, the metal speciation is poorly taken into account while in the case of models used in other fields e.g. geochemical models, this is taken into account. So models can be usefully integrated into tiered assessment approaches, but they may not fully reflect reality as at present many important processes are sometimes excluded. Hence, bearing in mind their limitations, they should be carefully used for the higher tier assessments. The uncertainty of input parameters should be considered and documented as much as possible.

Validation with experimental data is useful and from time-to-time necessary to justify the concepts used. Models are essential in regulatory risk assessment, but many require updating and would benefit from further 'validation' of generic input parameters to ensure they are still realistic and representative. Models' default parameters may be quite old and should be updated with actual information from reliable studies. It would be useful if they could also take longer term fate and behaviour of substances into account (adsorption, aging and movement through the soil profile) for better comparison with long-term effect studies.

For example in future, a landscape-based modelling in combination with GIS (a geographic information system) mapping specifying soil types and climatic conditions would facilitate a higher accuracy of PEC values. Future potential could be a more sophisticated handling of spatial aspects based on geographic information (distribution of key environmental parameters such as temperature, rainfall, soil type, pH, organic carbon in soil). Furthermore, as mentioned above, existing exposure modelling tools do not always consider all the processes taking place in soil (i.e. advective/diffusive transport, bioturbation, sorption, absorption/volatilisation, degradation).

Currently, simplistic approaches are used in modelling exposure. Simplistic approaches are very useful in the regulatory context, particularly for concluding low risk at the screening level, but may be insufficient for higher tier assessments. In future, more and more sophisticated numerical models that include the main relevant processes and which can be spatially highly resolved will/should be used. Before the implementation of any new modelling, it should be considered whether the new methodologies will increase the ability to meet protection goals, compared to those currently utilised. Complex modelling tools might not be necessary. They could be developed/used, but only if there is a protection need. Most exposure calculations are simple conceptual models and this is probably adequate to achieve the level of protection required.

There are tools and methods available to be used as intermediate tiers from lab to field in the exposure assessment. The available FOCUS soil models (PELMO, PEARL) could principally be used as intermediate tiers for the exposure assessment. It is important to address and take account of both nature/properties of the chemical and of the receiving matrix (e.g. soil) in the exposure (fate) assessment of a chemical. Tools and tests to be used as intermediate tiers could involve direct measures of chemical concentration in soil gas, biodegradation tests, site specific toxicity tests, etc.

This is pure analytical chemistry in combination with a clever sampling strategy that exploits the geology of the location under assessment to the optimum. The current regulatory tests often study only one process/phenomenon in isolation whereas in the environment, for example, different biotic and abiotic degradation/dissipation processes occur simultaneously and synergistic or antagonistic effects are possible, which can lead to a different exposure level from that predicted on the basis of reaction rates obtained for isolated processes. For example, photodegradation is generally not addressed by the standard biodegradation tests. Therefore, perhaps the field relevance of the laboratory tests could be increased (e.g. soil degradation studies on a set of different soil types). However, the applicability for regulatory purposes needs to be carefully assessed taking

into account the purpose of the assessment (e.g. general/local conditions) and variation in environmental conditions.

As previously indicated, bioavailability of chemicals depends on their speciation in soil, in particular on the distribution between soil particles and soil porewater, on 'within porewater' speciation, and on bioaccessibility of chemicals on particles. Regarding speciation in porewater, geochemical models are available for metals for extrapolating from laboratory to field conditions. The main limitation is the characterisation of organic matter in soil (e.g. distribution between humic acids and fulvic acids).

Passive sampling techniques (e.g. diffusive gradients in thin-films for metals, hydrophobic membranes for organics) could also be used for describing speciation (and bioavailability) of chemicals in soil pore water. Regarding bioaccessibility of chemicals, laboratory protocols are available for simulating conditions occurring in the gastrointestinal tract (GIT). Dynamics of chemicals in field conditions (not reproduced in laboratory conditions where soil is homogenised) can be simulated by models combining chemical processes (e.g. sorption/desorption) and physical processes (e.g. advective/diffusive transport, etc.).

There are a wide range of intermediate scale studies that can be used to develop an understanding of how specific processes interact and how these are influenced by more realistic conditions. Examples of such test systems are:

- Soil degradation studies using intact soil cores in the laboratory. This approach better conserves the soil microbial population and hence can provide more realistic degradation rates and routes. Such cores can be used in combination with UV and non-UV emitting light sources to evaluate the influence of phototrophic soil organisms and photodegradation. The studies are conducted under controlled conditions enabling the significance of individual variables to be assessed.
- More sophisticated laboratory/semi field tests:
  - Laboratory incubation test with sieved soil incubated under varying temperature conditions mimicking natural fluctuations;
  - Laboratory incubation test with sieved soil which is "fed" with organic matter easily accessible to soil micro-organisms (e.g. alfalfa flavour) mimicking the plant root exudates;
  - Perfused cores;
  - Laboratory incubation test with undisturbed soil columns (different sizes possible) with irrigation mimicking rainfall;
  - Laboratory incubation test with undisturbed soil columns and irradiation mimicking natural sunlight;
  - Pore water sampling.
- Small scale outdoor soil degradation studies. These studies can often be conducted with radio-tracers and enable the soil degradation to be studied under more realistic environmental conditions.
- Lysimeter studies are similar to the above, but are designed to assess the movement of compounds down the soil profile to a specified depth (often 1m) where the leachate is captured and the amount of compound and degradation products is determined. The weakness of this approach is that labile reaction intermediates are preserved and quantified in the same way as stable products.
- Semi-field aquatic fate-mesocosm studies enable the fate of compounds to be studied in water/sediment studies in the presence of aquatic plants under realistic environmental conditions. Radio-tracers can be used enabling most of the degradation products to be tracked and quantified. These studies provide much more realistic rates and routes of degradation to be determined.

- Microcosm and mesocosm studies, where the fate of a substance could also be investigated and not only the toxicity endpoints of species, on recovery and/or on community level.

For effect, and fate and behaviour studies appropriate sampling schedule, sampling techniques and analytical methodologies should be applied to allow the results to be used with confidence in the risk assessment.

### **Exposure assessment at landscape level**

In the current risk assessment procedure for soil organisms, landscape level approaches are not (yet) taken into account. Landscape level approaches would require the availability of data on effects of landscape structure on soil organisms. These data are not always available. Landscape level approaches might be particularly important for soil organisms that also have aboveground life stages. The recent EFSA opinion on non-target arthropods contains a modelling approach that might be helpful. A landscape level approach would need modelling exposure at the landscape level including both in-field and off-field exposure.

The landscape level is considered to be a highest tier of the assessment and quite often the principle of expert judgement applies here. The Guidance from EFSA<sup>3</sup> implies that spatially distributed modelling could be developed based on databases from the European Soil Data Centre. However, there is little practical experience of this available and it should be ensured that such developments are proportionate to the risks involved. It is of outmost importance to define what the protection goals required to be met are (e.g. "unpolluted reference landscape"; in any case, any protection goal chosen would need to be clearly defined) and/or the aims of the modelling should be defined.

To estimate exposure on a landscape level, geographic data are needed which indicate the spatial variability of the relevant compartment, e.g. maps of soil properties, meteorological characteristics, or agricultural practices. Different institutions and agencies of the European Union like the JRC, EEA, or EFSA provide such geographic data for Europe. Data with a finer spatial resolution are commonly available from national institutions on a country level. Generally, data that are more precise lead to exposure assessments that are more accurate.

Exposure assessment at a landscape level would probably require statistically representative data for relatively large areas. Therefore, geostatistical methods would be beneficial if "point sampling" is done. If spatial variation is considered important (e.g. to obtain information on the maximum exposure level) then a sufficient amount of samples need to be taken and analysed. The data can be processed further with geostatistical methods/software, e.g. to study the spatial dependence of exposure from the source.

