

SCIENTIFIC OPINION

Scientific Opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations of plant protection products in soil¹

EFSA Panel on Plant Protection Products and their Residues^{2, 3}

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ABSTRACT

Based on consultation with Member States, EFSA asked the Panel to prepare a revision of the Guidance Document on the persistence of plant protection products in soil (SANCO/9188VI/1997 of 12 July 2000) as scientific knowledge in this field has evolved in recent years. Therefore the Panel developed a revised methodology for the assessment of exposure of soil organisms to such products. Based on a previous Opinion of the Panel, this methodology has been developed both for the concentration in total soil and the concentration in the soil pore water. The goal of the exposure assessment has been chosen to be the 90th percentile of the exposure concentration in the intended area of use in each of the three regulatory geographical zones (North, Centre, South). The exposure-assessment methodology is restricted to spray applications to annual crops under conventional or reduced tillage (excluding tillage systems with ridges and furrows). The Panel proposes a tiered approach. Tier 1 is based on a simple analytical model. Tier 2A is based on simulations with numerical models. To keep the approach as simple as possible, the Panel based Tiers 1 and 2A for each regulatory zone on only one scenario each for the concentration in total soil and for that in pore water. These scenarios are to be used for all these annual crops and for all plant protection products in each regulatory zone. Tiers 2B and 2C are also based on the simple analytical model but in these tiers a specific crop or crop group and an individual plant protection product are considered. Tier 3 is based on simulations with numerical models but, as in Tiers 2B and 2C, a specific crop or crop group and a specific plant protection product are considered. All tiers aim to assess the same exposure assessment goal. Given the complexity of the calculations in the different tiers, efficient use of this tiered approach in the regulatory process is impossible without software tools. Therefore the Panel recommends developing user-friendly software tools for the calculation of the exposure concentrations in the different tiers.

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KEY WORDS

Exposure assessment, soil, plant protection products, soil organisms, ecotoxicological effects, tiered approaches, crop interception.

SUMMARY

The European Food Safety Authority (EFSA) asked the Panel on Plant Protection Products and their Residues to prepare a revision of the Guidance Document on persistence of plant protection products in soil (SANCO/9188VI/1997 of 12 July 2000) as scientific knowledge in this field has evolved in recent years. Therefore the Panel developed a revised methodology for the assessment of exposure of soil organisms to such substances, which is needed as part of the effect assessment for soil organisms. To ensure an adequate link between exposure and effect assessment, the Panel explored in a previous Opinion (EFSA, 2009) the ecotoxicologically relevant types of concentrations to be considered. As a result of this previous Opinion, the methodology is developed both for the concentration in total soil and that in the soil pore water.

Development of a scientific methodology for assessment of exposure of organisms to plant protection products and their soil metabolites requires a detailed definition of the exposure-assessment goal. This definition is a risk-management decision. The proposed methodology is provisionally based on the goal to assess the 90th-percentile concentration considering all agricultural fields within a regulatory zone (North, Centre, South) where the particular active ingredient is applied. This goal is considerably less differentiated in space than those for the current EU exposure-assessment methodologies for leaching to groundwater and exposure of aquatic organisms. This was done to keep the regulatory approach for exposure of organisms in soil as simple as possible.

The proposed exposure-assessment methodology is restricted to spray applications to annual crops under conventional or reduced tillage (excluding tillage systems with ridges and furrows). The Panel proposes to base this methodology on a tiered approach. Tier 1 is based on a simple analytical model. Tier 2A is based on simulations with numerical models. To keep the approach as simple as possible, the Panel based Tiers 1 and 2A for each regulatory zone on only one scenario each for the concentration in total soil and for that in pore water. These scenarios are to be used for all these annual crops and for all plant protection products in each regulatory zone. Tiers 2B and 2C are based again on the simple analytical model but in these tiers a specific crop or crop group and a specific plant protection product are considered. Tier 3 is based on simulations with numerical models but, as in Tiers 2B and 2C, a specific crop or crop group and a specific plant protection product are considered. All tiers aim to assess the same exposure endpoint, i.e. the 90th percentile of a certain type of concentration⁴ considering all agricultural fields within a regulatory zone where the particular active ingredient is applied.

Based on discussions at the IRIS workshop (attended by Member States and stakeholders), it was a boundary condition that the proposed exposure-assessment methodology can be applied by taking median or average substance properties (such as the degradation half-life in soil and the sorption coefficient) from the dossiers. Such substance properties are uncertain and inclusion of this uncertainty leads to probability density functions of concentrations that show more spread. As a consequence, this boundary condition led to the need to base the scenario-selection procedure on the 95th-percentile concentration instead of the 90th-percentile concentration.

There appeared to be distinct differences between the properties of the scenarios selected for (i) the concentration in total soil and (ii) the concentration in pore water. So it was necessary to use different scenarios for these different types of concentration.

Peak concentrations in total soil and in pore water were calculated with numerical models for the Tier-2A scenarios. The calculations were carried out for applications on bare soil in sugar beet and winter wheat for a number of example substances. The concentration differences between the three regulatory zones appeared to be no more than a factor of two. These differences are comparatively small in view of the considerable differences in climate and soil properties between the three zones.

⁴ Type of concentration is the concentration scenario considered in the risk assessment, e.g. the concentration in total soil averaged over the top 5 cm or the concentration in the pore water averaged over the top 20 cm.

The concentration in total soil decreased in the order North-Centre-South whereas the concentration in pore water usually decreased in the order South-Centre-North.

The area of the crop within a regulatory zone appeared to have a distinct effect on the 95th-percentile concentration. Therefore in the Tier-1 and Tier-2A assessments (which are based on the total area of annual crops in a zone), the concentrations have to be multiplied with a so-called 'crop extrapolation factor' to ensure that these assessments are conservative enough. This crop extrapolation factor depends on the type of concentration, the regulatory zone and the area of the crop considered. The Panel assessed this factor for 12 crops using maps of their density at a resolution of 1×1 km² for the whole EU and found the required factor to range from 1.02 to 1.79. If no map is available of the density of the particular crop, the crop factor has to be based on the 100th-percentile concentration considering the whole area of annual crops in a regulatory zone. The range of crop factors based on this 100th percentile was from 1.3 to 3.2. These findings indicate that the effect of the area of the crop on the exposure endpoint may be in the same range as the differences between the regulatory zones.

Tier-2A calculations carried out on a number of example substances, with the numerical models PEARL and PELMO, showed distinct differences between concentrations calculated with these models. So in tiers based on calculations with numerical models (Tiers 2A and 3), the choice of the model is also a source of uncertainty. If the margin of safety for the assessment of effects on organisms in soil is less than a factor of two, risk managers could consider the necessity of performing calculations with both PELMO and PEARL and of using the highest exposure concentration of the two models.

The Panel notes that other models are equally adequate and encourages the parameterising of the scenarios also for numerical models other than PELMO and PEARL. The only requirement is that the process descriptions in these numerical models have a similar or higher level of detail than those in PELMO and PEARL (PRZM and MACRO fulfill this requirement).

For active substances, registration dossiers contain at least four studies on the degradation half-life in soil and the sorption coefficient. The proposed exposure-assessment methodology is based on the use of the geomean of the relevant statistical population of these substance properties which may differ from the geomean of the sample population derived from the data in the dossier. The Panel developed a procedure to assess the uncertainty in the soil exposure concentrations resulting from the limited number of studies on the degradation half-life in soil and the sorption coefficient in the dossiers. Preliminary calculations showed that this uncertainty depends strongly on (i) the type of concentration, (ii) the substance properties, and (iii) the ecotoxicological averaging depth. In these calculations, it was assumed that only four studies were available for the degradation half-life in soil and the sorption coefficient and the uncertainty ranged from negligibly small to about 50% higher or lower concentrations. Using the above procedure, calculations on the uncertainty resulting from the available number of *DegT50* and *K_{om}* values in the dossier could be included on a routine basis in the exposure assessment if deemed necessary by the Standing Committee on Food Chain and Animal Health (SCFCAH).

The proposed exposure-assessment methodology is based on the population of all agricultural fields within a regulatory zone grown with the crop or group of crops that are considered for the plant protection product within the EU registration procedure. So to apply the exposure assessment methodology for EU registration, the list of possible annual crops for this registration has to be defined. This definition is a risk-management decision. The Panel recommends that the SCFCAH comes to a decision regarding this list of crops. After this decision, it is advisable to develop maps for as many of those crops as possible (if not yet available as a CAPRI crop), using the CAPRI methodology. It is recommended to do this at the same 1×1 km² scale as that used for this guidance development in order to facilitate use of these maps in higher tiers of the proposed methodology (these maps are likely to be useful also in other exposure-assessment methodologies).

The tiered approach contains many tiers and the procedures to be followed in each tier are complicated. Thus efficient use of the approach in regulatory practice is impossible without appropriate software tools. Therefore the Panel recommends developing user-friendly versions of numerical models that can calculate exposure concentrations for the six Tier-2A scenarios. Furthermore, the Panel recommends developing a single user-friendly software tool that can perform the following tasks: (i) calculation of the Tier-1 PECs, (ii) calculation of the Tier-2B 95th-percentile PECs, (iii) calculation of the Tier-2C 95th-percentile PECs using output from Tier-2A simulations for the soil load including wash-off, and (iv) selection of the grid cell corresponding to the 95th-percentile PEC as needed for the scenario development of Tier 3. When this tool becomes available, the Panel recommends checking iteratively the consistency of the tiered flow chart considering the three regulatory zones, all types of concentration, all relevant crops and the relevant range of substance properties.

The Panel recommends checking (using again this user-friendly tool) whether the proposed shift from the 90th to the 95th spatial percentile to account for the uncertainty in *DegT50* and *K_{om}* is appropriate considering the three regulatory zones, all types of concentration, all relevant crops and the relevant range of substance properties.

The development of the exposure-assessment methodology would have been much easier and much more straightforward if appropriate tools for spatially distributed modelling with numerical models had been available. Because this was not the case, the proposed methodology had to be based on a number of simplifying assumptions. The development of such tools has now become feasible since maps of relevant data are now available for the whole EU at a resolution of 1×1 km². Therefore the Panel recommends developing such tools.

The tiered approach to assess 90th-percentile concentrations has been developed considering only parent substances because developing a methodology that also included soil metabolites was considered too complex as appropriate tools for spatially distributed modelling with numerical models are not yet available. Nevertheless, the Panel also recommends using this tiered approach for soil metabolites in the absence of a better alternative. However, risk managers should be aware that there is no guarantee that exposure endpoints for soil metabolites are close to the 90th percentile.

The half-life for decline of the dislodgeable foliar residue (DFR) on plants, resulting from both degradation on plant surfaces and uptake by plants (but not considering losses due to volatilisation), is an input parameter for the numerical models, and may have a large effect on soil exposure concentrations of substances sprayed on full-grown crops. This half-life is not part of the EU data requirements and therefore is usually not available in dossiers; thus a default half-life is needed. The Panel recommends using a default half-life of 10 d (based on a previous EFSA Opinion). The Panel recommends the collection and analysis of all relevant literature data on the decline of the DFR in order to further underpin the default value of the DFR half-life.

The Panel recommends using an estimator of the median *K_{om}* for all exposure assessments (e.g. soil and aquatic organisms, leaching to groundwater) and using for that purpose either a bias-corrected geomean estimator or the conventional geomean.

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BACKGROUND AS PROVIDED BY EFSA

During the review process of the substances of the second list, several concerns were raised regarding the Guidance Document on persistence in soil. A number of Member states have expressed interest in a revision of the current Guidance Document on persistence in soil during the general consultation of Member States on Guidance Documents in answer to the request by the Director of Sciences of EFSA in letter 3 July 2006 sent *via* the Standing Committee on the Food Chain and Animal Health. Further the former EFSA PRAPeR Unit noted that the Guidance Document needed to be brought in line with the FOCUS degradation kinetics report (SANCO/100058/2005, version 2.0, June 2006).

FOCUS (1997) developed the first guidance at EU level for exposure assessment in soil. This included a simple approach for estimating PEC_{SOIL} but FOCUS (1997) did not develop first-tier scenarios (in contrast to subsequent FOCUS workgroups that developed such scenarios for surface water and groundwater as development of soil scenarios was a lower priority at that time). FOCUS (2006) developed detailed guidance on estimating degradation rate parameters from laboratory and field studies, but did not develop exposure scenarios. Nevertheless there is need for such scenarios in view of ongoing discussions in peer review experts groups regarding PEC_{SOIL} as current approaches at EU level just represent the range of climatic conditions covered by available field dissipation and/or accumulation studies and member states would like tools to be able to extrapolate to a wider range of climates present in the EU.

The existing Guidance Document on Persistence in Soil (9188/VI/97 rev 8) published in 2000 did not include scenarios. The intention with the new guidance document is to update the existing Guidance Document on Persistence in Soil to include European exposure scenarios for soil and to provide guidance on best practice for using the results of field experiments and soil accumulation studies in the exposure assessment.

The revision will not include guidance that is in the existing guidance document but has been replaced by newer guidance e.g. in FOCUS (2006). Some parts of the current guidance will not be considered in the revision e.g. for non-extractable residues, as these sections are better dealt with separately. The revision will also exclude risk-management guidance and hazard cut-offs e.g. PBT classification as this is not within the mandate given to EFSA.

Member States and stakeholders have been and will be consulted through web-conferences and stakeholder workshops to collect comments during the revision of the Guidance Document.

TERMS OF REFERENCE AS PROVIDED BY EFSA

The Scientific Panel on Plant Protection Products and their Residues (PPR Panel) of EFSA was asked in November 2007 by EFSA to prepare a revision of the Guidance Document on persistence in soil (SANCO/9188VI/1997 of 12 July 2000).

ASSESSMENT

1. INTRODUCTION

1.1. Background to development of the guidance

FOCUS (1997) developed the first guidance at the EU level for the exposure assessment of soil organisms to plant protection products. This included a simple approach for estimating PEC_{SOIL} (Predicted Environmental Concentration in soil) but it did not develop scenarios for numerical models (in contrast to subsequent FOCUS workgroups which developed such scenarios for surface water and groundwater). FOCUS (2006) developed detailed guidance on estimating degradation rate parameters from laboratory and field studies, but also did not develop exposure scenarios. Nevertheless there is need at the EU level for such scenarios in view of ongoing discussions in peer-review experts groups on PEC_{SOIL} . The existing Guidance Document on Persistence in Soil (9188/VI/97 rev 8) published in 2000 did not include scenarios. Therefore the Panel has revised the existing Guidance Document on Persistence in Soil by developing tiered exposure-assessment approaches for soil organisms in which European exposure scenarios play an important role. This approach is based on development of scenarios representing realistic worst-case conditions for the three regulatory zones North/Centre/South (Figure 1), as included in Annex 1 of the new regulation concerning the placing of plant protection products on the market (Anonymous, 2009).

EFSA (2010a) described the outline of the proposed guidance for the soil exposure assessment and indicated that the guidance will in the first instance be limited to spray applications to annual crops under conventional and reduced tillage (excluding tillage systems with ridges and furrows). EFSA (2010d) described how field dissipation studies can be used to refine the estimation of the half-life for degradation in the top 30 cm of soil at 20°C and moisture content at field capacity which is an important substance property in the tiered exposure-assessment approach. This document gives guidance for the soil-exposure assessment for these spray applications, this guidance being based on the tiered exposure-assessment scheme described in Chapter 2.



Figure 1: Map of the three regulatory zones used in the registration procedure of plant protection products in the EU.

1.2. General principles of tiered approaches

The Panel considers tiered approaches to be the basis of environmental risk-assessment schemes that support the registration of plant protection products. A tier is defined as a complete exposure or effect assessment resulting in an appropriate endpoint (in this case a PEC_{SOIL}). The concept of tiered approaches is to start with a simple conservative⁵ assessment and only to do additional more complex work if necessary (so implying a cost-effective procedure both for notifiers and regulatory agencies).

The general principles of tiered exposure approaches are:

- i. lower tiers are more conservative than higher tiers,
- ii. higher tiers are more realistic than lower tiers,
- iii. lower tiers usually require less effort than higher tiers
- iv. in each tier, all available relevant scientific information is used
- v. all tiers aim to assess the same exposure goal.

In short, the tiered exposure assessment needs to be internally consistent and cost-effective and to address the problem with higher accuracy and precision when going from lower to higher tiers. These principles permit moving directly to higher tiers without performing the assessments for all lower tiers.

1.3. Relationship between effect and exposure assessment in the guidance development

The guidance aims to develop exposure-assessment methodologies for assessment of ecotoxicological effects on soil organisms at the EU-level. So the exposure assessment is considered to be part of the assessment of terrestrial effects.

EFSA (2010c) described the framework for the risk assessment for aquatic and terrestrial organisms. The risk assessment requires two parallel tiered flow charts (Figure 2), one for the effect assessment

⁵ In the context of this Opinion, 'conservative' means 'on the safe side with respect to the risk assessment'.

and one for the exposure in the field. Each flow chart is based on a ‘reference tier’ to which lower tiers are calibrated; in the example shown, the reference tiers of the field-exposure and the effect flow charts are at exactly the same level. However, the reference tiers may be at different levels because both flow charts stand on their own and because it suffices if each flow chart is internally consistent.

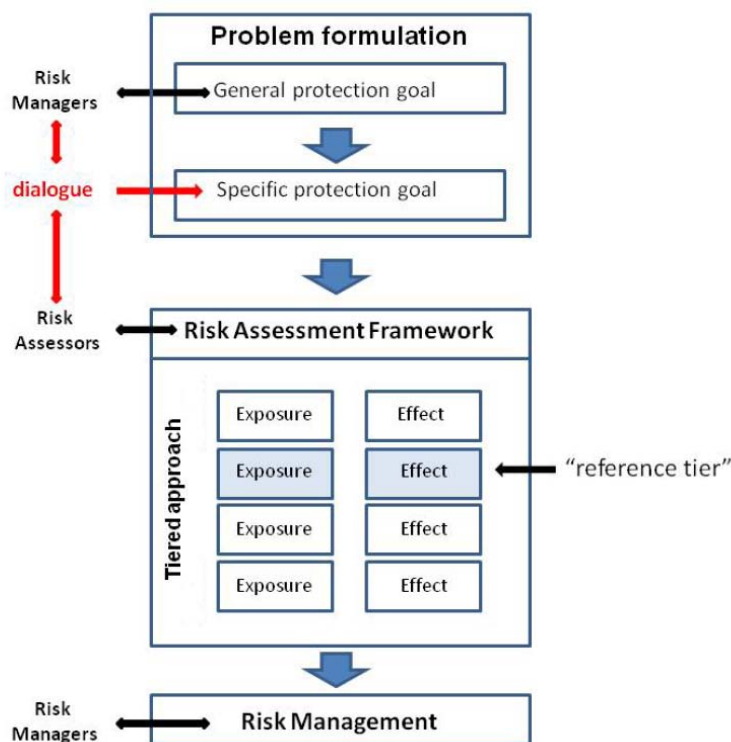


Figure 2: The tiered approach used in a risk-assessment framework and its relationship to problem formulation, protection goals and risk management in the process of developing both specific protection goals and risk-assessment guidance (adapted from EFSA, 2010c). Note that the ‘Exposure’ tiers in this scheme deal only with field exposure and not with exposure in ecotoxicological studies.

As described by EFSA (2010c), the risk assessment requires that the exposure assessment has to consider all kinds of concentration that are relevant for assessing these effects. These concentrations are called Ecotoxicologically Relevant types of Concentration (ERC), and they are determined by the protection goal (EFSA, 2010c).

Considering in more detail the interactions between the flow charts for field exposure and effect (Figure 3), there are of course only arrows from field-exposure to effect tiers. All options for delivery of field-exposure assessments to effect tiers are possible (called the ‘criss-cross’ model by Boesten *et al.*, 2007). This is required to be flexible and cost-effective.