If spatial variation is not considered relevant for the purpose, then combined samples can be used to provide the average level of exposure. Perhaps, some integrated measurement methods can also be used (depending on the case or substance) such as analysis of soil runoff water or, in the case that volatilising substances are measured, tracer gas or micrometeorological measurements could be done to obtain landscape level information without the need for labour-intensive sampling from a high amount of measuring points.

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<sup>3</sup> European Food Safety Authority, 2015. EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2015;13(4):4093, 102 pp., doi:10.2903/j.efsa.2015.4093

Multimedia box models, where information on meteorology, land use, emission, soil organic carbon content, surface water fluxes, etc. at a resolution that reflects the necessities of the assessment is available and might be useful in developing tools for carrying out exposure assessments at a landscape level. The results obtained should be usefully backed up by monitoring data.

Sufficient data (e.g. in GIS) might be available to construct a landscape level tool, but the challenge will be to make sure that the calculations produce reliable and realistic results (enormous degree of validation would be needed). Models based on GIS are already available and used (e.g. groundwater assessment on national and European levels). For the soil exposure assessment at landscape level, large spatial and temporal data sets regarding soil profile, groundwater level etc. have to be available. However, it should be noted that soil and climatic data do not cover the whole of Europe and the quality of some data is low. Another problem is that – where data are available at country level – these can often not be combined, because different methods were used for collecting the data (e.g. different sampling depths, different analytical methods were used to measure the same parameter).

The availability of tools to calculate exposure on landscape level depends on the modelling approach for the exposure assessment. The implementation of simple analytical models to calculate exposure in soil is straightforward in every geographic information system (simple map algebra). In addition, the EFSA software tool PERSAM is able to calculate exposure on the landscape level based on analytical models.

However, the implementation of more sophisticated numerical models is not possible in most geographic information systems due to their inability to simulate dynamic processes (solution of differential equations). Spatially distributed versions of the numerical models PEARL and PELMO exist for most parts of Europe and could be used for the exposure assessment on the landscape level.

However, the availability of these spatially-distributed models to stakeholders is limited. In addition, the implemented GIS data in the models could be outdated; therefore, the models need to be revised to bring them up to date. The development of a new spatially-distributed numerical model within a specialised GIS environment would be a possible development.

## **2.3 Specific aspects of exposure/fate in the soil risk assessment**

### **Degradation/dissipation**

The key aspects when considering degradation/dissipation assessment vary by nature and may be grouped in a limited number of issues:

- Issues related to the representativity of lab tests with regard to the conditions in the field;
- Process-related issues like Arrhenius' equation to extrapolate across temperatures, soil water content, need to assess formation and identity of transformation products, need to assess biodegradation/mineralisation.

An issue that is often overlooked in degradation/dissipations assessment is when to include plants, sewage sludge or slurry/manure in soil degradation studies, possibly when performing and valuating field dissipation studies. For some types of substances, plants have been shown to enhance degradation and animals like earthworms by digging indirectly stimulate microbial activity by enhancing soil mixing and aeration. These

effects could be relevant for scenarios assessing the risks to agricultural soils, e.g. PPPs, biocides and REACH scenarios where crops are intentionally included.

It is recognised that there needs to be further agreement on triggers for higher tier exposure testing or modelling, following initial standard lab testing. The questions that need to be answered include: what are the most relevant simulation studies and whether/how to normalise for temperature, organic matter (OM) content etc. either in the tests or in subsequent modelling. In general, acceptable WoE requires suitable justification, but further general guidance and examples should be developed on what constitutes acceptable WoE justifications.

In many cases, modelling endpoints have to be normalised at an agreed temperature value. Therefore, it was seen appropriate to perform the study at the agreed temperature, e.g. 20°C. However, the distribution of temperatures in the region/country/continent might become important; therefore, normalisation to other temperatures (than 20°C) might be necessary. Regulatory assessment for a certain geographical area can be done at a temperature relevant to that area whereas, for example, for the laboratory characterisation of transformation products or routes, a different temperature can possibly be used. However, for reasons of coherence, the same reference temperature should be used for the assessment for both parent substance and metabolites unless differences are justified for ensuring realistic worst-case conditions. For example, taking into account degradation rates at 12°C appears as a reasonable worst case for predicted concentration calculations. However, for the relevant metabolite identifications, 20°C appears as a more appropriate worst case (again testing for stability of metabolites, may be required at different temperatures).

### **Animal testing**

There is a high level of consensus on the key properties that allow the identification of key exposure pathways that allow animal testing to be minimised confidently. The key issue is to either make sure that direct or indirect exposure to soil is unlikely, or that the chemical is not available for inducing adverse effects. Thus in general terms, data on exposure, sorption behaviour and degradation are required.

The most commonly mentioned key properties include:

- $K_{ow}/K_{oc}$ ;
- Biodegradation potential;
- Chemical reactivity;
- Volatility;
- Solubility as a function of pH;
- Leaching probability, as dependent on the dynamics of water in soil; and
- Soil properties affecting speciation, like pH, redox, OC.

Finally, there is a plea to apply as much as possible read-across considerations from similar compounds.

### **How might the background concentration of soil contaminants be incorporated into the risk assessment?**

Consideration of the risk associated with background concentrations of contaminants in soil may be useful in developing specific protection goals and/or risk management strategies to meet such goals.

It is important to define terms used as it is regularly a challenge to resolve what is in fact accepted as a background for both "natural" and "anthropogenic" conditions. It was commented that neither of the two terms are well defined and the result is that

background is a scientific/political decision. For example, for the US regulatory system it is typically determined on a state-by-state basis in regulation. These political considerations drive the risk management determinations.

It was noted that the background concentrations are often not well established. Furthermore, background concentrations can vary at the EU scale, at the national scale and at the local field scale. Therefore, using average background concentrations will tend to underestimate the risk in half of the cases. On the other hand, using maximum concentrations will clearly over-estimate the risk in most of the cases. It will be difficult to incorporate this into a regulatory process working for all of Europe unless the risk characterisation is mapped according to geographical conditions.

The choice of the relevant background concentration can depend on whether the purpose is local site-specific or generic risk assessment. For example, the highest available background concentration could be the starting point and if the result indicates unacceptable risk, it can be possible to refine the PEC e.g. by using site-specific data for local risk assessment, if appropriate for the purpose, identifying which areas may be at risk.

As a simple first tier screen it was suggested that the PEC values could be compared to the background concentration. Where the PEC values suggest a negligible increase in the actual concentrations regarding the background levels, it could be concluded that the risk from the additional source can be considered negligible. However, this should be considered on a case-by-case basis as there may be occasions where this approach is not appropriate, e.g. due to differences in bioavailability between the background and newly released chemical. Use of the added risk approach has already been applied for metals and it was also proposed in general for other type of substances. On the other hand, it was stated that background concentration cannot be incorporated as its typical site-specific information.

It was pointed out that the background concentration of a chemical (e.g. metal) may increase (within natural limits) the natural tolerance of the acclimated or adapted organisms. For essential metals, for example, homeostatic regulation allows to regulate internal element concentration. The possible acclimation/adaptation of communities to different (natural) metal background concentrations has been poorly considered in applied ecotoxicology.

Background concentrations are already taken into account for the risk assessment of substances that are present in the environment, in a case-by-case approach. For example, the issue of background levels was discussed at length in ESR assessments for zinc and nickel amongst others. The background concentration is only relevant for persistent substances. In the new EFSA Guidance document, simulations are run for long periods of time to calculate a plateau concentration.