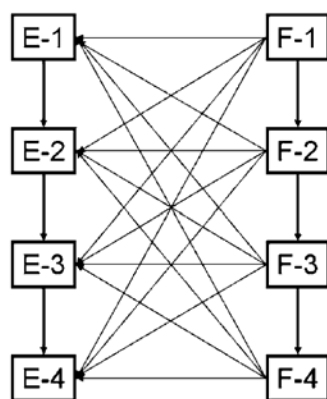


Figure 3: Possible routes through the combined effect and field-exposure flow charts for a terrestrial effect assessment. The boxes E-1 to E-4 are four effect tiers and the boxes F-1 to F-4 are four tiers for assessment of exposure in the field ('F' from 'field'). Downward arrows indicate movement to a higher tier. Arrows from right to left indicate delivery of field-exposure estimates for comparison with effect concentrations in the effect flow chart (after Boesten *et al.*, 2007).

Figure 4 shows in detail how the interaction between exposure and effect assessment works for an arbitrary combination of an effect and a field-exposure tier (by zooming in on an arbitrary combination of an effect and field-exposure tier from Figure 3). The standard procedure in ecotoxicological experiments is to use a range of concentrations to derive a concentration–response relationship. Assessment endpoints within effect tiers have to be expressed in terms of the same type of ERC as the endpoints of the field-exposure tiers. For instance, if the type of ERC was defined as the concentration in the soil pore water then this has to be used in the risk assessment both for evaluating the results of the ecotoxicological experiment and for estimating the exposure in the field. This implies that there are two equally important types of exposure assessments required for the risk-assessment procedure. The first assessment (in the field-exposure box in Figure 4) involves estimating the exposure (in terms of a certain type of ERC) that will occur in the field resulting from the use of the plant protection product in agriculture. This is part of the field-exposure flow chart (Figure 2) and is often referred to as the Predicted Environmental Concentration (we use 'PEC' because this is the most common term but this does not exclude use of measured field concentrations in higher exposure tiers if these measured concentrations are more appropriate). The second exposure assessment (in the effect box in Figure 4) is a characterisation of the exposure (defined in terms of the same type of ERC) to which the organisms were exposed in all ecotoxicological experiments. This second exposure assessment is part of all tiers in the effect flow chart. Both exposure assessments and their interaction with the ecotoxicological activities (Figure 4) require that experts in both fate and ecotoxicology have to co-operate closely for the exposure assessment in such experiments.

This guidance proposal is restricted to exposure assessment in the field.

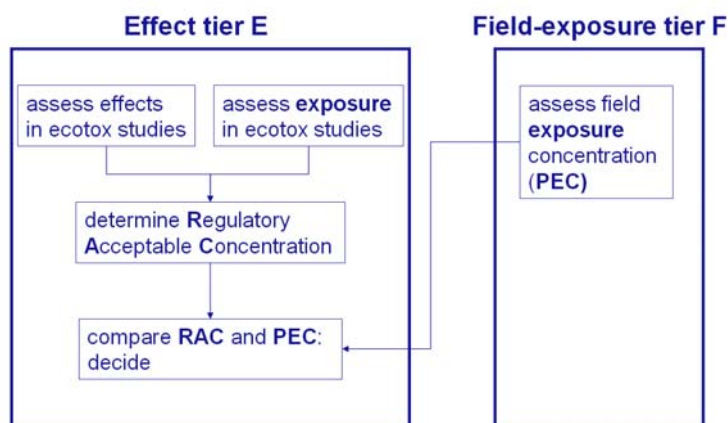


Figure 4: Schematic representation of the two types of exposure assessments which are needed in any combination of tiers of the effect and field-exposure flow charts (after Boesten *et al.*, 2007). Note that ‘Field-exposure tier F’ is identical to the ‘Exposure’ tiers in Figure 2.

1.4. Specification of the exposure-assessment goal

1.4.1. Introduction

EFSA (2010c) indicated that the first step of linking exposure to effects is to define the type of ERCs that are needed. EFSA (2009) indicated that the following types of ERC are needed:

- i. the concentration in total soil (sorbed plus dissolved) expressed as mass of pesticide per mass of dry soil (mg kg^{-1}) averaged over the top 1, 2.5, 5 or 20 cm of soil for various time windows: peak and time-weighted averages (TWA) for 7, 14, 21, 28 and 56 d
- ii. pore-water concentration (mg L^{-1}) averaged over the top 1, 2.5, 5 or 20 cm of soil for the same time windows.

EFSA (2010c) furthermore indicated that the spatio-temporal dimensions of the exposure assessment need to be considered and that this requires specification of (i) the spatial unit, (ii) the spatial statistical population of these units, (iii) the multi-year temporal statistical population of concentrations, and (iv) the percentile of the spatio-temporal statistical population of concentrations to be used in the risk assessment. As described by EFSA (2010c), these are essential specifications of the protection-goal dimensions because the risk is only assessed for the spatio-temporal variability of the systems that are included (e.g. if a 90th percentile of the spatio-temporal population of concentrations is considered in the exposure assessment, then for the remaining 10% of the systems the exposure concentrations are higher than the provided endpoint of the exposure assessment). Therefore the proposed specifications of the items (i) to (iv) are described in Sections 1.4.2 to 1.4.5.

Older soil ecotoxicological studies often expressed exposure only in terms of the applied rate (in kg ha^{-1}). The Panel has reservations whether this is an appropriate procedure for linking exposure to effects. However, if such studies have to be used, the Panel proposes performing the exposure assessment on the basis of the concentration in the top 20 cm of soil (see Appendix I for details).

1.4.2. Specification of the spatial unit

The specification of the spatial unit has two aspects: the type of spatial unit and its area over which exposure concentrations may be averaged. We propose that the type of spatial unit is any agricultural

field where the target crop is grown. As described by EFSA (2010e), an alternative definition could be to restrict the spatial unit to only agricultural fields in which a certain animal group is present i.e. the soil ecoregion approach. EFSA (2010e) developed a modelling approach for defining soil ecoregions within Europe in an attempt to improve the realism of exposure scenarios. Biological information on four soil-animal groups (earthworms, enchytraeids, collembolans and isopods) was used to assign each species to different life forms, representing depth horizons in which they occur. Based on information from three countries covering a North-South gradient (Finland, Germany, Portugal), species presence-absence data were modelled using pedological and climatological information. Ecoregion maps were produced for earthworms and enchytraeids for most of the countries and these revealed marked differences between the countries. However, because comparable information from other EU countries was not available, the approach could not be extended to the entire EU territory. So the proposed type of spatial unit (which does not distinguish between agricultural fields with different dominant animal groups) should be seen as an interim solution that needs to be improved once the soil ecoregion approach has been extended to the whole EU.

The second aspect is the surface area of the spatial unit over which exposure concentrations may be averaged, for which the Panel proposes to use the whole surface area of an individual agricultural field growing the target crop. So the assessment procedure will not account for the spatial variability within an individual field because the Panel considers this level of detail currently not sufficiently relevant for the risk-assessment schemes regarding ecotoxicological effects.

1.4.3. Specification of the spatial statistical population of the spatial units

The next item of the spatio-temporal dimensions is the spatial statistical population of the spatial units. The first aspect of this population is the total area to be considered. For example, this could be the whole EU, one of the regulatory zones North-Centre-South or a Member State. Another example for the total area to be considered can be derived from the development of groundwater scenarios by FOCUS (2000) who divided the EU into nine climatic zones. In the initial stage of the development of the guidance, EU Member States were given opportunity to comment on the project plan. Several Member States indicated that the exposure-assessment procedure should be kept as simple as possible. If scenarios were to be developed for each of nine different climatic zones, this would lead to a complicated procedure. Therefore the Panel proposes to consider three total areas, *viz.* the three regulatory zones North/Centre/South (Figure 1).

The second aspect of the spatial statistical population of the spatial units is the definition of the target crop or the target crop groups. So, for example, does the exposure assessment apply to tulips or to all flower crops? EFSA (2010a) recommended that the Commission should provide the list of crops or crop groups to be considered for the soil exposure assessment. This has not yet happened. Therefore the Panel proposes two lists: (i) one based on the so-called CAPRI crops or crop-group list (Leip *et al.*, 2008) for which EU crop maps are available at a scale of 1x1 km² (see maps in EFSA, 2010b), (ii) the list of all other crops or crop groups. The exposure-assessment methodology will describe procedures for both lists. CRD (2006) and Ctgb (2011) give respectively the crop lists for the UK and Dutch registration of plant protection products which may serve as examples for the future EU list of crops. The list of annual crops provided by CRD (2006) contains many crops that are grown on a small scale e.g. canary flower, borage, choi sum, Florence fennel (Appendix II). The list of annual crops provided by Ctgb (2011) is even more detailed containing for example nine types of dry-harvested peas. So considering crops or crop groups other than the CAPRI crops is likely to be an element of the exposure-assessment methodology.

The third aspect of the statistical population of the spatial units is whether the population is limited to fields grown with the target crop where this active ingredient is applied or whether all fields grown with the target crop are included. The ratio between the total surface areas of these two statistical populations is called the fraction of the target crop treated. So far, it has been common practice to limit

the population to fields where this active ingredient is applied and the Panel proposes to follow this practice. Assessment of the fraction of the target crop treated may become relevant if post-registration monitoring is included as a higher tier. Some Member States have collected statistical data on this fraction (see footnote on p. 29 of EFSA, 2008).

1.4.4. Specification of the multi-year temporal statistical population of concentrations

As described in Section 1.4.1, the ERC is a peak or a TWA concentration for time windows up to 56 days. The conventional procedure is to consider the highest value within one calendar year for multiple applications in the same crop or for applications in different crops on the same location in the same calendar year (for example, the latter occurs for herbicide applications in maize and carrots in the Netherlands).

However, in crop rotations there may of course also be years without application of the particular active ingredient. Let us assume the following example of a four-year application sequence:

- year 1: 0.5 kg ha⁻¹ in carrots and 1.0 kg ha⁻¹ in maize
- year 2: 0.7 kg ha⁻¹ in sugar beet
- year 3: no applications
- year 4: no applications.

So this sequence is repeated every four years. For each year the exposure assessment will deliver e.g. the annual peak concentration as the PEC. So in this case, each four-year application sequence will generate four PECs. The question is then: which PEC-year combinations are part of the temporal statistical population of concentrations and which are not?

The Panel proposes to consider as part of this population only the PEC for the year that generates the highest PEC value of the years in the repetition sequence (in this example four years). The background to this proposal is that the temporal statistical population of concentrations may otherwise contain a large fraction of zero or very low concentrations that are generated by the years without applications or low application rates. Adding such a large fraction of zero or low concentrations seems not meaningful for an adequate risk assessment. The Panel does not preclude that, at a later stage, low or zero concentrations in years without applications may play a role in the assessment of the long-term recovery of the soil ecosystem but considers this not relevant for the specification of the temporal statistical population of the peak concentrations.

As will be shown later, differences between peak concentrations in different application years are comparatively small because differences in weather from year to year have only a limited effect on them. Let us consider a plant protection product that is applied only every four years. So the total temporal population of PEC values at one location would then consist of 75% of low values (no application years) and 25% of high values. But these high values are close to each other. In such a case, the dilution of the statistical population with 75% low values is expected to have only a small effect on the PEC value that is selected from these 25% of high values. The definition of the temporal statistical population of PEC values is a risk-management choice that has to be agreed by the risk managers but this is expected to have only a limited effect on the outcome of this risk assessment. However, the Panel emphasises that this limited effect of the definition of the temporal statistical population is only valid for the exposure assessment of soil organisms considered in this Opinion (e.g. this does certainly not apply to the assessment of leaching to groundwater).

1.4.5. Specification of the percentile of the spatio-temporal statistical population of concentrations

Based on the definitions of (i) the ERC, (ii) the spatial unit, (iii) the spatial and temporal statistical population of concentrations (Sections 1.4.1 to 1.4.4), we can consider now the specification of the required percentile of the spatio-temporal statistical population of concentrations.

The development of the FOCUS groundwater scenarios was based on 90th-percentile PEC values within agricultural areas using the plant protection product in each of nine climatic zones across the EU (FOCUS, 2000). Based on this, nine groundwater scenarios were developed with each of these being intended to deliver the 90th-percentile PEC for one of the climatic zones. The development of the FOCUS surface-water scenarios was based on similar considerations but not on a fixed overall percentile of the population of concentrations to be expected (FOCUS, 2001). Based on this history, the Panel checked with risk managers at Member-State level (via the consultation of the project plan) whether a 90th-percentile exposure concentration should be used here and their response confirmed this. Provisionally, therefore, the Panel aims to select a 90th percentile from the spatio-temporal population of PEC concentrations. However, as part of its planned work, the Panel will review the suitability of the 90th percentile for meeting the overall protection goals, taking account also of the degree of conservatism in other parts of the risk assessment (e.g. effects assessment). The outcome of this will be provided to risk managers, whose role it is to decide on the level of protection to be achieved in practice.

1.5. Limitations of the exposure-assessment methodology

The exposure assessment for annual crops differs from that for permanent crops because the soil systems of these crops differ e.g. permanent crops will often have a litter layer whereas this is usually not so for annual crops. Moreover EFSA (2009) indicated that different types of crop need different types of ERC (see Figures 4 and 5 of EFSA, 2009). The exposure assessment for tillage systems with annual ploughing differs from that for no-tillage systems because the ploughing may have a large 'diluting' effect on the concentrations in the top centimetres. The exposure assessment depends also on the application technique of the plant protection product: for instance a seed treatment will lead to high exposure concentrations around the seeds and low concentrations in most of the surrounding soil whereas spraying onto soil will lead to concentrations that are more or less uniform across the soil. Therefore different exposure-assessment methodologies are needed for different combinations of crops, tillage systems and application techniques. Based on statistical data of EU agricultural practice collected by EFSA (2010a), this guidance focuses on spray applications to annual crops under conventional and reduced tillage (assuming annual ploughing to 20 cm depth and excluding tillage systems with ridges and furrows; Figure 5) and does not consider covered crops.

The guidance is limited to exposure assessment for terrestrial effects within the treated field (so off-crop exposure assessment will not be provided). As described in Section 1.3, the guidance is limited to field exposure and thus does not consider exposure assessment in ecotoxicological experiments (Figure 4). It does also not include guidance for assessment of persistence triggers or for PBT (Persistence Bioaccumulation Toxicity) classification.

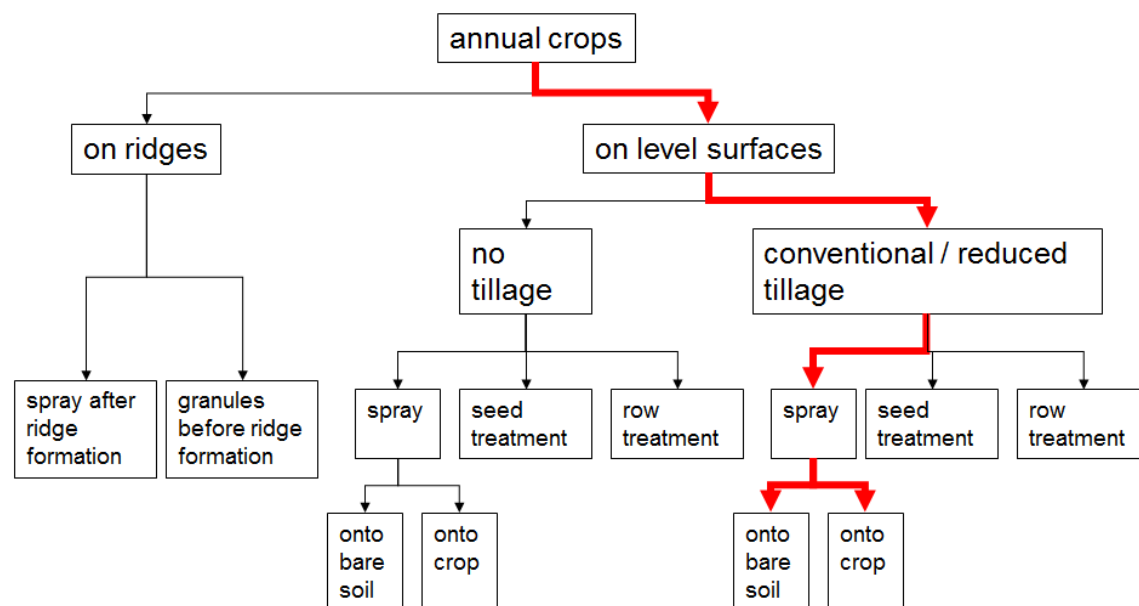


Figure 5: Overview of tillage systems and application techniques for annual crops. The bold red lines indicate the selected combinations for the development of the exposure-assessment methodology. The box ‘on level surfaces’ indicates that the tillage does not lead to ridges and furrows.

1.6. Overview of the structure of the Opinion

Chapter 2 describes the proposed tiered approach for exposure assessment for spray applications to annual crops under conventional and reduced tillage. Chapters 3 to 6 describe the development and parameterisation of the different tiers. Chapter 7 provides guidance on input parameters for crop interception and substance properties to be used in the different tiers. Chapter 8 describes the uncertainty of the exposure assessment resulting from the limited number of measurements of *DegT50* and K_{om} available in dossiers.

2. TIERED APPROACH FOR SPRAY APPLICATIONS IN ANNUAL CROPS WITH REDUCED OR CONVENTIONAL TILLAGE

The Panel proposes a tiered assessment scheme (Figure 6) both for the assessment of the concentration in the pore water and for the concentration in total soil. The schemes for the two types of ERCs (the concentration in total soil and the concentration in pore water) are identical but the contents of the tiers differ so there are two parallel tiered assessment schemes. The tiered scheme applies to spray applications to annual crops under conventional or reduced tillage but will at a later stage hopefully also be useful for other types of application or other tillage systems.

The scheme is designed to minimise the work load for the exposure assessment by providing three fixed scenarios for (i) a simple model in Tier 1 and (ii) numerical models in Tier 2A and by offering the option to continue in Tiers 2B and 2C with the simple model. Tiers 1, 2A, 2B, 2C and 3 are based on modelling approaches and on one scenario per regulatory zone North-Centre-South for each of the two types of ERC. Tier 4 is a spatially distributed modelling approach based on calculations with many scenarios for each of the zones; this is currently not yet operational but should be seen as a desirable future development. Tier 5 is a post-registration monitoring approach that does not consider scenarios.

Tiers 1 and 2A are based on the spatial statistical population of all annual crops as the target crop group. This is of course not a realistic target crop or crop group for a regulatory exposure assessment. So it should be considered as a virtual target crop group. This was done to be able to have in lower tiers one fixed scenario for each regulatory zone irrespective of the target crop or crop group that is assessed. Using all annual crops as the target crop group is expected to result in a robust procedure because this spatial statistical population is the sum of the populations of all the crops and so it should be 'on average' correct. The alternative to this single fixed scenario per regulatory zone would have been to select and parameterise one scenario for each crop or crop group which would have required much more work and this was impossible within the time frame of the mandate of this Opinion. However, the target crop or crop group has of course an effect on the spatio-temporal population of the exposure concentrations so there is *a priori* no guarantee that a scenario calculation based on all annual crops is conservative enough. For example, if a minor crop such as celery is mainly grown in a region of the central zone that has a lower temperature than average, the concentration in total soil calculated for such a crop area may be systematically higher than the concentration calculated for the population of all annual crops in the central zone. Therefore in Tiers 1 and 2A, crop extrapolation factors are introduced (Table 1). As described in Section 1.4.3, the Panel will describe exposure-assessment procedures both for the CAPRI crops or crop groups and for other crops. EFSA (2010b) showed that crop extrapolation factors for the other crops need to be higher than for CAPRI crops or crop groups, and so guidance for both types of factors will be provided for Tiers 1 and 2A.

Tiers 1 and 2A are based on one scenario per zone for each ERC considering the entire surface area of arable land within a zone and assuming that the K_{om} and $DegT50$ of the substance do not depend on soil properties such as pH and clay content. This assumption is not defensible for all plant protection products and their metabolites in soil (the K_{om} and $DegT50$ may be, for example, a function of pH). Therefore higher tiers are included should these substance parameters be a function of soil properties. For these cases, Tiers 2B, 2C and 3 are proposed (Figure 6). In Tiers 2B, 2C and 3, the area of use can be restricted to specific crops and dependencies of K_{om} and/or $DegT50$ on soil properties can be included in the scenario-selection procedure.