In summary, the following issues were raised to improve the understanding of the role of background concentrations in the risk assessment:

- There should be sufficient and reliable data on the background concentrations of the chemical and its bioavailability;
- Background concentrations should be presented clearly and as open information;
- Monitoring data collection;
- Use of the full application rate applied;
- Soil types and regions should be presented;
- The risk assessment should concentrate on the effects of increases of concentrations due to contemporary release of contaminants;



- Take into account the ability of soil organisms to acclimate to different, environmentally-relevant, background chemical concentrations;
- Soils with low and elevated background concentrations should be included in fate and effect testing;
- Total concentration may differ from the bioavailable concentration and therefore, for example, "ageing factors" can be used in some cases.

The US EPA Superfund Cleanup Program is an example of a regulatory programme where background considerations have been incorporated into the risk assessment. The Superfund Program developed a policy statement, *Role of Background in the CERCLA Cleanup Program*<sup>4</sup>. In this policy, background refers to constituents or locations that are not influenced by the releases from a site, and is usually described as naturally occurring or anthropogenic. In some cases, the same hazardous substance, pollutant, and contaminant associated with a release is also a background constituent. The policy [for US sites] further states that these constituents should be included in the risk assessment, particularly when their concentrations exceed risk-based concentrations, and that background information is important to risk managers because the Superfund Program, generally, does not clean up to concentrations below natural or anthropogenic background levels.

## 2.4 Inclusion of bioavailability and bioaccumulation in current and future soil ERA strategies

### Bioavailability

Current risk assessment ignores different non-extractable residue (NER) types, i.e. type I (xenobiotic, sequestered; potential for slow release), type II (xenobiotic, covalently bound, no/little chance for release), and type III NER (biogenic residues, amino acids, phospholipids etc.). Type I NERs should be considered in risk assessment, type III NERs would reduce the environmental risk.

Although methods for differentiation of the NER types are at hand, structural identification of residues is often missing. The threshold values are most often only used to trigger attempts to quantify the amounts in fulvic acids, humic acids and humin, which for environmental risk assessment is not enough.

For PPPs, the formation of residues is not taken into account except when the mineralisation is < 5% active ingredient and NER > 70%. In this latter case, further assessment/characterisation of NERs is required. The formation of NERs is usually not measured in field studies. Discussion is ongoing on the issue of whether binding of residues is a way of reducing risk, as this would imply that the NER is no longer bioavailable and therefore no longer contributes to adverse effects. In this respect, it is necessary that it is convincingly shown that NER formation is irreversible and that the NER does not present a hazard to the ecosystem.

In the case of the REACH and Biocidal Products regulations, there is insufficient documented guidance relating to NERs. Within REACH and the BPR, NER formation is mainly an (unresolved) issue for persistence determination in PBT assessment – see ECHA R11 Guidance.

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<sup>4</sup> OSWER 9285.6-07P, May 2002;  
<http://www.epa.gov/oswer/riskassessment/pdf/role.pdf>

There are key differences between how a soil simulation study is assessed for REACH, biocides and pesticides. The issue is how the data are used in subsequent modelling as well as with regard to the frequent availability of field dissipation studies for persistent pesticides. For PBT assessment within REACH and biocides, only degradation and not dissipation or NER formation is usually used. This is done differently for persistence assessment within the pesticide legislation.

In the US, exhaustive extraction of residues is required and if additional parent or degradation products of interest are extracted, they may be included in PEC calculations. Extraction of non-bioavailable residues in simulation studies can result in unrealistically slow apparent degradation rates if included in kinetics calculations. No account is taken of unextracted residues in field studies as these studies are designed to quantify defined chemical entities. The extraction methodologies used, need to be validated to demonstrate quantitative extraction.

The general premise is that adsorption and NER formation reduce availability and thus reduce adverse effects. Nevertheless, it is recognised that NER formation may not always be considered as a loss of effects on non-target organisms, as this may depend for instance on the exposure route (digestion). Stabilisation, therefore, needs to be assessed on a case-by-case basis by means of an appropriate bioassay, and in the case of shown irreversible binding, it may be assumed that no adverse effects will take place. As assessment of NER formation is hard to perform by means of harsh extraction methods that might modify the chemical structure of the contaminant, and the concept of time-dependent sorption was therefore introduced recently. A key obstacle in applying this concept is the lack of guidance.

With regard to bioavailability assessment correction can be done on either the exposure or effects side. Work previously done for the existing substance risk assessments of some metals (e.g. copper, zinc) has demonstrated the value of empirical bioavailability correction, informed and justified by mechanistic understanding of the processes concerned, and could be presented as an example.

For metals, there are several illustrations for how bioavailability can be incorporated into soil risk assessments. It is important to understand that effects are difficult to predict based on total soil concentrations. This observation has led to experimental work identifying that metal toxicity to plants, invertebrates, and microbial processes is influenced by key soil parameters, like pH and effective CEC (eCEC). Bioavailability-based approaches have been developed for risk assessments of Cu, Ni, and Zn, and other metals, recognising that the best metric for taking into account bioaccessibility/bioavailability depends on the target organisms.

For plants that take up chemicals from the root system, or for uptake through the dermis, the freely dissolved pore water concentration can be the best metric. For organisms ingesting soil particles, the physicochemical conditions in the GIT can affect the exposure. According to organisms, bioavailability characterisation should thus involve different kinds of tools (e.g. geochemical modelling, passive sampling, lab reproduction of the geochemical environment of the digestive system).

It is assumed that adsorption reduces availability and thus reduces the effect; however, this will also be taken into account in the effects test where soil is the matrix.

It has been suggested that solvent extraction with mild agitation may remove more than the bioavailable residue from soil. In many cases, a significant proportion of non-bioavailable residues are removed by most extraction methods used in simulation studies as historically the methodologies used have been designed to be as exhaustive as possible (for parent and degradation products).

## Bioaccumulation

There is a difference between bioaccumulation in soil organisms on one hand and food-chain (bio)accumulation in terrestrial organisms on the other hand. The first refers to the direct uptake of chemicals from soil by lower organisms like earthworms, isopods and springtails, and in plants, which are at the basis of food chains. The latter deals with the bioaccumulation of chemicals from soil in higher organisms, like carnivorous or herbivorous birds and mammals, but might also include e.g. reptiles and amphibians.

For pesticides there are suggested methods for terrestrial bioaccumulation (food chain) assessment in the EFSA PPR Guidance document on bird and mammal risk assessment (2009) and also in the biocide risk assessment guidance. This issue has been extensively discussed in the ECHA REACH PBT Expert Group (in relation to B determination in PBT assessment).

Models for estimating bioaccumulation in soil and terrestrial organisms are available. These models require information on properties of the chemical ( $\text{Log } K_{ow}$ ,  $\text{Log } K_{oa}$ ,  $\text{Log } K_{oc}$ , DT50), the soil (pH, %OC) and the organisms (lipid content; contact with soil).

Since exposure of soil organisms is mainly from pore water, the difficulty is in the fact that the bioaccumulation factor (BAF or BSAF) for organic chemicals is determined by binding of the chemical to soil on one hand and its uptake in the organism on the other hand. Both processes are determined by lipophilicity ( $K_{ow}$ ), making BAF/BSAF hard to predict. This may, for instance, lead to the apparent absence of bioaccumulation in earthworms while there is significant bioaccumulation of the same chemical in the food chain (e.g. birds). This problem also hampers the definition of trigger values for bioaccumulation in soil.

Bioaccumulation could be derived from a test carried out with a soil with low adsorption capacity (low organic matter or low cation exchange capacity (CEC) for ionisable substances). Thresholds could be based both on total concentration and on bioavailable or bioaccessible concentration.

Experimental determination of BAF is needed, but which species should be used for that? The only protocol available is for bioaccumulation tests with earthworms; there are no protocols for bioaccumulation tests on other soil organisms or organisms higher in the food chain.

Inclusion of kinetics (TK/TD) is recommended because of the link between bioaccumulation and toxicity; however, this link needs further investigation. Bioaccumulation tests reflect toxicokinetics (TK) of chemicals in the organism body.

Skipping the uncertainty due to toxicokinetics and focusing on toxicodynamics (TD) can reduce the global uncertainty of the assessment. Internal concentrations are then relevant to reflect the actual exposure of the organism and may be a better option than exposure concentrations for exposure-based waiving. Bioaccumulation aggregates the contributions of many routes of exposure and accounts for the bioavailability of the chemicals. Bioaccumulation thus allows a more relevant extrapolation between species. For 'complex' organisms, a question remains on the 'internal' concentration that should be considered (whole-body concentration used as a surrogate of the concentration at the site of toxic action vs tissue-residue approach).

Bioaccumulation of metals needs a different approach because of specific aspects like regulation of body concentrations, hyper-accumulating plants etc.

### 3 Effect assessment

#### 3.1 General overview

As already stated in the section for Topic 1, the general goals and principles of the soil risk assessment within the biocides, plant protection products (PPPs) and industrial chemicals (REACH) regulations are similar. Nevertheless, some particular aspects and requirements on the effect and the exposure assessment of biocides, PPPs and industrial chemicals differ. The table below illustrates some of the main differences (Table 2).

	Industrial Chemicals (REACH)	PPPs	Biocides
Emission	Assessed throughout the entire life cycle of the substance; tonnage-based approach	Mostly focused on the intended use (application and service life; consumption-based approach)	Mostly focused on the intended use (formulation of the biocidal product, application and service life; mainly consumption-based approach)
Exposure	Direct or indirect	Direct	Direct or indirect, depending on the product type
Effect and Risk Characterisation	PEC/PNEC approach; effects on indicator organisms and expected environmental exposures for defined environmental compartments are assessed; persistence and the potential for accumulation up the food chain are taken into account	TER (Toxicity Exposure Ratio), calculated for each species in the terrestrial compartment and for a given time period, which allows specific areas of concern to be identified for further refinement in a tiered approach	PEC/PNEC approach; effects on indicator organisms and expected environmental exposures for defined environmental compartments are assessed; persistence and the potential for accumulation up the food chain are taken into account

**Table 2. Some aspects of effect and the exposure assessment of biocides, PPPs and industrial chemicals**

#### 3.2 Species representativeness and sensitivity

The choice of species to be assessed and ecosystem functions to be protected is seen to be dependent on the potential route of exposure and impairment of ecosystem functions/services. This demonstrates the recognised perception of the link “species (biodiversity) – functions - services” and, implicitly, on how the use of the ecosystem service concept can/should be used to tailor the risk assessment.

The choice of species should also be specific to the regulatory schemes (i.e. plant protection products (PPPs), biocides, industrial chemicals (REACH)), wherein the species, functions and effect endpoints selected will be useful for relevant regulatory decision-making. Additionally, it was suggested that efforts for a harmonisation across different regulations should exist (e.g. in adopting similar risk characterisation approaches and assessment factors whenever relevant).

The main ecosystem **functions** traditionally considered for the selection of test species were the decomposition of organic matter, nutrient cycling, water storage and natural attenuation; these functions can be linked to relevant ecosystem services. Nevertheless, other services such as soil formation or pest control, and their related ecosystem functions, can also be very relevant triggering certain assessments. In terms of **taxonomic groups**, key drivers for these functions were identified: plants, invertebrates (both in-soil and epigeic) and microorganisms (bacteria and fungi, including mycorrhiza). Selection of test species could be done based not only on their role in the ecosystem, but also on the vulnerability concept (sensitivity and probability of exposure). This could be done based on behavioural and physiological traits for a broader range of relevant test-species. An appropriate test battery could be customised on a case-by-case basis, according to the physico-chemical properties of the substance.

Despite the need to assess the effects on organisms from different trophic groups and having different routes of exposure, the invertebrate groups most commonly referred are the ones usually used: earthworms/enchytraeids, collembolans, mites, and, to a lesser extent, larger detritivores (isopods) and predators (spiders, beetles).

The selection of test species included a combination of relevance, availability and practicalities; it should be noted that the selection has not always been explained in a transparent way. Larval stages of different insect species with part of their life cycle in soil were also noted. Testing at community level (enhanced laboratory tests, mesocosms) could also present a way to assess effects of interactions between species when exposed to chemicals.

For microorganisms, it was stressed that due to the unrecognised genetic diversity and the high functional redundancy for broad-scale processes (e.g. carbon transformation, ammonification) interest should focus on functional groups ensuring narrow niche processes (i.e. nitrification, denitrification, N<sub>2</sub>-fixation, sulphur-cycle, methane oxidation). These microorganism groups responsible for the above-mentioned processes could have a lower level of functional redundancy (lower diversity), and the functional significance of diversity shifts or losses after maximum exposure could be addressed.

**Exposure routes to be considered** include e.g. contact with soil, litter and/or soil pore water, ingestion of soil, and diet (litter and prey for predators). Regarding the **habitat(s)**, for PPPs the in-field assessment is considered the primary target, while an off-field risk assessment should be performed with the aim to protect biodiversity.

For all three regulatory frameworks (PPP, Biocides and REACH), persistence is not the only trigger for testing (as it was until 2014 in practice for the PPP Regulation), but the selection of test species should be also linked to the toxic mode of action of the substance as well as the sensitivity of the species/organism group.

For many non-persistent substances other species/groups should be tested, implicitly indicating that testing earthworms is not protective enough for other soil organisms with a different taxonomy. Additionally, testing other soil fauna groups (detritivores, insects) could be a way to take interspecies variability into account and to minimise uncertainties due to extrapolations. On the other hand, the need to make a comparative analysis of the sensitivity of tested species (mainly earthworms) and other groups before requiring

more tests may also be needed. For PPPs, testing of other species (*Folsomia* sp., *Hypoaspis* sp.) is already included in the new data requirements.

In relation to **the representativeness of currently tested species in the framework of approving PPPs**, it was noted that the current data requirements (testing earthworms, collembolans, mites and microorganisms) provide a sufficient level of protection towards soil functions and ecosystem services, including soil formation (as this service is the result of the activity of soil organisms that are tested).

On the other hand, there are also views that the current test battery is not protective enough because several organism groups playing a key role in different ecosystem services are not represented. There is a need to establish specific protection goals with a strong link between key ecosystem services and soil functions and the selection of test species. Another issue raised was the fact that some of the species/organisms tested, although being key drivers, are not the most sensitive to certain classes of PPPs (the case of earthworms for insecticides). Therefore, there is a need to include more test species/organism groups (e.g. organisms embracing different sensitivity and different mechanisms of toxicity – isopods, snails, enchytraeids, insects) into the test batteries.

When dealing with **interspecies variability**, the species sensitivity distribution (SSD) approach was mentioned (also in the ecological risk assessment (ERA)). However, this could only be achieved by having a large data set for the assessed substance. There is a need for guidance to make the development of SSDs an achievable goal. If there are no sufficient data to produce an SSD, assessment factors (AFs) are used instead and could be coupled with testing of key species. Furthermore, it is recommended that currently used AFs should be validated and the associated uncertainties should be quantified.

The link between species variability and soil variability is also important, pin-pointing the question of extrapolating effects to natural soils from the artificial soil used in some laboratory tests. Collecting further data using other species and performing mesocosm studies is proposed; along with the correction of toxicity data to standard soil properties to account for other sources of variation (e.g. bioavailability).