At Tier-2B and Tier-2C levels, a simple model is used (similar to Tier 1), whereas scenarios for numerical models are used at the Tier-3 level (similar to Tier 2A). Tiers 2B and 2C are included because a better selection of the 90th-percentile PEC may have more effect than a more detailed description of the processes in the numerical models and because derivation of such a percentile is relatively easy to do.

Because there are many different possibilities for the nature of the relationships between K_{om} or $DegT50$ and soil properties (e.g. the K_{om} may either increase or decrease with pH), and because there are many different crops, Tiers 2B, 2C and 3 will consist only of a description of the procedures to be followed.

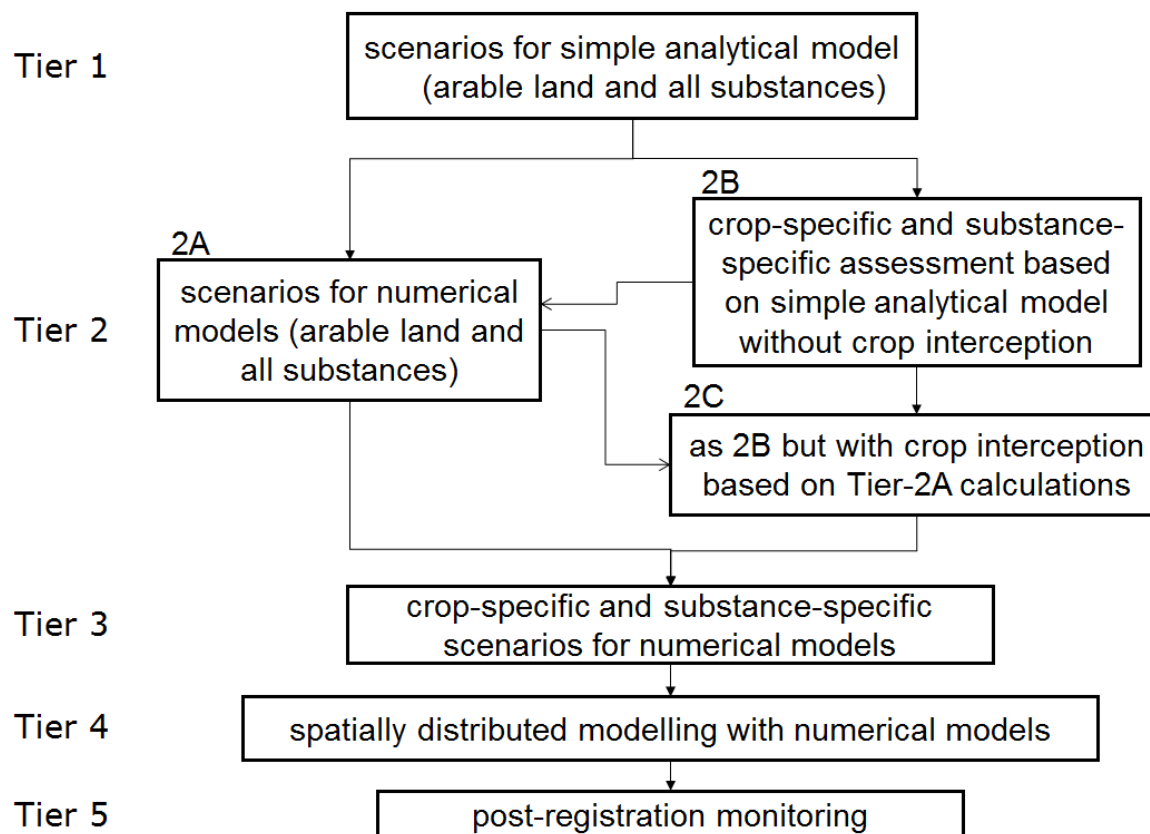


Figure 6: Tiered scheme for the exposure assessment of spray applications to annual crops under conventional or reduced tillage. The scheme applies both to the ERC ‘concentration in total soil’ and the ERC ‘concentration in pore water’. Tiers 1, 2A, 2B, 2C and 3 are all based on one PEC for each of the regulatory zones North, Centre and South and allow for application every 1, 2 or 3 years.

Tiers 1, 2B and 2C are based on this simple analytical model. In Tier 1, this simple model has the advantage that the required number of inputs is very limited and thus also the documentation of exposure assessments will require little effort. In Tiers 2B and 2C, the simple model has the advantage that the exposure assessment requires much less effort than in the alternative Tier 3. However, there is of course no guarantee that the simple model is conservative enough when compared with the more realistic numerical models used in Tier 2A (using the same scenarios as in Tier 1). Therefore a model adjustment factor is needed in all the tiers that use the simple analytical model (Tiers 1, 2B and 2C; Table 1).

The scenario-selection procedures in Tiers 1 and 2A are based on the assumption that the substance parameters $DegT50$ and K_{om} are not related to soil properties (e.g. soil pH). However, these tiers should also be conservative for substances whose K_{om} and/or the $DegT50$ do depend on soil properties. This will be assured by using conservative values of the K_{om} and/or the $DegT50$ of such substances herein.

Table 1: Overview of inclusion of the crop extrapolation factors, the model adjustment factor and crop interception of substance in the different tiers of Figure 6. Inclusion of the crop extrapolation factor implies that low extrapolation factors are used for CAPRI crops or crop groups and high extrapolation factors for other crops. ‘+’ indicates that the process or factor is included, ‘-’ indicates that it is not included and ‘±’ indicates that it may be either included or excluded.

Tier	Crop extrapolation factor	Model adjustment factor	Crop interception
1	+	+	-
2A	+	-	+
2B	±	+	-
2C	-	+	+
3	-	-	+
4	-	-	+

The flow chart (Figure 6) has two parallel branches in Tier 2. Tier 2A is based on three fixed scenarios for the numerical models with all annual crops as the target crop group and with this one set of scenarios for all substances. Tier 2B is based on an assessment of the 90th-percentile PEC with the simple analytical model considering both the target crop or crop group and the substance properties. So in this tier, the risk assessor has to perform a tailor-made exposure assessment. The assessment in Tier 2B is both crop and substance specific because this gives a more accurate result and because it is no more work to include both aspects in the assessment. In Tier 2B, crop interception is ignored (as in Tier 1) which is a simple and conservative approach.

Tiers 1 and 2B are based on the assumption that crop interception of the substance does not occur (Table 1). In Tier 2A this can be included because the numerical models are able to simulate crop interception and the subsequent loss processes at the plant surface including wash-off to the soil. Tier 2C offers the possibility to include crop interception in the assessment in case this would have a large effect on the exposure assessment. The only way to include this is to use results of Tier-2A scenario calculations for this purpose because the simple analytical model does not include plant processes such as wash-off. The advantage of including crop interception in Tier 2C over jumping to Tier 3 is that Tier 3 requires much more work because the numerical models need to be parameterised for the scenario selected in Tier 2A.

Note that the use of results of Tier-2A calculations in Tier 2C does not imply passing through Tier 2A in the flow chart. As described in Section 1.2, a tier is defined as a complete exposure assessment resulting in an appropriate endpoint. A tiered flow chart describes the flow of the decision-making process for the exposure endpoint, not the procedure to get to this endpoint. Therefore performing calculations with Tier 2A-scenarios does not imply passing through Tier 2A.

As indicated by arrows in the flow chart, the user may go from Tier 2B to Tier 2A and from Tier 2A to Tier 2C. These possibilities are included in the flow chart solely because they may be more efficient for notifiers (and consequently also less work for governmental risk assessors). There is no arrow from Tier 2A to Tier 2B because it is no more work to go immediately to Tier 2C after the exposure assessment of Tier 2A has been carried out (and thus the crop-interception information is available).

As will be described later, the crop extrapolation factors were derived from calculations with substances whose *DegT50* and *K_{om}* are not related to soil properties. This is the only practical option because it is impossible to include all possible relationships between *DegT50* or *K_{om}* and the various

soil properties. However, this has the consequence that there is no guarantee that the crop extrapolation factors in Tiers 1 and 2A are conservative enough for substances whose *DegT50* and the K_{om} are related to soil properties. As described before, conservative values of the K_{om} and/or the *DegT50* of such substances have to be used in Tiers 1 and 2A. Because for such substances these crop extrapolation factors are always used in combination with these conservative values, the Panel considers it very unlikely that the exposure concentrations derived from Tiers 1 and 2A will not be conservative enough.

As will be described later, the model adjustment factor for the possible differences between the simple model and the numerical models is based on comparison of Tier-1 and Tier-2A calculations for substances whose *DegT50* and K_{om} are not related to soil properties (for the same reason as described in the previous paragraph) and considering only the total area of arable land in a regulatory zone. So this has the consequence that this factor (as used in Tiers 1, 2B and 2C) may not be conservative enough for substances whose *DegT50* and/or K_{om} are related to soil properties or for other crop areas (and thus these tiers might give a less conservative result than Tier 3). However, the Panel considers this to be unlikely because (i) the model adjustment factor is needed to account for differences between the simple analytical model and the numerical models and (ii) the numerical models in Tier 3 are the same as in Tier 2A.

As described by EFSA (2010b), a tiered approach should be based on a reference tier that can act as a yardstick for lower tiers. In the flow chart (Figure 6), the only suitable candidate for this reference tier is Tier 4, i.e. the spatially distributed modelling with numerical models. However, this tier is not yet operational. If it were operational, Tiers 2A and 3 would probably be superfluous and the development of the exposure-assessment procedure would have been much more straightforward.

The tiered approach (Figure 6) contains many tiers and the procedures to be followed in each tier are complex. Thus efficient use of the approach in the regulatory practice is impossible without appropriate software tools. Therefore the Panel recommends that such tools be developed and made available.

3. DESCRIPTION OF THE SIMPLE ANALYTICAL MODEL

Tiers 1, 2B, and 2C are based on a simple analytical model (Chapter 2) that is parameterised for the three zones (North/Centre/South). As will be described later, this model is also used to select the Tier-2A and Tier-3 scenarios for the numerical models. So this analytical model plays a key role in the development of the exposure-assessment procedure. This model is described in this chapter (first in terms of a conceptual model and thereafter mathematically).

The simple analytical model is based on the following conceptual model:

- i. the substance is applied to the soil surface as a single dose (i.e. sum of all applications within one year) on the same date every year or every two or three years,
- ii. this dose may be corrected to account for crop interception and dissipation on plant surfaces based on other models or data
- iii. the only loss process from the soil is degradation and the degradation rate is a function of only soil temperature,
- iv. soil properties such as moisture content and temperature are constant in time,
- v. the model does not consider the time course of concentrations; instead the maximum of the exposure concentration after infinite time is considered,
- vi. the effect of tillage is accounted for by assuming complete mixing over the tillage depth of 20 cm (EFSA, 2010a) at the moment of tillage (each year in autumn or winter),
- vii. adsorption is described by a linear isotherm using the concept of a sorption coefficient that is proportional to organic-matter content (K_{om}),
- viii. the average exposure concentration over a certain depth is calculated from the sum of the concentration just before the last application and the dose divided by this depth
- ix. a flexible approach is taken for introducing relationships between $DegT50$ or K_{om} and soil properties when used for Tier 2B.

The consequence of this conceptual model is that the substance-specific input to the model is restricted to:

- i. half-life for degradation in top soil at 20°C and a moisture content corresponding to field capacity,
- ii. the organic-matter/water distribution coefficient (K_{om}),
- iii. the annual rate of application (i.e. the sum of the application rates within one growing season in case of multiple applications); for Tier 2C this has to be corrected based on calculations with numerical models,
- iv. when used for Tier 2B, relationships between $DegT50$ or K_{om} and soil properties as necessary.

The mathematical description is as follows for parent substances. Firstly the initial concentration in total soil directly after application is calculated:

$$C_{T,ini} = \frac{A}{\rho z_{eco}} \quad (1)$$

where $C_{T,ini}$ (mg kg⁻¹) is the initial concentration in total soil, A is the annual application rate (kg ha⁻¹ or mg dm⁻²), z_{eco} (dm)⁶ is the ecotoxicological averaging depth (i.e. 1, 2.5, 5 or 20 cm as specified in Section 1.4.1), and ρ is the dry soil bulk density (kg L⁻¹). In the second step, the background concentration ($C_{T,plateau}$ mg kg⁻¹), just before the next application after an infinite number of annual applications, is calculated:

⁶ The unit ‘cm’ is used for depths in the remainder of the text because this is more common than ‘dm’; here ‘dm’ is used as the unit for z_{eco} and similarly for z_{fil} after Eqn 2 to ensure consistency of units within Eqns 1 and 2 (1 dm = 10 cm).

$$C_{T,plateau} = \frac{z_{eco}}{z_{til}} C_{T,ini} \frac{X}{1-X} \quad (2)$$

where z_{til} (dm) is the plough depth (fixed at 20 cm based on EFSA, 2010a) and X is defined as:

$$X = e^{-t_{cycle} f_T k_{ref}} \quad (3)$$

where t_{cycle} is the time between applications (365, 730 or 1095 d), f_T is a factor describing the effect of soil temperature on the degradation rate coefficient, and k_{ref} (d^{-1}) is the first-order degradation rate coefficient at a reference temperature T_{ref} (i.e. 20°C) and the soil moisture content at field capacity. Although the soil temperature is constant in time, the factor f_T is needed because dossiers are based on degradation rate measurements at 20°C and f_T converts this rate to the rate at the scenario temperature. As follows from the combination of Eqns 1 and 2, the background concentration does not depend on the ecotoxicologically relevant averaging depth but depends only on the plough depth.

Eqn 2 can be derived as follows (Hill *et al.*, 1955). Let us assume that the substance is applied at the rate A every year on 1 January and that X is the fraction of the dose left at the moment of the next application. Based on the assumption of first-order kinetics, the amount in the soil just before the next application after an infinite number of application periods equals $A (X + X^2 + X^3 + X^4 + \dots)$. This is a geometric series. From the expression for the sum of an infinite geometric series, this amount is shown to be $AX / (1 - X)$. Eqn 2 is based on this expression combined with the conversion of the application rate A into a concentration in total soil mixed over the plough depth.

The dimensionless factor f_T describing the effect of temperature on degradation is given by:

$$T > 0^\circ C \quad f_T = \exp\left(\frac{-E}{R} \left[\frac{1}{T} - \frac{1}{T_{ref}}\right]\right) \quad (4a)$$

$$T < 0^\circ C \quad f_T = 0 \quad (4b)$$

where E is the Arrhenius activation energy, ($kJ \text{ mol}^{-1}$), R is the gas constant ($0.008314 \text{ kJ mol}^{-1} \text{ K}^{-1}$), T (K) is the soil temperature, and T_{ref} (K) is the temperature at reference conditions (20°C so 293 K). The Arrhenius activation energy in the model was set to 65.4 kJ mol^{-1} (EFSA, 2007). The coefficient k_{ref} is calculated from the degradation half-life by:

$$k_{ref} = \frac{\ln 2}{DegT_{50}} \quad (5)$$

where $DegT_{50}$ (d) is the degradation half-life in soil at the reference temperature.

The background concentration corresponds to the residue remaining immediately before the next application. So the maximum concentration in this model will occur directly after this next application and it can be calculated by:

$$C_{T,peak} = C_{T,ini} + C_{T,plateau} \quad (6)$$

where $C_{T,peak}$ ($mg \text{ kg}^{-1}$) is the maximum concentration in total soil.

The maximum concentration in the liquid phase is calculated from the maximum concentration in total soil assuming a linear sorption isotherm:

$$C_{L,peak} = \frac{C_{T,peak}}{\theta / \rho + f_{om} K_{om}} \quad (7)$$

where $C_{L,peak}$ (mg L⁻¹) is the maximum concentration in the liquid phase, θ (m³ m⁻³) is the volume fraction of liquid in soil at field capacity, f_{om} (kg kg⁻¹) is the mass fraction of organic matter, and K_{om} (L kg⁻¹) is the coefficient for sorption on organic matter.

The model includes also calculation of TWA concentrations. A TWA concentration is defined as the concentration that is averaged over a certain time period since the application time:

$$C_{TWA} = \frac{1}{t_{avg}} \int_0^{t_{avg}} C(t') dt' \quad (8)$$

where t_{avg} (d) is the time period since the application time over which concentrations are averaged and t' is a dummy time integration variable. Because it is assumed that the substance is degraded following first-order kinetics, the TWA concentration in total soil, $C_{T,TWA}$ can be calculated from:

$$C_{T,TWA} = \frac{1}{t_{avg}} \int_0^{t_{avg}} C_{T,peak} \exp(-f_T k_{ref} t') dt' \quad (9)$$

which gives:

$$C_{T,TWA} = \frac{C_{T,peak}}{t_{avg} f_T k_{ref}} [1 - \exp(-f_T k_{ref} t_{avg})] \quad (10)$$

The TWA concentration in the liquid phase, $C_{L,TWA}$, is calculated from an equation akin to Eqn 10 but with $C_{L,peak}$ instead of $C_{T,peak}$.

The model calculates concentrations of metabolites based on the conservative assumption that each metabolite is applied at the application time of the parent at a dose that is corrected for the kinetic formation fraction (using procedures in FOCUS, 2006) and the molar mass of the metabolite. It can be shown that this assumption is conservative for the peak concentration by considering the analytical solution for the time course of a metabolite that is formed and degraded following first-order kinetics after a single application:

$$C_{T,metabolite} = \frac{F_{f,l-p} k_{parent} \frac{M_{met,l}}{M_{parent}} C_{T,0,parent}}{k_{parent} - k_{met,l}} [\exp(-k_{met,l} t) - \exp(-k_{parent} t)] \quad (11)$$

where $C_{T,metabolite}$ (mg kg⁻¹) is the concentration of this metabolite in total soil, $F_{f,l-p}$ (-) is the formation fraction of this metabolite (i.e. the stoichiometric coefficient of the formation of this metabolite from the parent substance), $M_{met,l}$ is the molar mass of this metabolite (g mol⁻¹), M_{parent} is the molar mass of the parent substance (g mol⁻¹), k_{parent} is the degradation rate coefficient of the parent (d⁻¹), $k_{met,l}$ is the degradation rate coefficient of this metabolite (d⁻¹) and $C_{T,0,parent}$ (mg kg⁻¹) is the concentration in total soil of the parent at the application time and t is the time elapsed since application (d).

Assuming that the metabolite is applied at the start implies that an infinitely large degradation rate of the parent is assumed. For an infinitely large degradation rate coefficient of the parent, Eqn 11 reduces to:

$$C_{T,metabolite} = F_{f,1-p} \frac{M_{met,1}}{M_{parent}} C_{T,0,parent} \exp(-k_{met,1} t) \quad (12)$$

Comparison of Eqns 11 and 12 shows that the concentration calculated with Eqn 12 is for all times higher than that calculated with Eqn 11. So Eqn 12 is a conservative approach both for the peak concentration and TWA concentrations of metabolites.

So for soil metabolites, the calculation procedure is the same as described above with one exception: in Eqn 1 the annual application rate A is replaced by the equivalent annual application rate of the metabolite (and of course using the $DegT50$ and K_{om} of the metabolite instead of the parent). For a soil metabolite formed from the parent, this equivalent rate is given by:

$$A_{met,1} = F_{f,1-p} \frac{M_{met,1}}{M_{parent}} A \quad (13)$$

where A is the annual application rate of the parent substance (kg ha^{-1} or mg dm^{-2}) as before. For a second soil metabolite formed from this first soil metabolite, the equivalent application rate is given by:

$$A_{met,2} = F_{f,1-p} F_{f,2-1} \frac{M_{met,2}}{M_{parent}} A \quad (14)$$

where $F_{f,2-1}$ is the formation fraction (-) of this second metabolite as formed from the first metabolite and $M_{met,2}$ is the molar mass of this second metabolite (g mol^{-1}).