### **3.3 Selection of the most appropriate test method(s): From effect (hazard) assessment to risk assessment**

#### **Long-term toxicity testing on soil organisms**

Long-term toxicity testing should always be conducted for several reasons. First of all, long-term tests were found to provide more information (e.g. reproductive effects) and were also protective for acute effects. It was also noted that short-term tests on soil-dwelling organisms were usually not very sensitive. Moreover, long-term tests are environmentally more relevant, as they cover chronic sub-lethal (e.g. reproductive) endpoints and can address potential delayed responses caused even by short exposure as well as repeated pulses. For long-term multi-species test, the ultimate protection goals for ERA (i.e. protection of populations, communities and ecosystems) can also be measured directly.

This approach has been considered for PPPs where, according to the most recent version of the data requirements (Regulation EU/283/2013), only long-term tests are required. Finally, effects at higher levels of biological organisation could also be predicted by integrating these measures into relevant mechanistic effect models.

On the other hand, there is a view that long-term tests should be performed only when long-term exposure is expected. The following parameters are suggested as potential triggers for long-term tests in soil:

- compounds with high degradation time (DT50) in soil;
- compounds with potential for bioaccumulation;
- compounds with strong adsorption capacity;
- when continuous or multiple exposure can be expected;
- when a relevant metabolite cannot be tested separately;
- when no acute toxicity is observed, but impact on fertility and metabolism is expected.

Some experts propose a tiered approach, where acute toxicity testing should be used for screening only. In this case, the long-term testing should be done if the lower tier risk assessments indicate a long-term risk to the organism with no recovery potential (i.e. via lab-based multi-generation approaches). Low and intermediate risk assessment tiers would need to be appropriately calibrated to provide an efficient and protective risk assessment. Moreover, long-term tests were found to be necessary when a risk cannot be excluded using validated short-term test(s), are with agreed AFs (e.g. under REACH and biocides RCR > 1). The uses of the substance could also help on deciding between performing acute and long-term tests.

In addition, short-term bioassay(s) would need to be developed for PICT (Pollution Inducing Community Tolerance) to assess tolerance of community-mediated functional processes (e.g. carbon mineralisation, ammonification, nitrification, denitrification and iron-oxidation).

### **Soil microorganisms**

Generally, soil microbial community is still considered as a black box. However, several test methods are available to measure both the structure and function of the soil microbial communities. The method applied should take into account specific protection goals, substance properties, and its use.

In general, nitrogen and carbon transformation test guidelines (OECD 216/217) are considered as suitable but not always sufficient to assess the risk of a substance to soil microorganisms. These methods were seen as appropriate for biocides, industrial chemicals (REACH), PPPs, and the ecosystem services concept.

Both inhibition and stimulation of essential soil microbial processes should be considered, as all effects (positive or negative) should be seen as a disturbance of soil functioning and represent an impact and change from the "steady state". Moreover, increase in nitrification/carbon dioxide release could lead to an increase in decomposition of organic substances and changes in the composition of the local soil.

A 'positive' effect could lead to inhibition or alteration of other processes, or to change of the microbial community structure. For example, all effects (decreases or increases) are considered as a relevant effect for biocides. On the other hand, increases in activity leading to stimulation in mineralisation processes was seen as a short-term effect due to increased amounts of nutrients for the microorganisms (but not affecting the soil function as such).

Considering that nitrogen and carbon transformation are not the only relevant soil microbial-mediated processes, alternative test methods were proposed for assessment of microbial effects in soil:

- Potential nitrification rate (as in the metal risk assessment);
- Bioassays determining effects on nitrogen and carbon cycling;

- Minicontainer test, Organic matter breakdown;
- Microbial activity: Substrate Induced Respiration (SIR) test, and ATP;
- Soil microbial biomass;
- Structure of soil microflora;
- Several biodiversity indicators, including functional diversity, as listed in the recent FP7 project (Ecofinders).

Due to functional redundancy, methods investigating effects at structural level indicators were seen as more reliable since effects may stay "hidden" when the studied function remains (but the microbial diversity may be highly affected). Therefore, short-term effects on microbial communities (both in terms of diversity and function) should be investigated, since even a recovery of the function can indicate a narrowing of the community which almost certainly shows a system less resilient to additional stressors (e.g. climate change).

Some aspects to be considered when developing specified protection goals were identified:

- Fertility and agronomic function of soil;
- Biodiversity (other test methods than mineralisation should be used);
- Structural and functional diversity;
- Microbial activity;
- Consideration of relevance in local versus landscape effects.

However, regardless of the selected test method, it has to be taken into account that soil characteristics such as pH and soil composition affect the exposure and interaction between the chemical and soil microorganisms.

### **Bioavailability in hazard assessment**

When addressing applicability of the test methods it is important to discuss how to account for bioavailability in the soil hazard characterisation. Even if the definition of bioavailability has to be improved, bioavailability should be taken into account in mesocosms and field validation studies. Moreover, experimental studies could be developed to estimate the bioavailability of the substance in the soil and/or in the organism. As an example, extraction protocols performed under acidic conditions could be proposed to estimate the bioavailability of the compound in the gut of earthworms.

It is still not clear how to determine the highest realistic bioavailability that is not equal to 100% for every potentially exposed soil type. Using an average for all soil types would clearly result in an underestimation of the risk for certain types of soil. Conversely, it is possible that substances which would bind tightly to soil particles would not be bioavailable anymore.

It is also important to stress that bioavailability should be considered not only as dependent on  $K_{ow}$ ,  $K_{oc}$ , etc., but also on the distribution of the substance, the species tested and the location of the soil organism (including their interaction with the chemical, e.g. via feeding). For example, rain could facilitate transport of substances to macropores where they would "stick" preferentially in burrow walls coated with soil organic matter. In this case, worms living in those burrows (e.g. *Lumbricus terrestris*) would be more exposed than worms crawling around in the soil (e.g. *Octolasion cyaneum*). Moreover, the activity pattern of soil organisms (e.g. low activity periods of diapause or quiescence) could also affect bioavailability of the substances from the soil.

For PPPs, there are guidance documents such as the bird and mammals guidance that includes some calculation proposals on a practical basis. There is also a bioaccumulation



tier 1 test for earthworms and enchytraeids that can be used to feed-in the data in these equations rather than the default values, which are always more conservative.

Further discussion is needed to identify whether exposure within current standard soil test guidelines is sufficiently representative of most field situations and, if not, whether any suitable corrections could easily be made.

The use of AFs is also important. These were proposed to be used alone or in combination with study results, if enough knowledge about the proper factor is available. Several conditions were identified:

- In PPPs framework, if artificial soil is used for testing, only 2-5% peat content should be used. The default correction factor of 2 should be removed if measured evidence shows similar bioavailability in different natural soils from agricultural areas;
- In biocides, tests in soil organisms are required if the risk assessment for the terrestrial compartment, based on the equilibrium partitioning method indicates a concern for the terrestrial compartment, or if there is direct or long-term exposure. For substances with strong adsorptive properties, special consideration is given (e.g. an additional AF of 10 is applied).
- In the REACH framework for substances with strong adsorptive properties, special consideration is given (e.g. an additional AF of 10 is applied).

Therefore, the use of AFs could be investigated to take bioavailability into account.

Models were identified as potential tools to predict bioavailability to identify key conditions (e.g. pH < 5) for different classes of compounds and then potentially apply an assessment factor. There are concerns on how an AF could be flexible enough to address variability in bioavailability under different environmental conditions. Uncertainties related to bioavailability issues could be accounted for by linking exposure to effect through toxicokinetic-toxicodynamic (TK-TD) studies and subsequent modelling. Using mechanistically-based effect models such as TK-TD or population models may not necessarily decrease uncertainty, but would visualise otherwise hidden uncertainties and force us to be explicit about how we deal with them. Application of (mechanistic, semi-mechanistic or empirical) bioavailability models linked to soil parameters and validated in representative soils also represents a potential tool to address bioavailability.

QSARs might also be useful tools to address bioavailability (e.g. QSAR coupling molecular, physico-chemical and biological endpoints). Structural equation modelling (SEM) approaches could also be used<sup>5</sup>.

There are several illustrations for how bioavailability of metals can be incorporated into soil risk assessments. It is important to understand that effects are difficult to predict based on total soil concentrations.

To assess the bioavailability of metals in soils, two phenomena on the ecotoxicity of metals to soil organisms have to be considered:

- The bioavailability and toxicity of metals to soil organisms is dependent on the equilibration time of metals in soil and the leaching of excess ions. Toxicity response from tests under typical laboratory conditions (i.e. no leaching and a maximum of a few days equilibration after spiking with a soluble metal source

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<sup>5</sup> There are CEFIC LRI project s currently running that address how to assess the effect of bioavailability on toxicity of a chemical (ECO-25) and also how to predict bioavailability using QSAR tools based on structural alerts (ECO-24)

- before the start of the ecotoxicity assay) and from tests under field conditions (slow accumulation of metals, long-term equilibration, leaching through percolating rain water) should be compared to derive an AF for this discrepancy.
- The toxicity response is dependent on the soil physico-chemistry (e.g. pH, cation exchange capacity, organic carbon content, clay content). Toxicity should be tested in a set of soils covering a representative range of soil properties to derive regression models between toxicity and soil properties.

Therefore, soil-specific quality standards corrected for bioavailability are calculated by applying bioavailability corrections that account for:

- (i) differences in metal toxicity between freshly spiked soils and field contaminated soil, and
- (ii) effect of soil properties on the bioavailability and toxicity of metals.

For several metals (Cd, Co, Cu, Pb, Mo, Ni and Zn) there are models, tools and guidance available to assess the bioavailability and ageing of metals in the environment<sup>6,7,8</sup>. A summary of the available models is found in Smolders et al. (2009)<sup>9</sup>. These models have been applied in the REACH risk assessments of the above metals. Corrections for bioavailability are made at the local, regional and EU level, using geo-references and harmonised data on the soil parameters influencing bioavailability, available from the GEMAS database.

### **Exposure aspects in laboratory and field ecotoxicity studies**

It was noted that for fertilisers in most cases ecotoxicological studies in soil are not needed due to their properties (e.g. highly soluble, not persistent). If the studies are needed, the equilibrium-partitioning method seems to work well.

For PPPs, testing exposure is not analytically verified and nominal concentrations are used. This means that the predicted environmental concentration (PEC) is calculated (in mg/kg soil dry weight) based on the applied amount in the field and some specific factors, such as soil depth and bulk density.

For each test, the respective amount per soil sample in the individual test vessels is calculated, and this amount is weighed-in. Assuming that this is done under the conditions of Good Laboratory Practice (GLP), no further analytical verification was even considered necessary. This could be seen as the most conservative approach (i.e. 100% of the applied amount ending up in the test vessel, evenly distributed in the soil sample). Sometimes this approach is seen as too conservative, at least in higher-tiers (intermediate between laboratory and semi-field tests) where degradation or ageing of the chemical during the test should be considered (time-weighted (TWA) average concentrations might also be an option).

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<sup>6</sup> Metals Environmental Risk Assessment Guidance (MERAG, <http://www.icmm.com/page/1185/metals-environmental-risk-assessment-guidance-merag>)

<sup>7</sup> US Environmental Protection Agency. 2007. Framework for metals risk assessment: USEPA Office of the Science Advisor, Risk Assessment Forum, Washington DC. EPA 120/R-07/001. <http://www2.epa.gov/sites/production/files/2013-09/documents/metals-risk-assessment-final.pdf>

<sup>8</sup> PNEC value calculator for these metals (<http://www.arche-consulting.be/en/our-tools/soil-pnec-calculator/>).

<sup>9</sup> Smolders E, Oorts K, Van Sprang P, Schoeters I, Janssen CR, McGrath SP, McLaughlin MJ. 2009. Toxicity of trace metals in soil as affected by soil type and aging after contamination: Using calibrated bioavailability models to set ecological soil standards. *Environ Toxicol Chem* 28: 1633–1642.

This could lead to the conclusion that measuring exposure during the test would be more realistic. It could be done, for example, in its own test vessels run in parallel to those with organisms. There is however, no consensus on when to measure it: only at the beginning, at the end or in between (measurements of stock solutions did not get much support). It is also not clear how to implement this information in risk assessment procedures.

The situation is quite different for metals compared to organic chemicals, mainly due to the higher amount of information regarding their behaviour in the soil. Free metal ions in the soil pore water represent the available fraction that is causing toxicity. Despite the fact that within the last 15 years many different extraction methods have been proposed, there is still no standard method applicable to most metals and soil types, meaning that these approaches are rarely (if at all) used in risk assessment. Instead, it seems that measuring the total metal concentration in soil and using the bioavailability models and so-called leaching/ageing-factors to take bioavailability into account is right now the most appropriate approach. However, in the long run the determination of the PEC (and also the PNEC) as a percentage of the labile form is desirable.

It is assumed that the bioavailable fraction of a chemical is the one relevant for risk assessment, meaning that taking bioavailability into account would considerably improve risk assessment in soil. However, with the exception of the discussion on metals almost no detailed proposals were made on how this could be done in practice – one exception was the proposal to exclude non-extractable residues (NERs) from the bioavailable fraction.

Since soil properties have a strong effect on the fate and availability of chemicals (and on the behaviour of test organisms), “representative” soils have to be identified, well characterised and recommended even in lower tier testing. Finally, there is one special case: when determining exposure of plants, the application rate is used. However, since exposure might be highest at the middle part of the stem (i.e. decreasing to the top and base) more elaborated estimates should be developed.

All of the above refers to laboratory testing. Regarding field studies there is no consensus on whether exposure in the field should be measured in the study (the earthworm field test was mentioned as an example for this approach). To facilitate the evaluation of these measurements, information from higher-tier fate studies should be used more intensively than in the past.

### **Ecological modelling software tools used in soil ERA**

There is a common opinion that modelling tools will play a big(ger) role in risk assessment procedures in the future (see Hunka et al. 2013<sup>10</sup>). At the same time, it is stated that in the different areas (e.g. PPPs, fertilisers) there is not much going-on in developing, validating or even using such models. Validation of effect models is in its early stages, despite recent activities of different stakeholders, such as the European Commission (FP7 project CREAM), SETAC (Modelink workshops), or EFSA (publishing minimum standards of good modelling practice).

Some favour the opinion that modelling is too complex for regulatory purposes (test and field data are considered to be more robust) and not protective enough (FOCUS SW/GW is provided as an example). On the other hand, those who favour the use of models in

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<sup>10</sup> Hunka A, Meli M, Thit A, Palmqvist A, Thorbek P, Forbes V. 2013. Stakeholders' perspective on ecological modelling in environmental risk assessment of pesticides: Challenges and opportunities. *Risk Analysis* 33: 68–79.

regulatory ERA often refer to good experiences made with fate models (e.g. ESCAPE 2.0, GREAT-ER, SESOL, PRZM). TK-TD models as well as the EPM are mentioned in this context.