Figure 7 shows an illustrative calculation for a system with a parent and two sequential metabolites. As would be expected, the steady-state level for the parent is exactly equal to that calculated with the kinetic model, whereas the steady-state levels of the metabolites overestimate the modelled maxima.

The simple analytical model ignores leaching losses. This is considered defensible because the soil is mixed every year over the 20 cm tillage depth and because it is unlikely for parent substances that a large fraction is leached below 20 cm depth. Thus leaching is expected to have only a minor influence on the steady-state level of the peak concentration calculated by the model. As a consequence, rainfall or irrigation are not input parameters to the model and thus play no role in calculations carried out with the model. The Panel acknowledges that there may be exceptional cases where leaching may have a significant effect on the accumulation levels in top soil (e.g. mobile parent substances or substances used in irrigated crops with many applications within a single growing season for $z_{eco} = 1 \text{ cm}$). Inclusion of all exceptional cases in the tiered exposure-assessment methodology would only be possible if Tier 4 (i.e. the spatially distributed modelling; Figure 6) were operational which is not so.

The principles of the tiered approach prescribe that lower tiers are more conservative than higher tiers. The model is very simple so there is *a priori* no guarantee that this model is conservative enough when compared to simulations with sophisticated numerical models (as in Tiers 2A and 3). There is also the possibility that it is more conservative than these numerical models. Therefore a model adjustment factor was introduced in the model:

$$C_{Y,cal} = F_{mo} C_Y \quad (15)$$

where C_Y is the uncalibrated value of either $C_{T,peak}$, $C_{L,peak}$, $C_{T,TWA}$ or $C_{L,TWA}$, $C_{Y,cal}$ is the calibrated value of each of these quantities and F_{mo} (-) is a model adjustment factor (see Section 5 for the assessment of this factor).

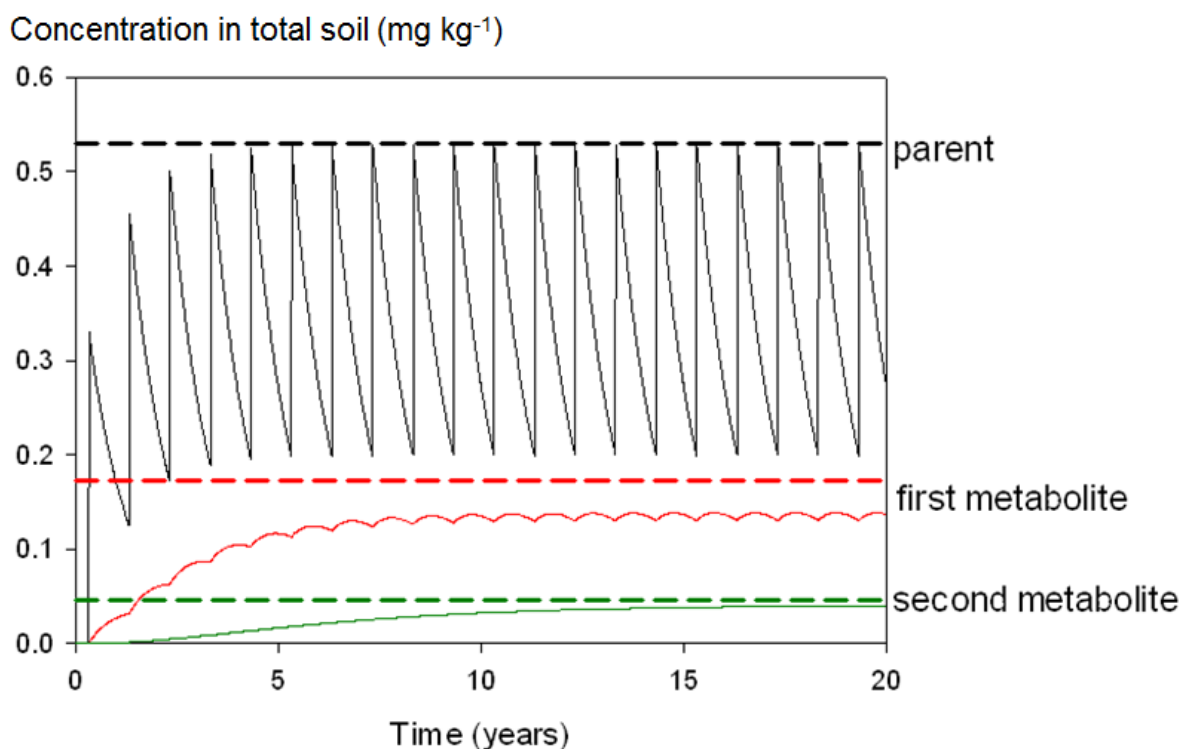


Figure 7: Comparison of (i) the time courses of the concentration in total soil of a parent and two sequential metabolites as calculated with a kinetic model based on first-order kinetics of degradation and formation with (2) the steady-state levels of the peak concentration as calculated with the simple analytical model based on Eqn 6 for the parent, Eqns 6 and 13 for the first metabolite and Eqns 6 and 14 for the second metabolite. Calculations were made for $A = 1 \text{ mg dm}^{-2}$, $t_{\text{cycle}} = 365 \text{ d}$, $\rho = 1.5 \text{ kg L}^{-1}$, $z_{\text{eco}} = 20 \text{ cm}$, $z_{\text{til}} = 20 \text{ cm}$, $T_{\text{ref}} = 20^{\circ}\text{C}$, $T = 10^{\circ}\text{C}$, $F_{f,1,p} = 0.3$, $F_{f,2,1} = 0.3$, $M_{\text{parent}} = 300 \text{ g mol}^{-1}$, $M_{\text{met},1} = 200 \text{ g mol}^{-1}$, $M_{\text{met},2} = 100 \text{ g mol}^{-1}$, DegT50 of parent of 100 d, DegT50 of first metabolite of 200 d and DegT50 of second metabolite of 400 d. The solid lines are calculations with the kinetic model and the dashed lines are the steady-state levels.

The simple analytical model is based on the assumption of a soil temperature that is constant over time. The selection of the soil temperature for Tier-1 scenarios will be based on analyses of meteorological time series of temperatures. The question is then how this constant temperature can best be derived from such time series. The most straightforward procedure is of course to derive simply the arithmetic mean temperature from a time series. However, the relationship between the rate coefficient and the temperature is described with the Arrhenius equation (Eqn 4) which is a non-linear function of the temperature. Therefore it is considered more appropriate to derive a mean temperature using an averaging method that gives the same weight to each daily or monthly temperature as would the Arrhenius equation. EFSA (2010b, p. 40) derived the expression for calculating this Arrhenius-weighted average temperature:

$$T_{\text{Arr}} = - \frac{E}{R \ln \left[\frac{1}{t_{\text{end}}} \int_0^{t_{\text{end}}} G dt \right]} \quad (16)$$

with

$$T_{mts} \geq 0^{\circ}\text{C} \quad G \equiv \exp\left(-\frac{E}{RT_{mts}}\right) \quad (17a)$$

$$T_{mts} < 0^{\circ}\text{C} \quad G \equiv 0 \quad (17b)$$

where T_{Arr} is the Arrhenius-weighted mean temperature (K), t_{end} is the length of the time period considered (d), and T_{mts} is the temperature of the meteorological time series (K) which varies of course with time. The principle behind Eqn 16 is that a decline calculation based on the time series of the temperature will give exactly the same fraction of the dose at time t_{end} as a calculation based on a constant temperature with value T_{Arr} .

To illustrate how Eqn 16 works, calculations were made for $E = 65.4 \text{ kJ mol}^{-1}$ (EFSA, 2007) and a soil temperature that fluctuates sinusoidally around 10°C within a year. Figure 8 shows that T_{Arr} increases with increasing amplitude of the sinus (with the exception of a small decline just after an amplitude of 10°C which is caused by the discontinuity in Eqn 17 at $T = 0^{\circ}\text{C}$). The background of the increase is that a year with an annual average temperature of 10°C and an amplitude of e.g. 20°C will result overall in a faster degradation than a year with a constant temperature of 10°C because the Arrhenius equation implies that the degradation rate coefficient increases approximately exponentially with temperature above 0°C (see Eqn 18 of Boesten & van der Linden, 1991). Therefore the speeding-up effect at soil temperatures above 10°C is larger than the slowing-down effect at soil temperatures below 10°C . The differences between T_{Arr} and the arithmetic mean of 10°C are small for annual amplitudes up about 5°C (Figure 8) but the difference may be considerable for higher amplitudes; thus one may expect that the difference between T_{Arr} and the arithmetic mean of 10°C will be larger for continental than for temperate climates within the EU.

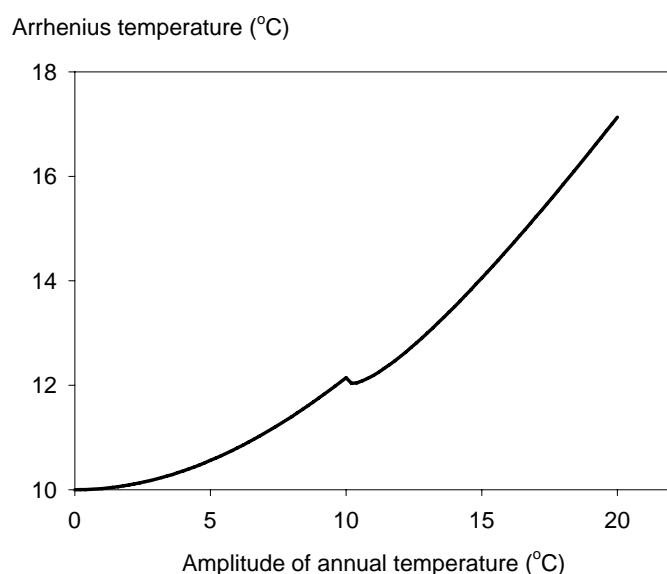


Figure 8: Arrhenius-weighted mean temperature as defined by Eqns 16 and 17 as a function of the amplitude of an annually sinusoidally fluctuating soil temperature for an Arrhenius activation energy of 65.4 kJ mol^{-1} ; amplitude is defined as the difference between the maximum (or the minimum) and the mean of the sinus. The arithmetic mean temperature of the sinus was 10°C .

The simple analytical model can also be used for a first assessment of the time needed to approach the background concentration (i.e. the plateau level). Let us consider the amount in soil after n applications, just before the $n+1^{\text{th}}$ application. This equals $A(X + X^2 + X^3 + \dots + X^n)$. We define $C_{T,n}$ as

the concentration in total soil after n applications, just before the $n+1^{\text{th}}$ application. Using the expression for the sum of a geometric series, $C_{T,n}$ can be calculated:

$$C_{T,n} = \frac{z_{eco}}{z_{til}} C_{T,ini} \frac{X - X^{n+1}}{1 - X} \quad (18)$$

Let us define a ‘fractional equilibrium’, φ , defined as the quotient of Eqn 18 divided by Eqn 2:

$$\varphi = 1 - X^n \quad (19)$$

So, for example, $\varphi = 0.9$ means that the concentration is 90% of the plateau value just before the next ($n+1^{\text{th}}$) application. Using Eqn 3 and defining an effective half-life $DegT50_{eff} = \ln 2 / (f_T k_{ref})$, Eqn 19 can be rewritten:

$$\varphi = 1 - \exp\left(-\ln 2 \frac{n t_{cycle}}{DegT50_{eff}}\right) \quad (20)$$

Figure 9 shows φ as a function of the quotient $n t_{cycle} / DegT50_{eff}$. The product $n t_{cycle}$ is the total time elapsed since the first application and so this quotient can also be seen as the number of half-lives elapsed since the first application. The fractional equilibrium approaches its maximum value of 1 closely after 4 to 5 half-lives (Figure 9). To illustrate the effect of t_{cycle} , let us consider a substance-scenario combination with $DegT50_{eff} = 1$ year. If this substance is applied every year ($t_{cycle} = 1$ year) then Figure 9 shows a fractional equilibrium of 0.5 just before the second application (i.e. $n = 1$). However, if this substance is applied every three years ($t_{cycle} = 3$ year) then the fractional equilibrium is about 0.9 (0.875 is the exact figure). So for applications every three years, the plateau value is approached after fewer application cycles than for applications every year. Eqn 20 shows that fractional equilibrium is a function of the product $n t_{cycle}$, which is the total time elapsed since the first application. So it is only this total time that matters ($n = 1$ and $t_{cycle} = 3$ years will give exactly the same φ as $n = 3$ and $t_{cycle} = 1$ year).

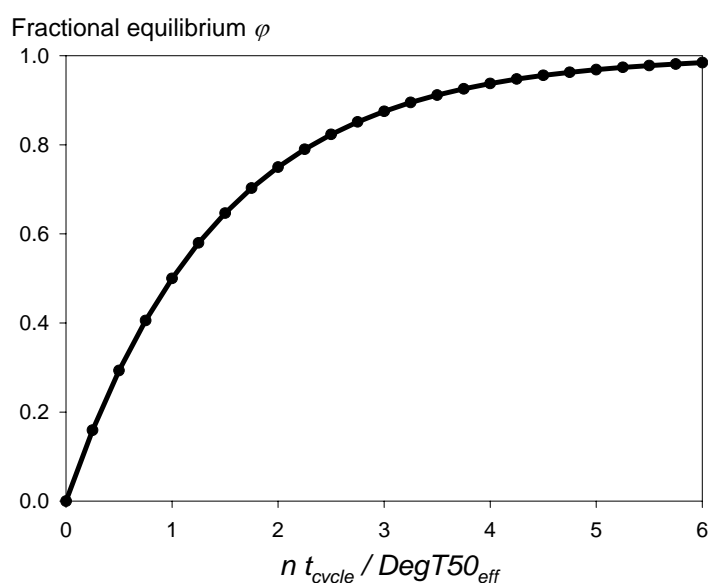


Figure 9: The fractional equilibrium φ as a function of the quotient of total time elapsed since the first application ($n t_{cycle}$) divided by the effective half-life $DegT50_{eff}$ (based on Eqn 20).

4. DEVELOPMENT AND PARAMETERISATION OF THE TIER-2A SCENARIOS

4.1. Introduction

As described earlier, Tier 2A will be based on one scenario per regulatory zone (North-Centre-South) for each of the two types of ERC (concentration in total soil and concentration in pore water) and it can be used for all annual crops and all substances. It will deliver concentrations averaged over depths of 1, 2.5, 5 and 20 cm of soil and both peak and TWA concentrations for time windows up to 56 days.

In principle, the scenario selection depends on the averaging depth and the time window considered. To keep the exposure assessment as simple as possible, it was decided at an early stage to limit the Tier-2A scenarios to one per type of ERC and one per regulatory zone. The scenario-selection procedure described below will include the full range of averaging depths (1 to 20 cm). The scenario selection was based on only the peak concentration. As shown by calculations reported in Section 6.1, the selected scenarios are also conservative for TWA concentrations of parent substances.

The scenario-selection procedure is based on the simple analytical model considering parent substances only. So there is no guarantee that selected scenarios are appropriate for soil metabolites. This is further discussed in Chapter 9.

The spatio-temporal population of concentrations is a function of both substance properties such as the *DegT50* or the K_{om} and the scenario properties (e.g. organic-matter content of the soil). So there is interaction between the scenario selection and the procedure to generate substance properties from dossier data to be used as input for the scenario calculations. During the IRIS-workshop in 2009, two options were discussed with Member States for the *DegT50*: use a median *DegT50* or e.g. a 90th-percentile *DegT50*. The conclusion was that a median *DegT50* is to be preferred because the accuracy of a 90th-percentile *DegT50* derived from dossier data is much less than that of a median *DegT50* so derived. Therefore use of median substance properties was a boundary condition for the development of the scenarios. FOCUS (2006) and EFSA (2010d) proposed using a geomean *DegT50* value. EFSA (2010d) proposed using a lognormal distribution for the *DegT50* (with a coefficient of variation of 0.5). Because the median is considered to be a good estimator of the geomean for lognormal distributions, use of a median *DegT50* for the development of the scenarios is consistent with this guidance. Consequences for the guidance for the K_{om} are discussed in Section 7.2.

4.2. Scenario selection

4.2.1. Overview

The scenario-selection procedure has been described in detail by EFSA (2010b), and so here only a summary is given. The selection consists of four steps: (i) data compilation, (ii) selection of model for vulnerability mapping, (iii) handling of uncertainty in soil and substance properties in the scenario-selection procedure, and (iv) selection of the scenarios that meet this target percentile for the range of substances to be considered.

4.2.2. Data compilation

The data used (available free at <http://eussoils.jrc.ec.europa.eu/library/Data/EFSA/>) were maps at a resolution of 1×1 km² of the whole EU of the following properties:

- i. land-use mask to indicate presence of annual crops
- ii. organic-matter content of the top 30 cm of soil based on the OCTOP map (i.e. an EU wide map of the Organic-Carbon content in the TOP 30 cm of the soil; Jones *et al.*, 2005).
- iii. dry bulk density of the top 30 cm of soil using a pedotransfer function based on organic-matter content,

- iv. volume fraction of water at field capacity (ie $pF = 2$) using a pedotransfer function based on soil textural class,
- v. monthly average air temperatures taken from the period 1960 to 1990 from the WorldClim database.

To ensure consistency within the dataset, all of the geographical data in the database have been harmonised in the Lambert-Azimuthal Equal-Area (LAEA) ETRS 1989 projection system.

The land-use mask for the presence of annual crops was based on CORINE land-cover classes 211 and 212, and on land-cover information from 1990 and 2000. Only grids that showed annual crops in both years were included in the mask. No threshold was considered in this grid-selection procedure. CORINE data were converted from the original $100 \times 100 \text{ m}^2$ resolution to the $1 \times 1 \text{ km}^2$ resolution by taking the dominant land use within each $1 \times 1 \text{ km}^2$ grid cell. Dominant land use was assessed considering the categories annual crops, grass, permanent crops, rice and non-agricultural. Only grid cells with annual crops as the dominant land use were included in the land-use mask. Dominant land use is defined as the land-use class with the largest surface area in the grid cell. For instance, 'annual crops' is the dominant land use if the surface area in a grid cell is distributed as follows: 30% annual crops, 20% grass, 20% permanent crops, 10% rice and 20% non-agricultural. Only cells with the dominant land use 'annual crops' were included to minimise the organic-matter map containing grid cells with extreme values from non-arable areas.

The map of organic-matter content of the top 30 cm was obtained by applying a conversion factor of 1.72 to the organic-carbon contents of the OCTOP map (Jones *et al.*, 2005). Within the OCTOP map, the organic-carbon content of a given pixel was derived from that of individual land uses available at a higher spatial resolution. Jones *et al.* (2005) and EFSA (2010b) used different procedures for the aggregation of, respectively, the organic-carbon and land-use maps that were available at a higher spatial resolution. The Panel considers it likely that the organic-matter content so derived is systematically too high for the area of annual crops in northern Europe and too low in southern Europe. Jones *et al.* (2005) used a pixel-thinning procedure in which the result of one randomly chosen pixel was assumed to represent the entire $1 \times 1 \text{ km}^2$ grid cell, whereas EFSA (2010b) used the dominant land use to represent the entire $1 \times 1 \text{ km}^2$ pixel. These different procedures may cause the aggregated map of organic-matter content for arable land (at a resolution of $1 \times 1 \text{ km}^2$) to be unduly influenced by organic-matter contents derived for forest and grassland (with higher organic matter than the area of annual crops) and for sparsely vegetated areas and bare rocks (with lower organic matter than the area of annual crops). The former is more likely to occur in northern Europe and the latter in southern Europe. So the OCTOP map is likely to overestimate the organic-matter content for arable soils with higher organic-matter content in northern Europe; such overestimation leads to underestimation of the soil bulk density and hence the exposure assessment is expected to overestimate the 90th-percentile concentration in total soil. For southern Europe, the OCTOP map is likely to underestimate the organic-matter content for arable soils with lower organic-matter content; such underestimation leads to underestimation of sorption and hence the exposure assessment is expected to overestimate the 90th-percentile concentration in pore water. The best solution to overcome this scale problem would have been to derive an OCTOP map specifically for arable land, but this was not possible within the given time frame.