The PNEC calculator developed by a consulting company and specifically designed to help perform an ERA for metals<sup>75</sup> under REACH was recommended for consideration, as well as the target lipid model for soils and sediments (Redman et al. (2014)<sup>11</sup>). Like in all comparable approaches, this tool strongly focuses on the inclusion of different soil properties. In fact, such models address mainly the bioavailability of chemicals, using both their properties as well as environmental variables. In general, both SSDs as well as multivariate tools were recommended as standards for effect evaluation.

Another "key term" linked with great expectations is ecological modelling, focusing on population dynamics. Different models for Collembola and earthworms are available, if not yet validated. Microbes are also mentioned as an organism group that could/should be modelled. Developing ecological population models for anecic earthworm species is recommended because of their ecological relevance as key species (i.e. ecosystem engineers). There is an opinion that ecological population models probably have the highest value when addressing the landscape level, incorporating different soil types as well as also long-term population effects and the potential for recovery.

It seems that there are high expectations regarding the use of modelling in soil ERA but further efforts are needed to develop, validate and standardise these tools.

### **Ecological assessments at landscape level**

Apart from the case of soil organisms with limited mobility, there is a general agreement regarding inclusion of the landscape level to the ecological risk assessment. This topic (with the exception of the PPPs community) has not been discussed very much so far.

Two (groups of) tools are seen as potentially useful in this context: modelling and field surveys. For both approaches a lot of basic ecological and taxonomic knowledge is necessary, and this kind of information is very heterogeneously available in Europe. This is especially true for the soil compartment, where basic properties (including the distribution of chemicals, particularly metals) have been mapped. Only in the last years has harmonised data become available at the European scale (e.g. GEMAS, LUCAS).

Even worse is the situation regarding soil biology where (despite some recent efforts, e.g. via FP7 projects) the distribution, diversity and abundance of many organism groups in wide parts of Europe is only scarcely known.

Modelling is most often mentioned as a useful tool for the landscape level, but in most cases it is not really clear to what exactly "landscape models" are referring to. Ecological modelling (niche modelling, habitat suitability) could be used as a starting point. One example for a model successfully predicting distribution patterns of invertebrates, mainly bees, is InVEST (integrating valuation of environmental services and tradeoffs), which may be modified for soil organisms.

More ideas are provided when it comes to existing models already used on the landscape level, but only rarely in the context of ERA: here both geographical information systems (GIS) and climate models (including the distribution of chemicals via air, e.g. fertiliser

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<sup>11</sup> Redman AD, Parkerton TF, Paumen ML, McGrath JA, den Haan K, Di Toro DM. 2014. Extension and validation of the target lipid model for deriving predicted no-effect concentrations for soils and sediments. *Environ Toxicol Chem* 33: 2679–2687.

emissions) have to be mentioned. In the context of adapting the ecosystem services approach, such modelling exercises are becoming more and more popular, meaning that they could be used to assess the impact of individual PPPs or agricultural practice in general. However, the lack of appropriate data sets for validating these models and the often inappropriate temporal and spatial resolution presents serious obstacles.

Field surveys/monitoring are proposed both as a method to validate modelling results as well as a source of basic ecological/biodiversity data. Especially the latter are difficult to obtain due to the decreasing number of experts in this field. However, current increases in the use of barcoding and meta-barcoding approaches may mean that, by using these new methods, not only shifts in diversity after chemical impact but also their functional significance could be evaluated. In this context, a European network of permanent soil monitoring sites (already existing in a few countries) in different land use types would be helpful, where both exposure and effects could be determined at the same time and place.

Some ideas presented seem to be difficult to be included in ERA on the landscape level (e.g. PICT, EUSES (European Union System for the Evaluation of Substances), IBM (individual-based models)). It seems that ecological risk assessments on the landscape level are useful, but that more discussion and research is needed for its implementation into regulatory activities.

### **Tools and tests to be used as intermediate tiers from lab to field in the effect assessment**

The need to include an intermediate tier between laboratory tests and field studies in soil risk assessment for PPPs is strongly supported.

The proposed tools could be classified in the following four groups (starting with laboratory level methods and ending with modelling approaches):

- Complex laboratory studies: multi-generation tests (probably with species already used as standard test organisms) or microcosms/mesocosms. The latter could be used for including species-interaction as a new endpoint. They could be combined with modified exposure conditions, e.g. using aged residues or specific PPP formulations such as granules. The duration of the test should be longer than in the commonly used tests. Even a whole tiered strategy could be an option, classifying the methods described here so far as laboratory level, followed by "real" intermediate tests, such as the Terrestrial Model Ecosystems (TME), and the field as the highest tier.
- Semi-field test methods: Complex "mesocosms" are important to consider because of their community approach and ecological relevance (e.g. regarding the inclusion of species interactions, food-chain studies or functional tests like the Bait-Lamina-Method). TME is most frequently noted, probably because a draft test guideline is available.
- Elaborated test result evaluations: The better use of already existing laboratory test results is the reason why SSDs are recommended as an intermediate tool. However, it is clear that SSDs require more data than usually available. New tests with other species have to be developed, standardised and validated before they can be used for this purpose.
- Modelling: Several proposals exist in this area, starting with relatively simple models (e.g. TK-TD or IBM), and ending with quite complex predator-prey or community models. Mechanistic effect models could also be used to select appropriate hypotheses which could be tested in semi-field or field tests.

Independently from the respective methods, it was clear that all these tools can only be used in regulatory risk assessment after they have been validated using different

scenarios, preferably by the OECD. Actually, standardisation of these approaches is seen as an urgent necessity. Assuming that this work has successfully been done, the inclusion of intermediate methods as part of a tiered testing strategy is generally supported.

### **3.4 Challenges for soil toxicity assessment and soil classification criteria**

#### **Links between exposure and effect assessment in the context of soil risk assessment**

There is a common opinion that there is a need to improve the current link between exposure and effect assessments. One of the first steps that can improve the integration of exposure and effects assessments is the use of exposure assessments to select appropriate/relevant test species for effects assessment. Not every possible non-target organism is exposed in the same way after the soil has been exposed to a hazardous substance. The most exposed trophic level and/or taxonomic groups should be determined based on exposure pathways and the substance's fate in the soil, and within those, suitable model-organisms should be selected for effects testing, considering the mode of action and expected sensitivity of different taxa/species when the information is available.

It is observed that very often ecotoxicity studies are made with nominal concentrations instead of measured concentrations. Measured concentrations and concentrations corresponding to the real exposure levels would provide more realistic information on the exposure and effect assessment. Both exposure and effect assessment would need to be based on the same 'form' and speciation of the substance.

Another way to better link exposure and effects assessment is to ensure that both are based on comparable dose estimates. Currently, both exposure and effects assessments are generally based on total soil concentrations. Not only the total soil concentration of the substance should be taken into account, but also the extractable, available and/or bioavailable fraction. Along this line, tissue residue determinations can help define the chemical bioavailable fraction. Aging, leaching and fixation effects are also important, especially in metals and metalloid assessment. Ecoregion-type assessments and "geochemical mapping" have been recommended for metals, since different species exist on different soils and these species may be adapted to different metals.

This link can also be improved by considering soil properties, such as soil type, organic matter (OM) and organic carbon (OC) content. For example, normalising exposure and effects data for soil OC/OM, the application of an AF for high OC/OM soils and high Log  $K_{ow}$  for organic chemicals could improve the assessment. It could be worthwhile to consider the concentrations in soil pore water and/or to test endpoints in pore water concentration followed by determining the route that poses the highest risk.

The link from laboratory data to field data should be improved by, e.g. establishing more realistic exposure scenarios in the ecotoxicological test systems (including whole community or field studies) and more realistic exposure measurements and calculations. More flexibility is needed in lab, semi-field, and field test systems, and ecological modelling in risk assessment should be considered. The need for adoption of monitoring schemes, especially if used for validation of modelling activities was also observed.