When overlaying the re-projected OCTOP data with the generalised land-use data derived from CORINE2000 about 700 pixels (i.e. 0.04% of the total of 1,800,836 pixels) appeared to have zero organic-carbon contents. These zero values should be considered as artefacts and they were discarded when necessary.

The dry bulk-density map was calculated from the organic-matter map using the following pedotransfer function (Tiktak *et al.*, 2006):

$$\rho = r_1 + r_2 f_{om} - r_3 \sqrt{f_{om}} \quad (21)$$

where r_1 , r_2 and r_3 are regression parameters ($r_1 = 1.800 \text{ kg L}^{-1}$, $r_2 = 1.236 \text{ kg L}^{-1}$ and $r_3 = 2.910 \text{ kg L}^{-1}$). Eqn 21 implies that ρ is a continuously decreasing function of organic-matter content ($\rho = 1.80 \text{ kg L}^{-1}$ at $f_{om} = 0$, $\rho = 1.52 \text{ kg L}^{-1}$ at $f_{om} = 0.01 \text{ kg kg}^{-1}$ and $\rho = 1.00 \text{ kg L}^{-1}$ at $f_{om} = 0.10 \text{ kg kg}^{-1}$).

4.2.3. Selection of the model for vulnerability mapping

The chosen model has to be compatible with the available data. It was not possible to use numerical models for this purpose because they need e.g. daily meteorological time series. So therefore the simple analytical model described in Chapter 3 was used. An important assumption is that this simple model gives the same ranking of soil exposure concentrations of the $1 \times 1 \text{ km}^2$ pixels as those from a numerical model. EFSA (2010a) tested this using the PEARL model and a database consisting of 1051 scenarios from the EU-15 (Tiktak *et al.*, 2004) and three substances P1, P2 and P3 (Table 2), and found that the ranking was good enough ($R^2 > 0.97$) to justify the use of the simple model for vulnerability mapping. In this test it was assumed that the soil was ploughed 20 cm deep every year both in the PEARL calculations and in those with the simple analytical model. So there is no guarantee that the selected scenarios are also valid for shallower tillage depths (e.g. 5 cm).

Table 2: Properties of the substances P1, P2 and P3.

Substance code	<i>DegT50</i> (d) in top soil at 20°C and field capacity	K_{om} (L kg ⁻¹)
P1	15	15
P2	50	200
P3	200	1000

As described in Section 3, the simple analytical model does not calculate the time course of concentrations: it only calculates the all-time high exposure concentrations after infinite time. Thus it was impossible in the scenario-selection procedure to base the 90th percentile of the spatio-temporal population of concentrations (as defined in Section 1.4.5) on a percentile in time. Including time percentiles in the scenario-selection procedure would only have been possible if a numerical model had been used that includes climatic variability over the whole area of the EU. However such a model was not available. To overcome this problem, the Panel adopted the conservative approach of using a 100th percentile in time (i.e. the all-time high concentration as calculated with the simple analytical model) in combination with a 90th spatial percentile. As will be shown by calculations with numerical models in Section 4.5, there are generally only small differences between the peak concentrations from different years.

The simple analytical model considers only processes within the soil matrix. So above-ground plant processes, soil photolysis and volatilisation from soil do not play a role in the scenario-selection procedure and thus vulnerability maps will not reflect the effect of these processes. Using a model that includes these processes for scenario selection at the EU level is not possible on the basis of current knowledge. The consequence of this restriction is that the selected spatial 90th percentile may be inaccurate for substances whose behaviour is dominated by these processes. So the selection procedure is targeted to applications of substances in crops where most of the substance penetrates into the soil.

4.2.4. Illustrative calculations with the simple analytical model for the area of annual crops in the whole EU

The simple analytical model uses the Arrhenius-weighted mean temperature (Eqn 16). This was calculated from the maps of the mean monthly temperatures. The map of the Arrhenius-weighted temperature is also available at the JRC website (<http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/>). The difference between the Arrhenius-weighted mean temperature and the arithmetic mean

temperature generally increased from west to east (Figure 10). The background to this is that use of the Arrhenius-weighted mean temperature leads to higher temperatures in climatic zones where the difference between summer and winter is higher, as in continental and Mediterranean climates (Figure 8).

Figure 11 shows illustrative calculations of concentration maps calculated with the simple analytical model using the data available at $1 \times 1 \text{ km}^2$ for the whole EU for the substances P1, P2 and P3 (taken from EFSA, 2010b). The calculations are for an ecotoxicological averaging depth of 20 cm and it was assumed in the calculations that there is no uncertainty in the substance properties. The peak concentration in total soil ($C_{T,peak}$ from Eqn 6) is generally high in Northern Europe and low in Southern Europe. This is caused by the lower dry bulk density and the colder climate in Northern Europe. As could be expected from its longer half-life, substance P3 gives higher $C_{T,peak}$ values than substances P1 and P2. The peak concentration in the liquid phase ($C_{L,peak}$ from Eqn 7) shows an opposite spatial trend with high values in Southern Europe and low values in Northern Europe. The cause of this will be analysed in Section 4.2.6.

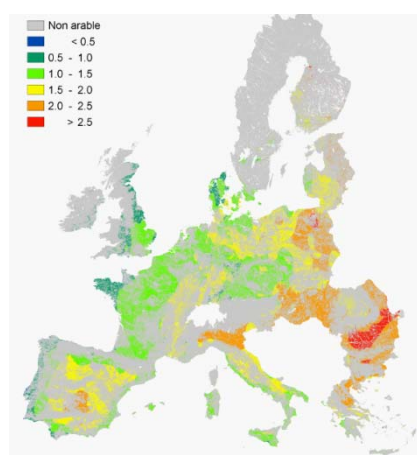


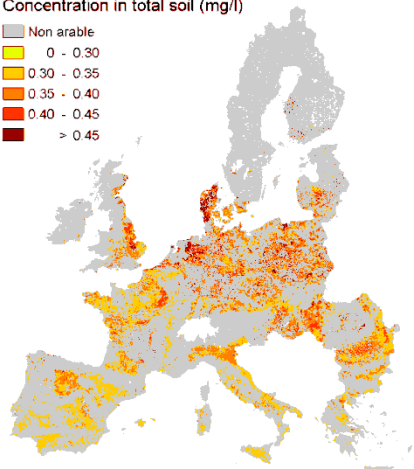
Figure 10: Difference between the Arrhenius-weighted mean temperature T_{Arr} (as defined by Eqn 16) and the arithmetic mean temperature calculated from monthly average temperatures for the years from 1960 to 1990 taken from the WorldClim dataset. ‘Non-arable’ means no annual crop.

Figure 12 shows the corresponding probability density functions for the regulatory zones North, Centre and South generated by these calculations. Indeed the concentrations in total soil show the highest values for the North and lowest for South, the opposite being the case for the concentrations in the pore water. In absolute terms the differences between the three zones are quite small. Let us consider the 90th-percentile values as an example. The North/South ratio of the concentration in total soil for this percentile ranges from 1.3 to 1.9 for the three substances and the South/North ratio of the concentration in the pore water ranges from 1.3 to 1.4. These are small differences between the three zones considering the considerable differences in climate and soil properties.

The probability density functions for the concentration in total soil are quite narrow (Figure 12): the 90th-percentile values are less than a factor two higher than the 10th-percentile values. The density functions for the concentration in liquid phase are wider: the 90th-percentile values are about a factor three higher than the 10th-percentile values. The maxima of the distributions for the concentration in the liquid phase are much higher than the 90th percentile (e.g. for P3, the 90th percentiles for the three zones are between 0.03 and 0.05 mg L^{-1} whereas the maximum is 6.6 mg L^{-1}). Further analysis showed that this maximum was caused by the grid cells with zero organic matter (as discussed in Section 4.2.2, these are artefacts in the organic-matter map).

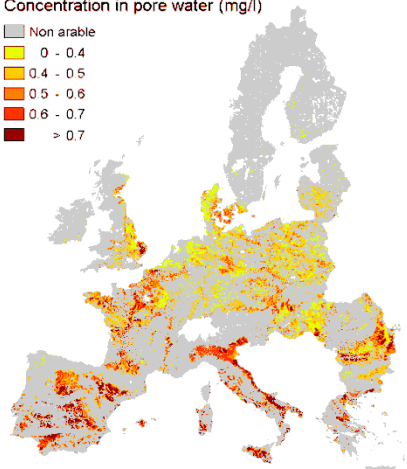
Substance P1: DegT50 = 15 d; K_{om} = 15 L/kg
Concentration in total soil (mg/l)

Non arable
0 - 0.30
0.30 - 0.35
0.35 - 0.40
0.40 - 0.45
> 0.45



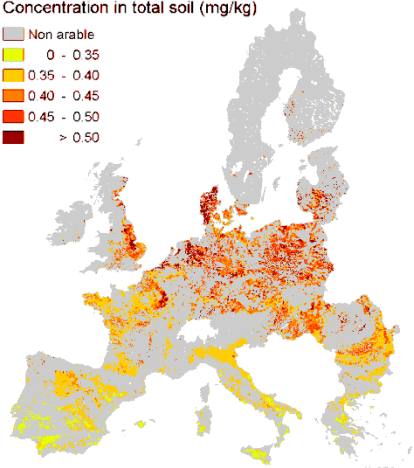
Substance P1: DegT50 = 15 d; K_{om} = 15 L/kg
Concentration in pore water (mg/l)

Non arable
0 - 0.4
0.4 - 0.5
0.5 - 0.6
0.6 - 0.7
> 0.7



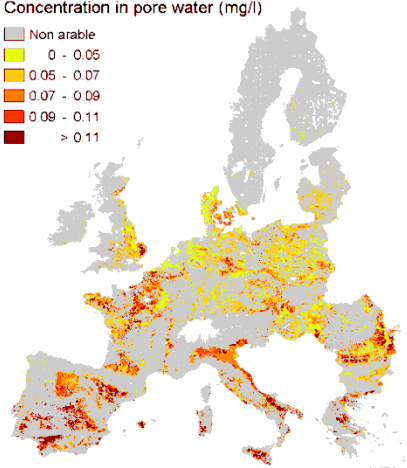
Substance P2: DegT50 = 50 d; K_{om} = 200 L/kg
Concentration in total soil (mg/kg)

Non arable
0 - 0.35
0.35 - 0.40
0.40 - 0.45
0.45 - 0.50
> 0.50



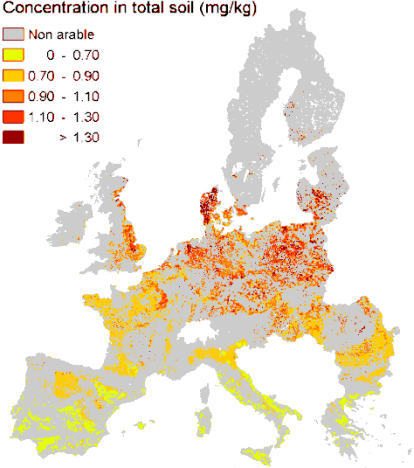
Substance P2: DegT50 = 50 d; K_{om} = 200 L/kg
Concentration in pore water (mg/l)

Non arable
0 - 0.05
0.05 - 0.07
0.07 - 0.09
0.09 - 0.11
> 0.11



Substance P3: DegT50 = 200 d; K_{om} = 1000 L/kg
Concentration in total soil (mg/kg)

Non arable
0 - 0.70
0.70 - 0.90
0.90 - 1.10
1.10 - 1.30
> 1.30



Substance P3: DegT50 = 200 d; K_{om} = 1000 L/kg
Concentration in pore water (mg/l)

Non arable
0 - 0.02
0.02 - 0.03
0.03 - 0.04
0.04 - 0.05
> 0.05

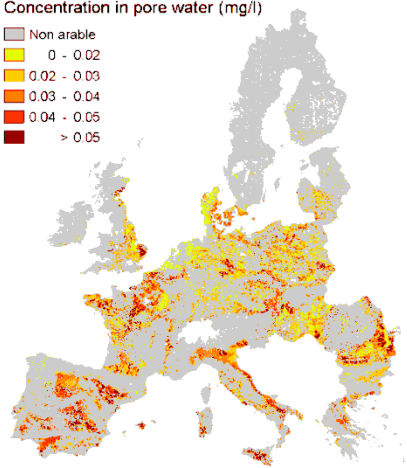


Figure 11: Peak concentration of the substances P1, P2, and P3 in total soil (left) and concentration in pore water (right) as calculated with the simple analytical model for an annual dose of 1.0 kg ha^{-1} , $z_{eco} = 20 \text{ cm}$ and $z_{til} = 20 \text{ cm}$ (taken from EFSA, 2010b). ‘Non-arable’ means no annual crop. Note that the resolution of the maps does not allow inspection of individual grid cells.

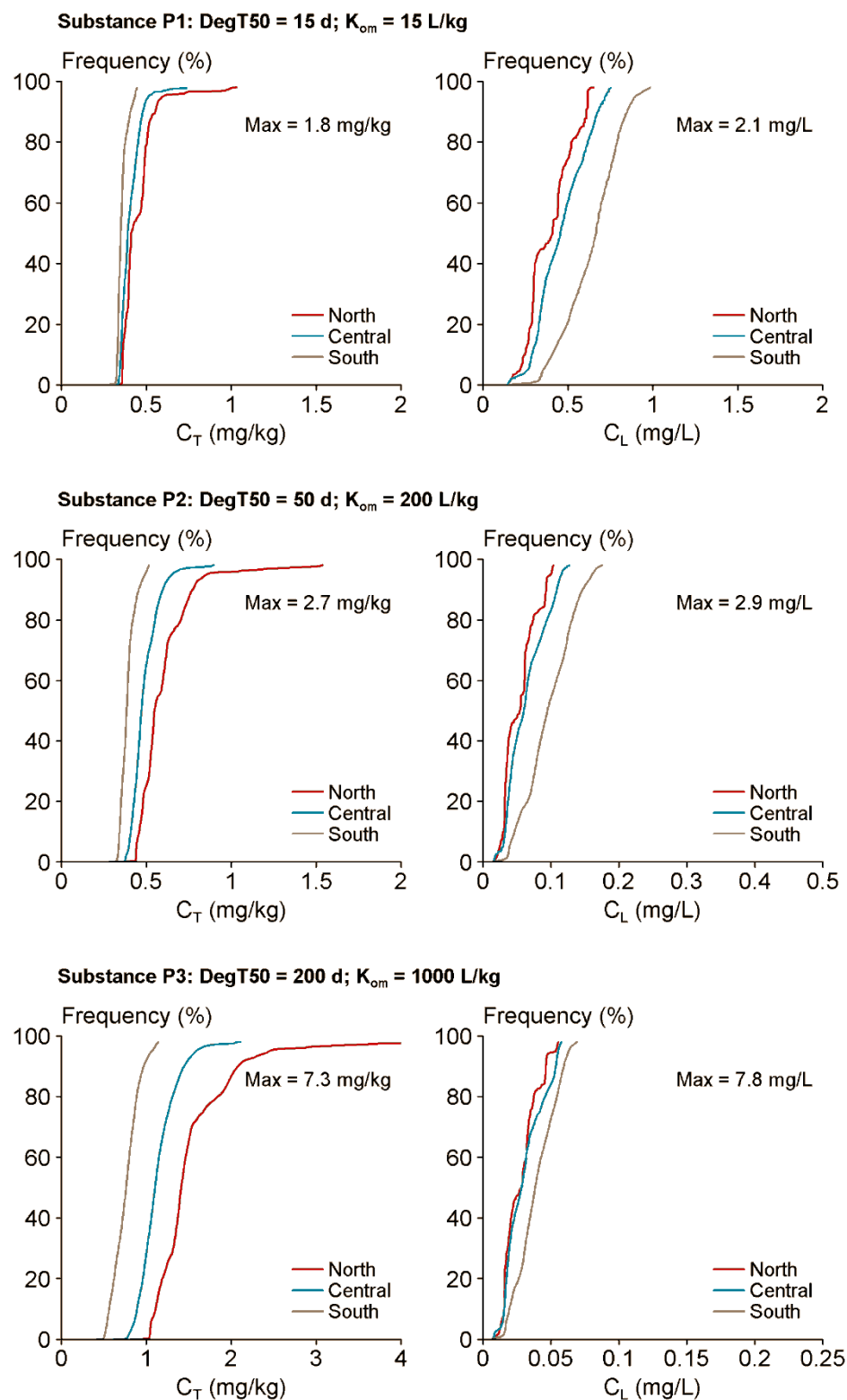


Figure 12: Spatial frequency distributions in the regulatory zones North, Centre and South of the peak concentration of the substances P1, P2, and P3 in total soil (left) and concentration in pore water (right) as calculated with the simple analytical model considering only annual crops for an annual dose of 1.0 kg ha^{-1} , $z_{eco} = 20 \text{ cm}$ and $z_{til} = 20 \text{ cm}$ (taken from EFSA, 2010b).

4.2.5. *Handling of uncertainty in soil and substance properties in the scenario-selection procedure*

The illustrative calculations (Figures 11 and 12) did not take into consideration any uncertainty in the soil or substance parameters of the simple analytical model. Including such uncertainties will lead to more diffuse maps and to probability density functions that show more spread (EFSA, 2010b). As described in Section 4.2.3, our target is to assess the spatial 90th-percentile PEC using the simple analytical model. So this 90th-percentile PEC will shift to higher values if uncertainty in soil and substance parameters is included. Therefore the effect of this uncertainty needs to be considered.

Ultimately Tier 2A has to consist of deterministic scenarios that can be used simply and so without the need to perform Monte-Carlo simulations for every exposure assessment. Moreover (as described in Section 4.1), a boundary condition was stipulated that the median substance properties (*DegT50* or *K_{om}*) from the dossier should be used in all tiers including Tier-2A scenario calculations. To fulfil these boundary conditions, EFSA (2010b) analysed the effect of uncertainties in soil and substance properties. Spatial probability density functions of concentrations of the substances P1, P2 and P3 were calculated with the simple analytical model for the EU-15 map described by Tiktak *et al.* (2004). This map (consisting of 1051 scenarios) was used because the data described in Section 4.2.2 were not then available to EFSA (2010b). Uncertainties in both soil properties and in substance properties were considered in the calculations. Peak concentrations in total soil and in pore water were calculated for ecotoxicological averaging depths (*z_{eco}*) of 1 and 20 cm.

The soil properties in the simple analytical model are (i) the organic-matter content, (ii) the volume fraction of water and (iii) the dry bulk density. EFSA (2010b) considered the uncertainty in the dry bulk density to have a larger effect on the probability density function of the concentrations than the uncertainties in organic-matter content and volume fraction of water. Therefore only uncertainty in dry bulk density was included. The uncertainty in the dry bulk density was simulated using a random term that was added to the bulk density. The random term was normally distributed with a mean of 0 and a standard deviation of 0.15 kg L⁻¹. The substance properties in the simple analytical model are the *DegT50* and the *K_{om}*. Based on Walker & Thompson (1977) and Allen & Walker (1987), the CV of both *DegT50* and *K_{om}* was assumed to be 0.25 and both were assumed to be lognormally distributed.

The calculations for these three substances using this database showed that the spatial 90th-percentile of the PEC calculated including these uncertainties corresponded to approximately the spatial 95th-percentile of the PEC calculated with the geomeans of the *DegT50* and *K_{om}*. This 95th percentile was the average of twelve values (three substances and four types of concentration) which ranged from 93 to 96. EFSA (2010b) concluded that the scenario-selection procedure should be based on the spatial 95th-percentile of the PEC. This enables exposure assessments in Tier 2A based on deterministic soil properties and the geomean or median *DegT50* and *K_{om}* values from the dossiers.

At a later stage, the Panel (EFSA, 2010d) considered a wider range of *DegT50* values than EFSA (2010b) and concluded that a CV of 0.5 for the *DegT50* within one of the three regulatory zones is more appropriate. Based on the literature review by Wauchope *et al.* (2002), the Panel considers also for the *K_{om}* a CV of 0.5 to be more appropriate than the value of 0.25 used in EFSA (2010b). Assuming a CV of 0.25 for both *DegT50* and *K_{om}* led to a shift from the 90th to the 95th spatial percentile. Assuming a CV of 0.50 for both *DegT50* and *K_{om}* will lead to a shift of the spatial percentile to a value between the 95th and the 100th percentile. A calculation for the peak concentration in the pore water of substance P3 and *z_{eco}* = 20 cm, assuming a CV of 0.50 and using the same procedure as for the CV of 0.25, showed a shift from the 96th to the 98th spatial percentile. The concentration at the 98th spatial percentile was about 30% higher than at the 96th percentile. It is expected that this shift in concentration for other cases (P1 or P2, other types of concentration) will be smaller (see Figures B9 and B10 of EFSA, 2010b). Given the time limitations, the Panel was unable to perform further calculations on the spatial shift with a CV of 0.50 and proposes to stick to the shift to the 95th spatial percentile. The Panel recommends performing at a later stage further calculations on

this spatial shift considering the maps for the regulatory zones that were also used for the scenario selection (see Section 4.2.2).

4.2.6. Selection of the scenarios

So the next step was to find scenarios (using the compiled data and the simple analytical model) that generate a 95th spatial PEC. As described in Section 4.1, the scenario-selection procedure will be based only on peak concentrations (so no TWA concentrations) considering the full 1-20 cm range of the ecotoxicological averaging depth, z_{eco} . The problem to be solved was that a spatial 95th-percentile scenario selected for a certain substance and a certain z_{eco} will differ from such a scenario selected for another substance or another z_{eco} . EFSA (2010b) adopted therefore the following scenario-selection procedure:

- Maps of the peak concentration in total soil and the peak concentration in the liquid phase were created for z_{eco} of 1 and 20 cm and for 19 parent substances with $DegT50$ ranging from 10 to 1000 d and K_{om} ranging from 10 to 1000 L kg⁻¹ (see Appendix III for the $DegT50$ - K_{om} combinations). Each concentration map (38 in total) was transformed into a vulnerability map by assigning to each grid cell the percentile corresponding to its concentration. For the calculation of this percentile, it was assumed that each pixel had equal weight. In principle, it would have been better to weight each grid cell with its fraction of surface area of annual crops. From each vulnerability map, the grid cells with a percentile between 95 and 97% were selected; this range was chosen in order to obtain enough pixels to choose from in the next step and to ensure that the resulting scenario was conservative enough in obtaining the spatial 95th-percentile PEC.
- In a final step, the 95-97% vulnerability maps of all 19 PPPs and the two ecotoxicological averaging depths were overlain and those grid cells that were common in all maps were considered candidate scenarios.

This procedure resulted in a large number of candidate scenarios for the regulatory zones South and Centre but only in a small number for the zone North. The selection was narrowed down by requiring that the candidate scenario should have both organic-matter content and an Arrhenius temperature that was within 1% of the mean of all candidate scenarios in a regulatory zone. This was done to avoid selection of scenarios with extreme properties. This procedure resulted in the scenarios with the properties shown in Tables 3 and 4.

For the peak concentration in total soil, the simple analytical model only contains as scenario parameters the dry bulk density and the Arrhenius-weighted mean temperature. By combining Eqns 1, 2, 3, 4 and 6, it can be shown that the concentration in total soil increases with decreasing bulk density and with decreasing temperature. So the selected scenarios in Table 3 should have comparatively low bulk densities and low temperatures and this is indeed the case. They have also relatively high organic-matter contents because the dry bulk density decreases with increasing organic matter (see Eqn 21). The organic-matter content of the scenario for the zone Centre (8.6%) was the spatial 89th percentile of the organic-matter frequency distribution in this zone. So the percentile of the organic-matter content of this scenario is less extreme than the target percentile of the concentration in total soil (i.e. 95th).

Table 3: Properties of the selected scenarios for the concentration in total soil. T_{arit} is the arithmetic mean temperature and T_{Arr} is the Arrhenius-weighted mean temperature.

Zone	Country in which scenario is located	T_{arit} (°C)	T_{Arr} (°C)	Texture	Volume fraction of water, θ (m ³ m ⁻³)	Dry bulk density, ρ (kg L ⁻¹)	f_{om} (%)
North	Estonia	4.7	7.0	Coarse	0.244	0.95	11.8
Centre	Germany	8.0	10.1	Coarse	0.244	1.05	8.6
South	France	11.0	12.3	Medium fine	0.385	1.22	4.8

For the peak concentration in the pore water, the relationships with the scenario parameters are somewhat more complicated. Let us consider these relationships in more detail. Eqn 7 can be rewritten as:

$$C_{L,peak} = \frac{A \left(\frac{1}{z_{eco}} + \frac{1}{z_{til}} \frac{X}{1-X} \right)}{\theta + \rho f_{om} K_{om}} \quad (22)$$

Eqn 22 implies that the effect of the Arrhenius-weighted temperature is the same as for the concentration in total soil: lower temperatures lead of course to higher concentrations. The effect of θ is only small because the product $\rho f_{om} K_{om}$ will usually be considerably larger than θ . The effect of f_{om} is not immediately clear because ρ is a decreasing function of f_{om} (Eqn 21). So the question is whether the product ρf_{om} decreases or increases with f_{om} . Calculations showed that this product is a continuously increasing function of f_{om} (at $f_{om} = 0$ $\rho f_{om} = 0$, at $f_{om} = 0.01$ kg kg⁻¹ $\rho f_{om} = 0.02$ kg L⁻¹, at $f_{om} = 0.10$ kg kg⁻¹ $\rho f_{om} = 0.10$ kg L⁻¹ and at $f_{om} = 0.20$ kg kg⁻¹ $\rho f_{om} = 0.15$ kg L⁻¹). So $C_{L,peak}$ is expected to decrease with increasing f_{om} and spatial 95th-percentile scenarios should therefore have low f_{om} values which is indeed the case (Table 4). The organic-matter content of the scenario for the zone Centre (1.8%) was the spatial 11th percentile of the organic-matter frequency distribution in this zone. So also here the percentile of the organic-matter content of the scenario is less extreme than the target percentile of the concentration (i.e. 95th, so the 5th for the organic-matter content).

Table 4: Properties of the selected scenarios for the concentration in the liquid phase. T_{arit} is the arithmetic mean temperature and T_{Arr} is the Arrhenius-weighted mean temperature.

Zone	Country in which scenario is located	T_{arit} (°C)	T_{Arr} (°C)	Texture	Volume fraction of water, θ (m ³ m ⁻³)	Dry bulk density, ρ (kg L ⁻¹)	f_{om} (%)	ρf_{om} (kg L ⁻¹)
North	Denmark	8.2	9.8	Medium	0.347	1.39	2.3	0.032
Centre	Czech Rep.	9.1	11.2	Medium	0.347	1.43	1.8	0.026
South	Spain	12.8	14.7	Medium	0.347	1.51	1.1	0.017

Once the scenarios have been selected, it is interesting from a regulatory point of view to analyse differences in the 95th spatial percentiles of $C_{T,peak}$ and $C_{L,peak}$ between the zones North, Centre and South. The concentration in total soil increases with decreasing bulk density and with decreasing temperature, and so the scenario properties in Table 3 imply that $C_{T,peak}$ values increase in the order North-Centre-South. The concentration in the liquid phase increases both with decreasing temperature and with decreasing ρf_{om} (see Eqn 22). The temperature decreases in the order South-Centre-North (Table 4) but note that ρf_{om} increases in this order. So these differences may compensate each other to some extent. EFSA (2010b) indicated that this compensating effect is caused by the opposite spatial

trends of organic matter and temperature in the EU. Calculations by EFSA (2010b) with the simple analytical model showed that differences in $C_{T,peak}$ values between the regulatory zones (based on Table 3) increased with increasing $DegT50$ and in the order South-Centre-North. Calculations also showed that differences in $C_{L,peak}$ values between the regulatory zones (based on Table 4) were mostly less than 20% and that the $C_{L,peak}$ increased in the order North-Centre-South (so opposite orders for $C_{T,peak}$ and $C_{L,peak}$ which is consistent with Figure 12).

4.3. Assessment of the crop extrapolation factors

The scenarios (Tables 3 and 4) were based on the 95th spatial percentile considering the total area of annual crops in each regulatory zone. However, the purpose of the exposure assessment is to consider either the total area of one of the CAPRI crops or crop groups or to consider the area of any other crop (Section 1.4.3). The 95th spatial percentile depends of course on the statistical population of 1×1 km² pixels considered.

To assess the effect of the crop area for CAPRI crop or crop groups, we define a 95th-percentile crop ratio as follows:

$$\xi = \frac{P_{95,x}}{P_{95,annual}} \quad (23)$$

where $P_{95,x}$ is the spatial 95th percentile of the concentration for the area of crop x and $P_{95,annual}$ is the spatial 95th percentile of the concentration for the total area of annual crops. This ratio ξ applies to either $C_{T,peak}$ or $C_{L,peak}$ and to a specific substance in a certain regulatory zone. To assess the possible magnitude of ξ , EFSA (2010b) made calculations with the simple analytical model for most of the CAPRI crops or crop groups (Table 5) that are grown annually on land with a level surface (so excluding potatoes). This was done for the substances P1, P2 and P3 (Table 2). Note that durum wheat and soybean are relevant annual crops but their crop extrapolation factors have not yet been calculated. The Panel expects to include results of these calculations in the final Opinion.

There are also CAPRI crop groups such as ‘other cereals’ or ‘other root crops’. The Panel did not include these in Table 5 because such a crop group does not seem well enough defined to be of use in the registration procedure of a plant protection product.

CAPRI maps are also available for e.g. rice, potatoes, citrus, permanent grass, fruit trees, olive groves, vineyards and nurseries. These are not relevant for the exposure assessment described here but they may be useful for the development of future exposure assessments.

Table 5: CAPRI crops or crop groups included in the assessment of the crop extrapolation factors. An ‘X’ indicates that the crop extrapolation factor was calculated for the combination of regulatory zone and crop.

CAPRI crop or crop group	North	Centre	South
Barley	X	X	X
Durum wheat			
Oats	X	X	X
Rye	X	X	X
Soft wheat	X	X	X
Maize	X	X	X
Rape and turnip rape	X	X	X

Sugar beet	X	X	X
Fibre and other oilseed crops (flax and hemp)	X	X	X
Soybean			
Vegetables	X	X	X
Dry pulses	X	X	X
Sunflower		X	X
Tobacco			X

Considering the ranges of ζ values found for each regulatory zone and for each type of concentration (Table 6), on average ζ is expected to be 1 for each type of concentration because the sum of the areas of the CAPRI crops or crop groups included in Table 5 is expected to be close to the total area of annual crops. So, as would be expected, minima are below 1 and maxima are above 1 (Table 6). The Panel proposes to use the maxima of each of this group of values as the crop extrapolation factors to be used in Tiers 1 and 2A (Table 1) for the CAPRI crops or crop groups included in the assessment of the crop extrapolation factors (see Table 5).

Table 6: Ranges of crop 95th-percentile ratios ζ as defined by Eqn 23 found for the CAPRI crops included in Table 5 and the substances P1, P2 and P3 for the three regulatory zones and for both the concentration in total soil and the concentration in the liquid phase.

	$C_{T,peak}$		$C_{L,peak}$	
	minimum	maximum	minimum	maximum
North	0.64	1.79	0.87	1.02
Centre	0.74	1.16	0.93	1.15
South	0.86	1.07	0.86	1.13

The next step is to assess the effect of the crop area for any other crop than the CAPRI crop or crop groups included in Table 5. As described in Section 1.4.3, the crop lists used by the UK and Dutch registration authorities are very detailed and so there may be many crops other than the CAPRI crop or crop groups. Crop maps are not available for other crops at the EU level and so the approach based on Eqn 23 is not possible. Therefore EFSA (2010b) calculated the ratio χ defined as:

$$\chi = \frac{P_{100,annual}}{P_{95,annual}} \quad (24)$$

where $P_{100,annual}$ is the 100th percentile of the concentration distribution (either $C_{T,peak}$ or $C_{L,peak}$) of a certain substance for the total area of annual crops in one of the regulatory zones. This ratio χ was calculated for the substances P1, P2 and P3 and the three regulatory zones using the probability density functions shown in Figure 12 (so three χ values for each type of concentration in each regulatory zone). The grid cells with zero organic-matter contents were excluded from the calculation of $P_{100,annual}$ for $C_{L,peak}$ because these generated extremely high χ values for $C_{L,peak}$ and because these zero organic-matter contents are considered artefacts of the organic-matter map (see Section 4.2.2).

The ratio χ was at most 1.41 for the concentration in the liquid phase and at most 3.2 for the concentration in total soil (Table 7). The Panel proposes to use the maximum values for each regulatory zone as the crop extrapolation factors for crops other than the CAPRI crop or crop groups included in Table 5.

Table 7: Ranges of the ratio χ (defined by Eqn 24) calculated using substances P1, P2 and P3 for the three regulatory zones and for both the concentration in total soil and the concentration in the liquid phase.

	$C_{T,peak}$		$C_{L,peak}$	
	minimum	maximum	minimum	maximum
North	2.68	3.20	1.22	1.41
Centre	1.92	2.13	1.11	1.33
South	1.96	2.60	1.29	1.39

4.4. Parameterisation of the Tier-2A scenarios

The parameterisation of the Tier-2A scenarios was based on the properties described in Tables 3 and 4. EFSA (2012) described the parameterisation of the Tier-2A scenarios in detail, and so here only a few important aspects of this parameterisation are described.

The scenarios were parameterised for the PELMO and PEARL models because these have been used since 2000 for the assessment of leaching to groundwater at the EU level (FOCUS, 2000, 2009). The MACRO and PRZM models have also been used for the leaching assessment at the EU level and they have additionally been used for the assessment of exposure of aquatic organisms (FOCUS, 2001). The scenarios have not yet been parameterised for MACRO and PRZM because this would have required that experts from the teams responsible for the development and maintenance of these models to assist the PPR Panel during the development process of this Opinion (for example, to write sub-routines that generate the specific model output that is required for this exposure assessment and to perform calculations with example substances) and this was impossible at this stage. However the Panel encourages parameterising the scenarios for numerical models other than PELMO and PEARL, the only requirement being that the process descriptions in such numerical models have a similar or higher level of detail than those in PELMO and PEARL (PRZM and MACRO of course fulfil this requirement).

The MARS climate database was used as the source for the meteorological time series. So for each of the six scenarios, the MARS weather time series selected was that closest to the scenario location (with the exception of the North- $C_{T,peak}$ scenario for which the Jokioinen weather series of FOCUS, 2009, was used; see EFSA, 2012, for background). MARS weather data for the period 1990-2009 were used, converting these to a 66-year time-series using the rules described in FOCUS (2000). However, the Tier-2A scenarios were selected using air temperatures from the WorldClim database from the period 1960 to 1990 (see Section 4.2.2). The arithmetic mean temperatures from the MARS weather series were 0.5 to 1.7°C higher than those from the WorldClim series (Table 8). The causes of this systematic difference are not clear; the differences are too large to be attributable to climatic change only. The Panel used the WorldClim database for the scenario selection because this database had a much higher resolution (1×1 km²) than the MARS database (25×25 km²). Therefore the Panel considered it inconsistent to base the mean temperature level of the scenarios on the MARS database. For example, WorldClim may have selected a pixel for a scenario in Table 8 that is systematically colder than the average of the corresponding 25×25 km² MARS unit because a colder temperature gives a higher PEC percentile. It is then inconsistent to use the average of the MARS unit. Moreover, the cause of the systematically higher temperatures in the MARS database is not yet explained, this being an additional argument in favour of the WorldClim database (because colder temperatures lead to more conservative exposure assessment).

Therefore the daily air temperatures from the MARS database were scaled in such a way that the arithmetic mean temperature of each Tier-2A scenario (20-year time period) is equal to the arithmetic

mean temperature of the WorldClim time series. So the daily temperatures for the Tier-2A scenarios were calculated as follows:

$$T_{day,scenario} = T_{day,MARS} + T_{arit,WorldClim} - T_{arit,MARS} \quad (25)$$

where $T_{day,scenario}$ is the daily mean temperature in the Tier-2A scenario, $T_{day,MARS}$ is the daily mean temperature from the MARS time series, $T_{arit,WorldClim}$ is the arithmetic mean temperature of the selected Tier-2A scenarios based on the 1960-1990 WorldClim time series, and $T_{arit,MARS}$ is the arithmetic mean temperature of the 1990-2009 MARS time series.

So whereas the scenario selection was based on the Arrhenius-weighted mean temperature (T_{Arr}), it played no role in the parameterisation procedure for the meteorological time series. This is correct because the role of this temperature was to characterise better the annual course of time of air temperatures at each pixel. Once the appropriate pixel has been selected, T_{Arr} plays no further role and use of the closest MARS weather station ensures an appropriate annual course of the air temperature.

Table 8: Properties of the selected Tier-2A scenarios. $T_{arit,MARS}$ is the arithmetic mean air temperature of the MARS meteorological time series of the scenario and $T_{arit,WorldClim}$ is the arithmetic mean air temperature of the WorldClim meteorological time series of the scenario. The column 'FOCUS climatic zone' indicates where the scenario is located (based on FOCUS, 2009).

Zone	Type of concentration	$T_{arit,MARS}$ (°C)	$T_{arit,WorldClim}$ (°C)	Member state	FOCUS climatic zone	Irrigated
North	Total soil	6.15	4.7	Estonia	Jokioinen	No
Centre	Total soil	9.73	8.0	Germany	Châteaudun	Yes
South	Total soil	12.35	11.0	France	Kremsmünster	No
North	Pore water	8.66	8.2	Denmark	Hamburg	No
Centre	Pore water	9.76	9.1	Czech Rep.	Châteaudun	Yes
South	Pore water	13.94	12.8	Spain	Seville	Yes

Irrigation was included in the scenario if the corresponding FOCUS climatic zone (FOCUS, 2009) is irrigated (Table 8) and if the crop considered is irrigated (FOCUS, 2009). The crop parameters for each scenario were based on those for the corresponding climatic zone of FOCUS (2009).

The Tier-2A scenarios are to be based on a time series of 20 years of daily meteorological data such as rainfall and temperature following the same procedure as FOCUS (2000). FOCUS (2000, 2009) used a warming-up period of 6 years in the leaching simulations before starting the evaluation period for the leaching assessment. For the soil-exposure assessment, the warming-up period needs to be long enough to ensure that the plateau value of the exposure concentration is closely approximated before the evaluation period starts. Considering that thereafter at least 20 years are simulated and the all-time high concentration is used as endpoint, it seems not necessary to be very strict with respect to the fractional equilibrium (as defined in Eqn 19) reached at the end of the warming-up period. After a period of time corresponding to three effective half-lives, the fractional equilibrium is about 0.90 (Figure 9). Let us consider this to be a sufficiently strict requirement. The Panel proposes to require that the warming-up period should be long enough for a $DegT50$ at 20°C of 2 years because this is likely to cover nearly all plant protection products. The Arrhenius temperatures for the different scenarios (Tables 3 and 4) can be used to approximate the $DegT50_{eff}$ values as used in Eqn 20 (Table 9). As described above, the requirement for the minimum length of the warming-up period is three effective half-lives; this results in warming-up periods ranging from 10 to 21 years (Table 9), i.e. considerably longer than the six years considered by FOCUS (2000, 2009). The Panel proposes using warming-up periods that are at least as long as the periods in the last column of Table 9 or to take other measures to ensure that the correct all-time high concentration is calculated. Possibly this can

also be ensured by assuming at the start of the calculations that the concentration in total soil in the top 20 cm is equal to the plateau concentration predicted with the simple analytical model, followed by a warming-up period of six years (which are discarded from the assessment as described before).

Table 9: Effective *DegT50* values for the different scenarios corresponding with a *DegT50* of 2 year at 20°C. These values were calculated with the Arrhenius equation for the Arrhenius-weighted mean temperatures as indicated using activation energy of 65.4 kJ mol⁻¹.