In addition, relevant (or worst-case) exposure scenarios, including both temporal and spatial variability (e.g. short versus long-term equilibration or zonal assessment), can be directly coupled to effects assessments in certain types of mechanist effects models. For

example, toxicokinetic-toxicodynamic models may allow predicting higher-level effects combined with population models.

Challenges in considering exposure and effects of multi-constituent substances, co-assessment of metabolites and chemical mixtures should also be pointed out. More evaluation work is required on measures of combined exposure in soils (e.g. sum of PEC/PNEC ratios, msPAF<sup>12</sup> for data-rich substances) to ascertain how well they perform in a risk assessment context. For PPPs, PEC<sub>soil</sub> is calculated according to the recommendations of the FOCUS soil guidance (1997). The new guidance document "Predicting environmental concentrations of active substances of PPPs and their transformation product in soil" will improve the ERA, since it will be performed through the TER calculations (ecotoxicological endpoint/PEC value). This system can be improved by introducing RACs<sup>13</sup> comparable to the new aquatic guidance document.

Finally, attention should be given to indirect exposure, as it is not always properly taken into account. For biocides, since the waiving of testing is linked to exposure, in the case of indirect exposure soil toxicity, tests are not required. Under the REACH Regulation, soil test requirements depend on the tonnage and on the direct or indirect exposure.

There is a common understanding that to achieve most of these improvements with a certain degree of harmonisation, development of new testing guidelines and a wider array of model-organisms is needed.

### **Adequate information supporting low toxicity to soil organisms when no aquatic toxicity is observed and no aquatic PNEC can be derived**

This issue is considered outside the remit of the PPPs regulatory framework where toxicity tests with soil organisms are always required, but is relevant for the other frameworks.

Overall, extrapolation from aquatic toxicity data to soil data seems problematic (unless where there is supporting scientific evidence). Some would only support it in specific cases, for example, for worms which have fast body-water exchange (in humid soils) and could resemble water organisms. A more reliable approach could be an extrapolation from toxicity data on non-target arthropods, i.e. from mites and aphids. Based on their experience in chemical risk assessment, some experts are of the common opinion that no aquatic toxicity information can be considered adequate to prove low toxicity to soil organisms.

A practical solution could be to perform toxicity tests on a few sensitive species or on key organisms that show no long-term (generational) impacts.

Screening tests could help to address relevant species and taxonomic groups in terms of soil toxicity (e.g. soil microorganisms, appropriate microtox test kit for soil samples, earthworms), fate and behaviour of the substances (e.g. capacity for soil adsorption), and possible exposure pathways (provided that there is a blank available for calibration of the area under investigation).

Extrapolation from aquatic toxicity data to soil data could be used for certain metabolites, providing that the same metabolites are formed in different soil types and environmental compartments. It is important to note that microbial functions may not be covered here.

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<sup>12</sup> msPAF = multisubstance Potentially Affected Fraction of species

<sup>13</sup> RAC = Regulatory Acceptable Concentration

Finally, the equilibrium partitioning approach with a sufficiently large AF could be applied. For the case of hydrocarbons, CTLBB (critical target lipid body burden) modelling can be performed using the TLM (target lipid model). This would help determine potential toxicity occurring above water solubility, meaning that the toxicity in soil would be unlikely if pore water exposure is assumed to be the main exposure route. However, exposure via ingestion is not addressed and should be considered if relevant (e.g. for substances with high  $K_{ow}$ ).

Although the need for further data and research on potential alternatives to testing with soil organisms is considered necessary, read-across with similar substances for which an aquatic PNEC is derived is still considered as a possible alternative to determine the toxicity to soil organisms when no aquatic toxicity is observed. This could be further supported by identifying the mode of action of the substance. Finally, development of QSARs for terrestrial species could also be considered.

### **Need for development of toxicity cut-off values for soil organisms which would be comparable with the quantitative T criteria in the context of PBT assessment under REACH**

When thinking about challenges for an assessment of soil toxicity, it is necessary to consider a need for a quantitative T criterion development for soil organisms in the context of the PBT assessment under REACH. Some views find development of cut-off values unnecessary or problematic due to the lack of the political interest to extend the current 'T' hazard criteria beyond the obligations of the current legal texts (based on marine or freshwater organisms and to an extent birds). Although it is considered to be an ambitious and challenging task, further discussion was seen beneficial.

When considering toxicity cut-off values for soil organisms, we have to bear in mind that the literature data on soil organisms is not as rich as that for aquatic toxicity. To derive the toxicity cut-off values for soil organisms, a thorough analysis of available soil toxicity data (including the pesticides database and mammalian data) with the help of modelling tools should be performed first. The EPM could also be considered. The lack of aquatic toxicity could be indicative of a low toxic potential to soil organisms except when the lack of waterborne toxicity is linked to very low aquatic solubility (ECETOC Task Force exists for this topic).

Soil is a very heterogeneous compartment and the outcome of soil toxicity studies based on total substance concentrations does not only depend on the intrinsic toxicity of a substance, but also on its behaviour and partitioning (and hence bioavailability) in soil. This complexity can be addressed e.g. by establishing different cut-off values for different soil types. Another approach could be to consider the partitioning criteria together with aquatic toxicity criteria, instead of soil toxicity criteria.

The selection of representative species is also considered very important. The cut-off toxicity value should probably be adapted for each species. All trophic levels should be taken into account. For biocides and REACH substances, a very small data set is available compared to PPP dossiers. To keep a harmonised approach on 'T' criteria, the data set should be the same for all regulations. In all cases, robust studies should be performed to have an idea on the impact of such decision.

There is also a suggestion to provide a long-term NOEC-based criterion similar to that for marine/freshwater organisms. Long-term would need to be defined, e.g. chronic in the context of existing standard toxicity tests such as 28-day earthworm reproduction, or a longer (more realistic), e.g. multi-species or multi-generation tests. The latter would be less acceptable in terms of costs but scientifically more robust.



There are some expert opinions that criticise the concept of deriving toxicity cut-off values, as a solely hazard-driven approach does not reflect general risk concept (i.e., risk being a function of both exposure and hazard). In this aspect, even very toxic chemicals will not cause risk if they are used in small amounts or are unlikely to end up in the environment at concentrations high enough to pose a risk. Therefore, the cut-off toxicity criteria should be accompanied by P and B criteria (P for soil is already part of the PBT and vPvB definitions in REACH and Biocides) and preferably compared with predicted worst-case environmental concentrations.

### **Need for development of criteria for classification and labelling of substances as hazardous to the terrestrial environment**

In general there seems to be no strong interest in having criteria for classification and labelling for the terrestrial environment, i.e. to extend the frame of the current CLP Regulation and Globally Harmonised System (GHS) to terrestrial wildlife.

Hazard classification should be determined on the basis of intrinsic characteristics for each substance, and the determining intrinsic toxicity to soil-dwelling organisms is found to be very challenging due to the contaminant - soil matrix interaction. It has been noted that, in terms of protecting our resources and ecosystem services, the use of the aquatic compartment as proxy for the soil compartment is not appropriate. A scheme for classification and labelling of substances with regard to soil toxicity would be relevant for all substances, but most important for substances most likely to end up in the soil compartment. However, fertiliser substances used to feed essential elements to the crops according to good agricultural practice should be exempted.

A useful resource for identifying elements to be evaluated when considering whether or not terrestrial classification is necessary (or even possible) is available for metals.<sup>14</sup>

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<sup>14</sup> Fairbrother A, Kapustka LA. 1997. Hazard Classification of Metals in Terrestrial Systems - A Discussion Paper. International Council on Metals and the Environment, 30 pp.