Zone	Country in which scenario is located	Type of concentration	T_{Arr} (°C)	$DegT50_{eff}$ (year)	3 $DegT50_{eff}$ (year)
North	Estonia	Total soil	7.0	6.9	21
Centre	Germany	Total soil	10.1	5.1	15
South	France	Total soil	12.3	4.1	12
North	Denmark	Pore water	9.8	5.3	16
Centre	Czech Rep.	Pore water	11.2	4.6	14
South	Spain	Pore water	14.7	3.4	10

4.5. Example calculations with numerical models for Tier-2A scenarios

Example calculations were made with FOCUS_PEARL(v4.4.4) and FOCUS_PELMO(v4.4.3) models for (i) the 19 example parent substances described in Section 4.2.6 and Appendix III, (ii) all six scenarios, (iii) concentrations in pore water and in total soil, (iv) peak values and 14 and 56 d TWA values, and (v) $z_{eco} = 1$ cm and $z_{eco} = 20$ cm (see EFSA, 2012, for details). In these calculations, the warming-up period was fixed at six years. Calculations were made for sugar beet and winter wheat and a dose of 1.0 kg ha⁻¹ applied one day before emergence of the crop every year. Emergence for sugar beet was between 15 April and 25 May for all scenarios except for pore water in the South zone where emergence was on 10 November. Emergence for winter wheat was between 20 September and 30 November. Sugar beet was irrigated for part of the scenarios as indicated in Table 8 and winter wheat was never irrigated (based on FOCUS, 2009).

As an example (Figure 13), for two types of concentrations the differences between the two models are usually less than a factor 1.5 but occasionally larger. The differences were generally larger for the concentration in pore water than for the concentration in total soil. The differences larger than a factor 1.5 occurred only for pore-water concentrations of substances with short half-lives and $z_{eco} = 1$ cm. These differences were caused by differences in the simulated soil moisture contents in the top 1 cm in the first weeks after application. Differences between the two models were nearly always less than twofold (see EFSA, 2012, for details).

So there may be distinct differences between Tier-2A concentrations calculated with different numerical models. The choice of the numerical model may thus have an effect on the outcome of the risk assessment, and hence an additional source of uncertainty. If the margin of safety for the assessment of effects on organisms in soil is less than a factor of two, risk managers could consider requiring Tier-2A calculations with both PELMO and PEARL and to use the highest exposure concentration of the two models.

The differences in peak concentrations between the three regulatory zones as calculated with PEARL or PELMO were always less than a factor of two for $z_{eco} = 20$ cm (Figure 14). For $z_{eco} = 1$ cm (results

not shown in Figure 14), the differences between the zones were usually smaller than those found for $z_{eco} = 20$ cm. The concentration in total soil decreased in the order North-Centre-South whereas the concentration in pore water decreased usually in the order South-Centre-North. These results are consistent with those found by EFSA (2010b) for the simple analytical model as discussed at the end of Section 4.2.6.

As described in Section 4.2.3, the Panel adopted the conservative approach of using a 100th percentile in time (i.e. the all-time high concentration as calculated with the simple analytical model) in combination with a 90th spatial percentile (note that in tiers that use numerical models the highest of 20 values is taken which is not a 100th but a 97.5th percentile). To assess the effect of this conservative assumption, PELMO and PEARL calculations were made for application of substances P1, P2 and P3 in sugar beet at a dose of 1.0 kg ha⁻¹ applied one day before emergence every year using $z_{eco} = 20$ cm for all six scenarios (Table 9) and the differences between the 20 annual peak values were inspected. As described in Section 1.4.5, the target was to obtain the 90th percentile from the spatio-temporal population of concentrations. The Panel considers it unlikely that such a 90th percentile would have been based on a time percentile that is lower than the 70th percentile. Therefore we compared the differences between the six highest concentrations (i.e. the 72.5th to the 97.5th temporal percentiles). For PEARL the 97.5th percentile of P1, P2, and P3 was on average only 6% higher than the 72.5th percentile (average of 18 cases considered). The range of this percentage was from 0 to 30%. For PELMO the 97.5th percentile of P1, P2, and P3 was on average only 4% higher than the 72.5th percentile (average of 18 cases considered). The range of this percentage was from 1 to 10%. So there are usually only small differences between the 72.5th and the 97.5th temporal percentiles of the peak concentrations. This indicates that the effect of this conservative assumption is usually small.

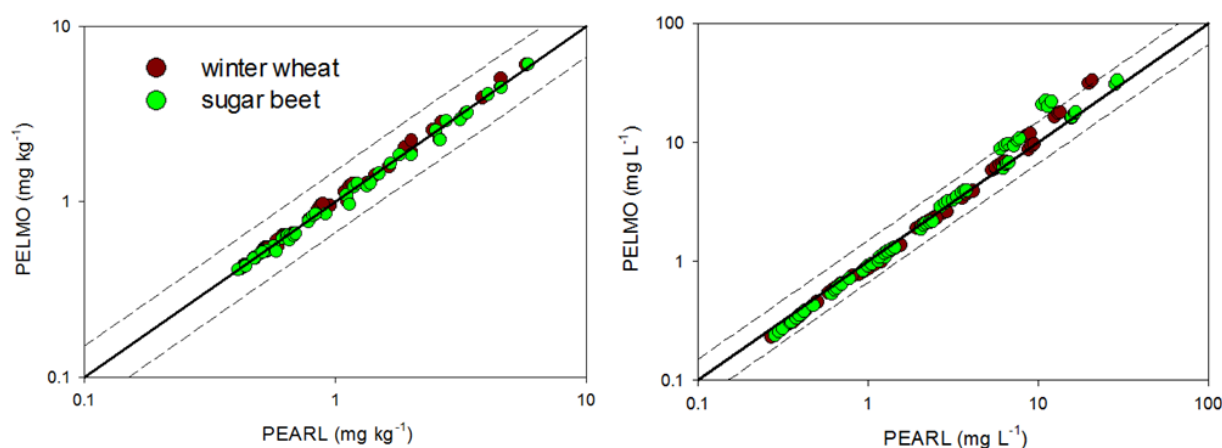


Figure 13: Comparison of two types of concentration calculated with the PELMO and PEARL models for the three scenarios and for the 19 example parent substances and for annual applications in two crops on the day before crop emergence. The left graph is for the peak concentration in total soil and $z_{eco} = 20$ cm and the right graph is for the 14-d TWA concentration in the liquid phase and $z_{eco} = 1$ cm. The solid line is the 1:1 line and the dashed lines are $PELMO = 2/3 \text{ PEARL}$ and $PELMO = 3/2 \text{ PEARL}$.

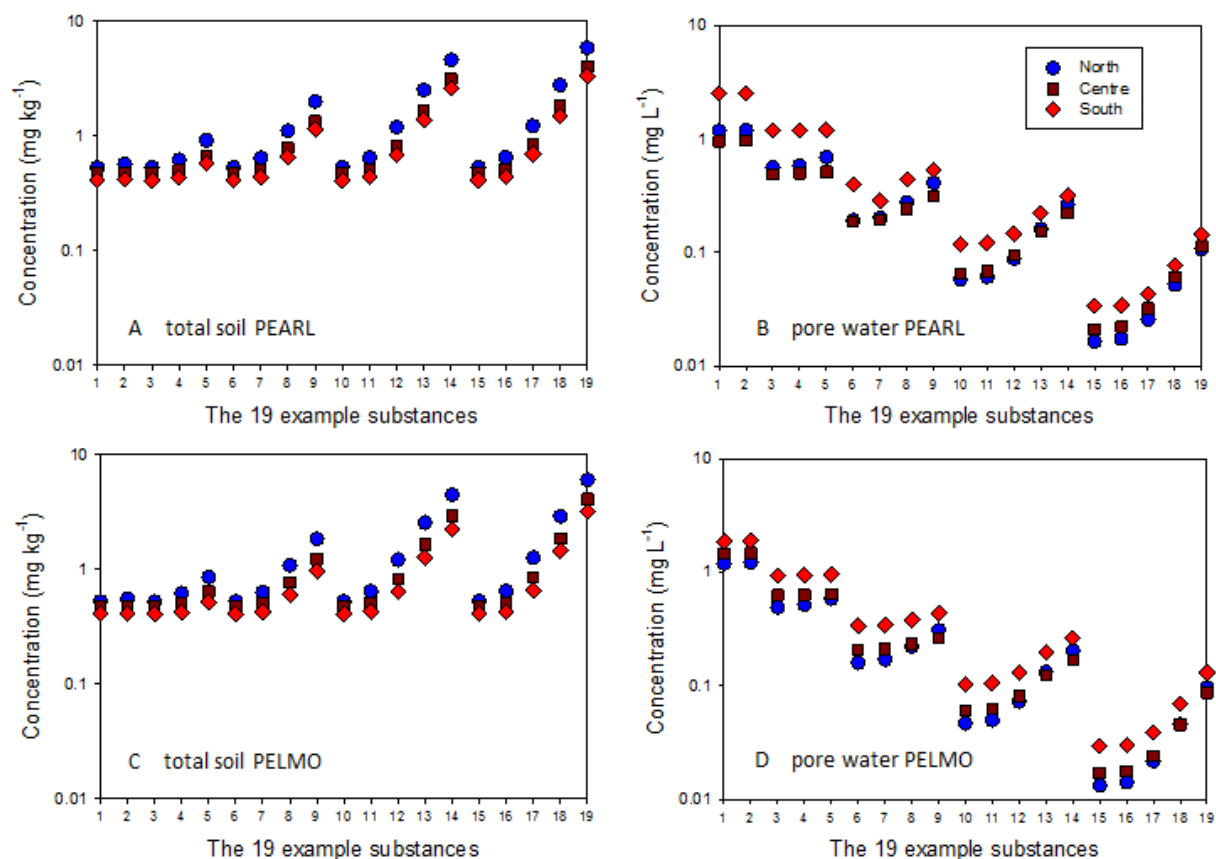


Figure 14: Peak concentrations in total soil (parts A and C) and in pore water (parts B and D) as calculated with the PEARL model (parts A and B) and with the PELMO model (parts C and D) for the three Tier-2A scenarios, the 19 example substances, annual application in sugar beet on the day before crop emergence, and $z_{eco} = 20$ cm.

5. PARAMETERISATION OF TIER 1 INCLUDING ASSESSMENT OF THE MODEL ADJUSTMENT FACTOR

Tier 1 was based on the simple analytical model as described before. The scenarios considered in Tier 1 were the same as in Tier 2A because this provides the best possible link between these two tiers. So the parameters for the Tier-1 model were set equal to those of the selected Tier-2A scenario described in Tables 3 and 4. The temperature in the Tier-1 model was the Arrhenius-weighted mean (T_{Arr}) from these tables because this ensures the best link with the Tier-2A scenarios.

The only remaining issue is the assessment of the model adjustment factor, F_{mo} (Eqn 15). This factor was assessed by performing calculations both for Tier-1 and Tier-2A scenarios. No crop safety factors were considered in these calculations because the same values of these factors are needed in Tier 1 and Tier 2A. So the comparison focuses on the differences between the two types of model in these two tiers.

The Tier-2A calculations were performed with the PELMO and PEARL models assuming a warming-up period of six years. The calculations were performed for the same cases as described in Section 4.6. In addition, calculations were also performed for a soil metabolite that was formed from the 19 parent substances. The properties of this metabolite were the same for all the parent substances: its $DegT50$ at 20°C was 100 d, its K_{om} was 50 L kg⁻¹, its formation fraction was 0.25 and its molar mass was assumed to be equal to that of the parent substance. In addition to the single application on the day before emergence, multiple applications within one year were also considered (1.0 kg ha⁻¹ one day before emergence, 1.0 kg ha⁻¹ at 30 d after emergence and 1.0 kg ha⁻¹ at 60 d after emergence). For these multiple applications, it was assumed that crop interception did not occur, as this approach kept the assessment of the model adjustment factor as simple as possible. For all these cases, Tier-1 calculations were also performed and plotted against the Tier-2A results (see EFSA, 2012, for these plots). Both peak concentrations and TWA values for 14 and 56 days were calculated both for $z_{eco} = 1$ cm and $z_{eco} = 20$ cm. From the plot for each zone and for each type of concentration, the maximum model adjustment factor was determined.

The warming-up period may have been too short for two of the 19 substances which had a $DegT50$ of 1000 days but this $DegT50$ is also larger than the upper limit of two years that was used to derive the required warming-up periods in Table 9.

The maximum model adjustment factor for the concentration in total soil was as low as 1.02-1.04 for the peak concentration for $z_{eco} = 1$ cm (Table 10). For all zones, the maximum factor for this concentration increased with increasing length of the TWA period to at most 1.6 for the TWA of 56 days (Figure 15A). The same trend was observed for the concentration in total soil for $z_{eco} = 20$ cm (Figure 15B). The maximum model adjustment factor for the peak concentration was at most 1.29, and so higher than the maximum for $z_{eco} = 1$ cm. The maximum model adjustment factor for the pore water did not show a clear increasing trend with increasing length of the TWA period (Figures 13C and 13D). However, nearly all factors for the pore-water concentration were higher than the corresponding factors for the concentration in total soil.

The Panel proposes the following values for the model adjustment factor F_{mo} :

$F_{mo} = 1.1$ for the peak concentration in total soil for $z_{eco} = 1$ cm;

$F_{mo} = 1.3$ for the peak concentration in total soil for $z_{eco} = 2.5, 5$ or 20 cm;

$F_{mo} = 1.7$ for all TWA concentrations in total soil for $z_{eco} = 1, 2.5, 5$ or 20 cm;

$F_{mo} = 2.0$ for all concentrations in pore water for the zones North and Central for $z_{eco} = 1, 2.5, 5$ or 20 cm

$F_{mo} = 3.0$ for all concentrations in pore water for the zone South for $z_{eco} = 1, 2.5, 5$ or 20 cm.

However, these should be applied with the restriction that the calculated Tier-1 TWA concentration is smaller than or equal to the Tier-1 peak concentration. This is done to avoid Tier-1 TWA concentrations for persistent compounds being higher than the corresponding peak concentrations.

These model adjustment factors are also valid for Tiers 2B and 2C as explained in Chapter 2. The restriction, that the calculated TWA concentration is smaller than or equal to the peak concentration, applies also to these tiers.

The assessment of the model adjustment factor as described above did not include calculation of crop interception and simulation of plant processes in Tier 2A. This is a conservative approach which was done to keep this assessment as simple as possible. So the differences between the concentrations calculated with the simple analytical model and those calculated with the numerical models (Table 10 and Figure 15) are not an accurate indication of the differences found in regulatory practice. For example, spray applications to fully grown crops may result in Tier-2A concentrations that are much lower than Tier-1 concentrations. More detailed information about the simulation results can be found in EFSA (2012).

Table 10: Maximum values of the model adjustment factor (F_{mo} as defined by Eqn 15) derived from the comparison between calculations with the simple analytical model and calculations with PELMO or PEARL for the different concentration endpoints.

Endpoint concentration	Ecotoxicological averaging depth z_{eco} (cm)	Zone	Model adjustment factor for concentration based on the specified endpoint		
			Peak	TWA of 14 d	TWA of 56 d
Total soil	1	North	1.03	1.07	1.27
Total soil	1	Centre	1.04	1.16	1.61
Total soil	1	South	1.02	1.13	1.41
Total soil	20	North	1.24	1.25	1.29
Total soil	20	Centre	1.29	1.30	1.61
Total soil	20	South	1.20	1.21	1.45
Pore water	1	North	1.62	1.64	1.17
Pore water	1	Centre	1.79	1.47	1.35
Pore water	1	South	2.64	2.13	1.90
Pore water	20	North	1.59	1.64	1.46
Pore water	20	Centre	1.72	1.63	1.86
Pore water	20	South	2.64	2.55	2.89

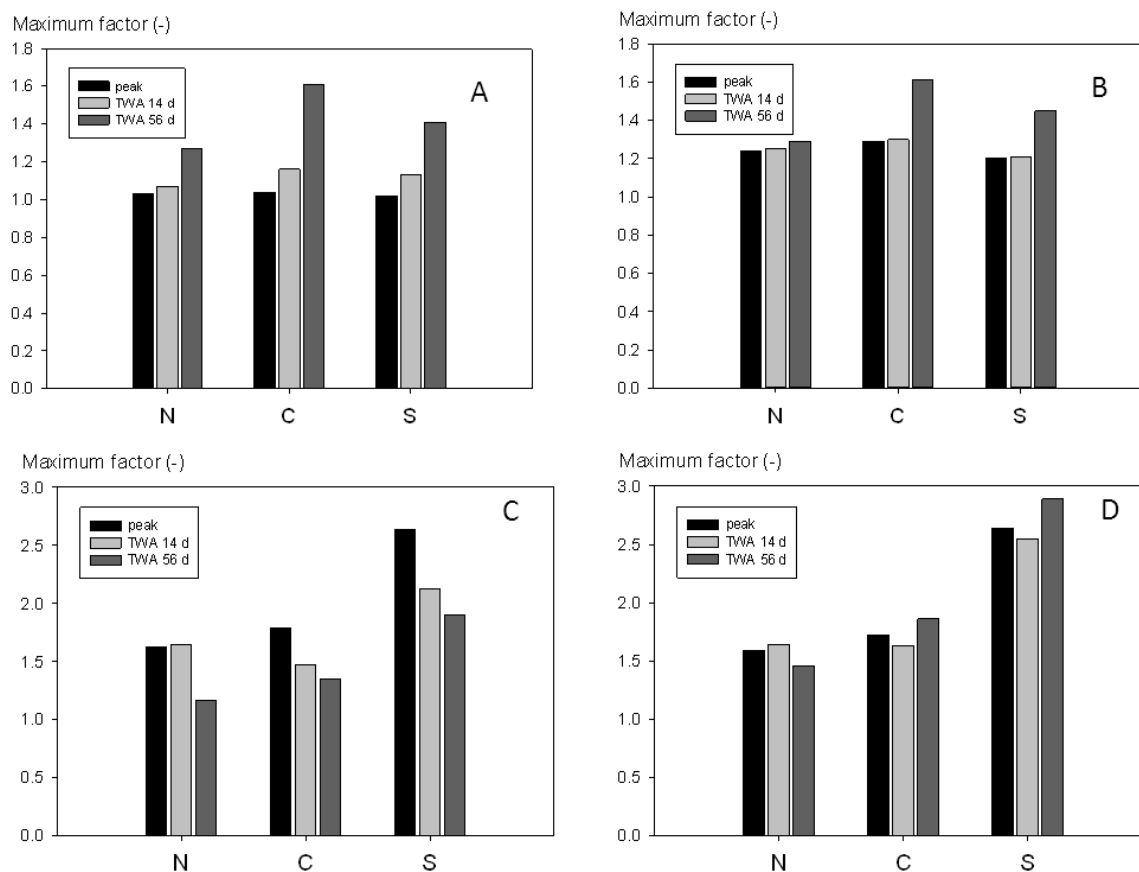


Figure 15: Maximum values of the model adjustment factor for the three zones and peak concentrations and 14-d and 56-d TWA concentrations as indicated. Parts A and B are for the concentration in total soil and $z_{eco} = 1$ and 20 cm, respectively; Parts C and D are for the concentration in pore water and $z_{eco} = 1$ and 20 cm, respectively. Note the difference in scale of the vertical axes between parts A/B and parts C/D.

6. DESCRIPTION OF THE OTHER TIERS

6.1. Tier 2B

Tier 2B provides the option of an exposure assessment with the simple analytical model for a particular crop and a particular substance (Figure 6). This has to be based on the spatial data described in Chapter 4 plus the following maps (at the resolution of $1 \times 1 \text{ km}^2$ available at the JRC website):

- pH measured in water (at a solid:liquid ratio of 1:2.5) of the top 30 cm of the soil
- fraction of area grown with one of the CAPRI crops or crop groups in a certain year.

As described in Section 1.4.3, the exposure assessment is developed for two spatial statistical populations: (i) one of the CAPRI crops or crop groups included in Table 5, and (ii) any other crop. If the exposure assessment is for a CAPRI crop or crop group included in Table 5 or if the crop map of the other crop is available to the risk assessor, the procedure is straightforward: calculate the 95th spatial percentile of the concentration and no crop extrapolation factors are needed. However, if for the other crop no map is available to the risk assessor, then the 95th spatial percentile has to be calculated using the K_{om} - $DegT50$ properties of this substance for the total area of annual crops and crop extrapolation factors have to be used as in Tier 1 and 2A.

The 95th spatial percentile for Tiers 1 and 2A was based on calculations with 19 example substances spanning a wide range of properties, and a pixel was selected that was in the 95-97th percentile range for all substances. In Tier 2B, the 95th spatial percentile is based on the K_{om} - $DegT50$ combination of this substance. So for substances whose $DegT50$ and/or K_{om} are not related to soil properties, it is possible that the Tier-2B scenario is more conservative than the corresponding Tier-1 or Tier-2A scenario. This could have been overcome by introducing something like a 'generic substance extrapolation factor' in Tier 1. The Panel did not do so because the 95-97th percentile range used for Tiers 1 and 2A is already on the safe side for the assessment of the 95th percentile. Thus it is considered very unlikely that Tier 1 is less conservative than Tier 2B as a result of substance properties outside those of the 19 example substances.

In Tier 2B, it suffices to calculate simply the 95th spatial percentile of the PEC of the required type of concentration without specifying the corresponding scenario. The procedure to find this 95th spatial percentile of the PEC with the simple analytical model is as follows:

- apply the land-use mask of the annual crops described in Section 4.2.2 to all maps.
- check the underlying maps and eliminate pixels that have unrealistic properties (e.g. zero organic-matter contents).
- based on the map of the relevant crop or crop group, create a map of the required type of concentration ($C_{L,peak}$ or $C_{T, peak}$ or any of the TWA averages) for the required ecotoxicological averaging depth (z_{eco}) and for the $DegT50$ - K_{om} properties of this substance.
- calculate from this concentration map the cumulative frequency distribution of PEC values. In this calculation the PEC of each $1 \times 1 \text{ km}^2$ pixel should get a weight that is proportional to the fraction of surface area grown with this crop or crop group.
- take the 95th-percentile PEC from this cumulative frequency distribution.

The scenario-selection procedure for the Tier-2A scenarios was based on $C_{L,peak}$ or $C_{T, peak}$ whereas in Tier 2B a spatial 95th-percentile of the PEC for one of the TWA concentrations is based on the spatial frequency distribution of this TWA concentration. Therefore it is possible in theory that a TWA concentration derived from Tier 2A or Tier 1 is less conservative than the TWA concentration from Tier 2B. Therefore the Panel made calculations with the simple analytical model for the 19 example parent substances as in Section 4.2.6, the six scenarios (Tables 3 and 4), $z_{eco} = 1$ or 20 cm, concentrations both in total soil and in the liquid phase and considering both peak concentrations and TWA concentrations for 7, 14, 28 and 56 days. For each of these 1140 combinations, the scenario PEC was calculated and also the spatial 95th-percentile of the PEC in the corresponding regulatory zone. The spatial 95th-percentile of the PEC so calculated was about equal to or lower than the scenario PEC.

So Tier-1 TWA concentrations are highly unlikely to be less conservative than Tier-2B TWA concentrations for parent substances.

Should a crop map be available, the Panel considers it defensible to use the Tier-2B procedure to refine the crop extrapolation factor for the type of concentration that is considered in Tier 2B and to use this refined factor in Tier 2A, thus replacing the conservative default values (the maxima in Tables 6 and 7) by a crop-specific and substance-specific value. This could be done by calculating the spatial 95th percentile of the PEC both for the crop considered and for the total area of annual crops. The crop extrapolation factor can then be calculated with Eqn 23.

6.2. Tier 2C

Tier 2C offers the possibility of incorporating the effect of crop interception in the PEC calculation with the simple analytical model carried out for Tier 2B. This has to be based on a conservative assessment of this effect based on simulations with the numerical models for the Tier-2A scenarios.

The numerical models simulate plant processes of the substance including wash-off. So simulations with these models for the Tier-2A scenarios generate annual amounts of substance that are washed off from the plants to the soil. In case of application every three years, the instruction is to sum up for every three-year period the amount that reached the soil surface at the moment of application and the amounts that were washed off to the soil. This gives 20 amounts because there are 20 three-year periods in such a case. Then take the maximum of these 20 values and to divide this by the total dosage in the application year, giving the maximum of the fraction that reached the soil, $F_{soil,max}$. For application every two years and every year, the instruction is to follow the same procedure to calculate $F_{soil,max}$ but now for two-year and one-year periods, respectively. The PEC of Tier 2C can be simply calculated from the corresponding PEC of Tier 2B with:

$$PEC_{2C} = F_{soil,max} PEC_{2B} \quad (26)$$

6.3. Tier 3

Tier 3 offers the possibility of simulating exposure concentrations with the numerical models for crop-specific and substance-specific scenarios focusing only on the type of concentration that is required. As a consequence, neither a crop extrapolation factor nor a model adjustment factor are needed in Tier 3 (see Table 1), which may lead to a considerably lower exposure concentration.

The Tier-3 scenario is selected with the simple analytical model using the procedure to find the scenario for the 95th spatial percentile:

- apply the land-use mask of the annual crops described in Section 4.2.2 to all maps.
- based on the map of the relevant crop or crop group, create individual maps for each endpoint (e.g. $C_{L,peak}$ or $C_{T,peak}$ or any of the TWA concentrations for z_{eco} of 1, 2.5, 5 or 20 cm) and for the $DegT50 - K_{om}$ properties of this substance; so this gives only one map that applies only to the type of concentration considered in one of the regulatory zones.
- transform the concentration map into a vulnerability map by assigning to each grid cell the percentile corresponding to its concentration. In the calculation of this percentile, each $1 \times 1 \text{ km}^2$ pixel should get a weight that is proportional to the fraction of surface area grown with this crop or crop group.
- select from the vulnerability map the grid cell with the percentile that is closest to 95%.
- use this grid cell to parameterise the scenario.

The consequence of this procedure is that different scenarios will be selected for different types of concentration.

The parameterisation of the Tier-3 scenario has to be based on the same procedures as followed for the Tier-2A scenarios (Section 4.4) with the exception of the selection of the time series of meteorological data. The procedure described in Section 4.4 would lead to the need to obtain new MARS weather data for each Tier-3 scenario which may be time consuming. To avoid this delay, the instruction is to take the MARS weather series from the corresponding climatic zone of the FOCUS groundwater scenarios (using the map of these climatic zones shown in Figure 16 which is available at <http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/>) and to scale the daily values of the minimum and maximum air temperature of this MARS weather series to the arithmetic mean monthly temperature of the corresponding Tier-3 scenario using an approach similar to Eqn 25:

$$T_{day,scenario} = T_{day,MARS} + T_{arit,WorldClim,month} - T_{arit,MARS,month} \quad (27)$$

where $T_{arit,WorldClim,month}$ is the arithmetic mean monthly temperature of the selected Tier-3 scenario based on the 1960-1990 WorldClim time series, and $T_{arit,MARS,month}$ is the arithmetic mean monthly temperature of the MARS time series taken from the FOCUS scenarios (given in Appendix IV). The monthly average temperatures of the WorldClim time series are available at <http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/>. Use of this monthly mean temperature is necessary to ensure that the Arrhenius-weighted mean temperature of the weather series is approximately equal to that of the selected Tier-3 scenario. This is necessary because there are considerable differences between the spatial patterns of (i) the difference between the Arrhenius-weighted mean temperature and the arithmetic mean temperature in Figure 10 and (ii) the FOCUS climatic zones in Figure 16. The justification for adjusting only the temperature of the weather series is that this is considered the most important meteorological variable influencing the soil exposure concentrations.

By analogy to the procedure for the Tier-2A scenarios, irrigation is included in the scenario if the corresponding FOCUS climatic zone is irrigated based on FOCUS (2009). The climatic zones Châteaudun, Piacenza, Porto, Sevilla, and Thiva are irrigated and the zones Jokioinen, Hamburg, Okehampton and Kremsmünster are not irrigated.

In view of the differences between the PEARL and PELMO models for the Tier-2A scenarios, the choice of the model is also a source of uncertainty for Tier-3 scenarios. If the margin of safety for the assessment of effects on organisms in soil is less than a factor of two, risk managers could consider requiring Tier-3 calculations with both PELMO and PEARL and to use the highest exposure concentration of the two models.

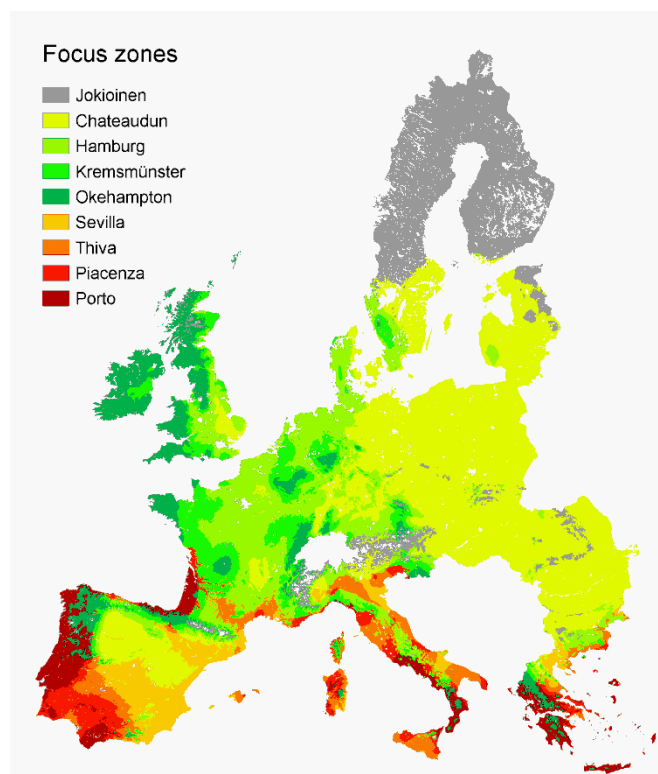


Figure 16: The nine climatic zones proposed by FOCUS (2009), each characterised by a combination of ranges of both annual rainfall and annual temperatures.

6.4. Tier 4

A further tier may be considered (Tier 4, Figure 6) which would consist of spatially distributed modelling with numerical models. Spatially distributed modelling has the advantage that the spatial 95th percentile of the PEC for all types of concentrations (pore water or concentration in total soil, peak or some TWA) of either the parent substance or any soil metabolite can be derived by statistical analysis of the output of the model runs, thus avoiding the need for simplifications in the scenario-selection procedure. Using the procedure described in EFSA (2010b), it is in principle possible to parameterise each 1×1 km² grid cell in the whole EU:

- i. All soil data needed for the numerical models can be derived from the organic-matter content and the soil texture using pedotransfer functions. The depth distribution of organic-matter content can be derived from the OCTOP map in combination with an average depth distribution for mineral and organic soils. The Panel considers this simplification acceptable, because the evaluation depth is 1 to 20 cm and the subsoil properties are not expected to have a big influence on the exposure in the top 20 cm;
- ii. The MARS database provides daily weather data at a resolution of 25×25 km². The temperature could be scaled to the WorldClim database to obtain temperature data series at a resolution of 1×1 km². If the full MARS database cannot be made available, it may be considered defensible to use a temperature-scaling procedure similar to the one described in Section 6.3.
- iii. Maps of major crops are in the CAPRI dataset, which is available at the JRC-site.

In view of computation time, it is not possible to perform calculations with a numerical model for each individual grid cell of the whole EU. It may therefore be necessary to reduce the number of grid cells for which calculations are done by clustering them into certain groups. There are different options for

such a clustering procedure. The Panel recommends conducting studies with spatially distributed models to assess which procedure is most appropriate at the European scale.

6.5. Tier 5

The Panel proposes to include post-registration monitoring as Tier 5. As described in Section 1.2, one of the principles of tiered approaches is that all tiers aim to assess the same exposure-assessment goal. In the context of the tiered approach of Figure 6, this means that all tiers aim to assess the spatial 90th percentile of the PEC_{SOIL} considering the spatial statistical population of agricultural fields (in one of the three regulatory zones) where the target crop is grown and in which this plant protection product is applied.

For Tier 5, this implies that this percentile has to be assessed via one of the following procedures:

- i. random sampling in combination with appropriate statistical assessment of the 90th percentile
- ii. some form of modelling combined with geostatistical analysis that enables a more targeted sampling strategy to assess this percentile (this includes also the use of existing data that are analysed afterwards).

The Panel expects that statistical analysis will show that hundreds of samples will be needed to assess the 90th percentile with sufficient accuracy on the basis of measurements alone. The alternative would be to use the analytical model to find the appropriate locations for monitoring studies. In this approach, monitoring studies should be carried out at locations that are identified by the analytical model to be at least 95th-percentile worst-case locations and that are randomly selected. To demonstrate that this condition is met, the notifier must report for each monitoring site the substance properties, soil properties, climatic conditions, application procedure and crop-management practices. Monitoring sites that do not meet these conditions should be excluded from the analysis. As described in Section 4.2.3, the scenario-selection procedure is targeted mainly at applications of substances in crops where most of the substance penetrates into the soil. So monitoring problems for substances that are dissipated to a large extent on plant or soil surfaces cannot be tackled using this alternative approach.

In line with the procedure that was used to simulate the overall 90th percentile of the PEC, the median value of the PEC at the individual monitoring sites should be used. Since the PECs at individual monitoring sites are expected to vary due to variation in K_{om} and $DegT50$ (normalised by temperature), the uncertainty on the calculated median PEC value should be considered. Using this information, it should be tested by statistical inference whether the derived PEC is significantly lower than the RAC.

Post-registration monitoring is likely to be meaningful only for plant protection products that show accumulation of residues at a time scale of at least 5 years. Interpretation of post-registration monitoring studies needs to take into consideration the fraction of the treated target crop included in such monitoring. If the results of the post-registration monitoring are obtained for a fraction of e.g. 50%, then the resulting 90th-percentile concentration has to be corrected via some procedure to obtain the 90th-percentile concentration corresponding to the spatial statistical population considering only fields treated with this active ingredient (because this was the target spatial statistical population as defined in Section 1.4.3).

7. GUIDANCE FOR SUBSTANCE PROPERTIES AND CROP-INTERCEPTION PERCENTAGES NEEDED FOR THE EXPOSURE ASSESSMENTS

7.1. Introduction

The exposure assessments in Tiers 1, 2A, 2B, 2C and 3 require information on substance properties and on crop interception at the application time(s). In general the Panel proposes to use for this purpose the guidance given by Anonymous (2011) and therein. The remainder of this chapter deals with items for which either Anonymous (2011) provided no guidance or for which the Panel proposes to improve the guidance provided.

The Panel recognises that K_{om} values obtained from batch adsorption studies for weakly sorbing substances may overestimate the true K_{om} considerably because of systematic errors resulting from loss processes from the liquid phase other than sorption in such studies (Boesten, 1990; Boesten *et al.*, 2009). Anonymous (2011) does not provide guidance to prevent this overestimation of K_{om} . However, the Panel is unable to improve the guidance on this aspect within the time frame of the mandate of this Opinion.

For the exposure assessment in soil, the degradation half-life ($DegT50$) in topsoil at 20°C and field capacity is an important input parameter of the simple and numerical models used in the tiered approach (Tiers 1, 2A, 2B, 2C and 3). The Panel proposes to use the guidance as provided by EFSA (2010d); for aspects that are not covered by EFSA (2010d), the Panel refers to Anonymous (2011) and FOCUS (2006).

7.2. Use of geomean K_{om}

As described in Section 4.2.5, the Panel proposes to use a CV of 0.5 and a lognormal distribution for the K_{om} . The reason for not using the normal distribution is that the variable (K_{om}) has only positive values, but its use with such a large CV would give a high probability of negative values.⁷ The scenario-selection procedure in Chapter 4 is based on the assumption that median substance properties will be derived from the dossiers as input parameters for the scenario calculations. The current guidance at EU level is to use an arithmetic mean K_{om} if less than nine values are available and the median K_{om} of the sample if nine or more are available (Anonymous, 2011, p. 26). For a lognormal distribution, the arithmetic mean is not an estimator for the median, whereas the geomean K_{om} can be so used. The geomean as an estimator of the median of the population also has better properties as the median of the sample, and hence this is the recommendation of the Panel for all sample sizes. A bias-corrected geomean estimator of the median of the population is:

$$K_{om,geo} = \exp\left(\frac{-\sigma^2}{2N}\right) \sqrt[N]{\prod_{n=1}^N K_{om,n}} = \exp\left(\frac{-\sigma^2}{2N}\right) \exp\left(\frac{1}{N} \sum_{n=1}^N \ln(K_{om,n})\right) \quad (28)$$

where $K_{om,n}$ is the n^{th} K_{om} value, σ is the standard deviation of the logarithms of the K_{om} values, and N is the sample size (total number of K_{om} values). The standard deviation σ is estimated with:

⁷ Very rarely, substances such as anions may have a small negative K_d and for these the concept of K_{om} cannot be applied.

$$\mu = \frac{1}{N} \sum_{n=1}^N \ln(K_{om,n})$$

$$\sigma = \sqrt{\frac{1}{N-1} \sum_{n=1}^N (\ln(K_{om,n}) - \mu)^2}$$
(29)

So if there are four K_{om} values 30, 52, 87 and 101 L kg⁻¹ then σ as calculated with Eqn 29 is 0.55 and the bias-corrected geomean (Eqn 28) gives 58.6 L kg⁻¹ whereas the arithmetic mean is 67.5 L kg⁻¹, the classic median of the sample is 69.5 L kg⁻¹ and the multiplicative median of the sample is 67.3 L kg⁻¹ (see EFSA, 2010d, for definition of classic and multiplicative median of the sample). Although Eqn 28 is formally a better estimate of the population median than the commonly used formula:

$$K_{om,geo} = \sqrt[N]{\prod_{n=1}^N K_{om,n}}$$
(30)

the Panel does not express a preference for one or other equation since the difference in the estimated median of the population by both is small compared with the uncertainty on the estimated median from a limited number of samples. The simpler Eqn 30 may be the easier choice and gives $(30 \times 52 \times 87 \times 101)^{0.25} = 60.8$ L kg⁻¹. In contrast, the arithmetic mean again gives higher estimates of the median, which is a general characteristic of these means. For small sample sizes (e.g. four K_{om} values in a dossier), the geomean and the arithmetic mean may differ by tens of percents. The same may apply to the difference of the geomean and the median of the sample as the above example shows.

The recommendation to use a geomean K_{om} does not only apply to the soil exposure assessment but also to other exposure assessments (e.g. leaching to groundwater and to surface water) because the Panel does not see any rationale of using an arithmetic mean for a quantity that is better described with a lognormal distribution.

7.3. Assessment of conservative K_{om} and/or $DegT50$ for substances whose K_{om} and/or $DegT50$ depends on soil properties

As described in Chapter 2, conservative values of the K_{om} and the $DegT50$ are to be used in Tiers 1 and 2A for substances whose K_{om} and/or $DegT50$ depend on soil properties such as pH or clay content. For such substances, quantitative relationships have to be established between (i) the K_{om} and/or the $DegT50$ and (ii) these soil properties and these relationships have to be based on statistical methods.

‘Conservative’ means that the calculated exposure concentrations are higher than the actual concentrations. For Tier 1, conservative implies that the K_{om} is low and the $DegT50$ is high. A low K_{om} is conservative because degradation is the only loss process in Tier 1, so the K_{om} influences only the distribution between the solid phase and pore water. The K_{om} has thus no effect on the concentration in total soil and a low K_{om} gives the highest concentration in the pore water. This assessment of parameter conservatism is valid both for parent substances and soil metabolites in Tier 1 because the simple analytical model used for soil metabolites therein is similar to that for the parent compounds (see Eqns 13 and 14).

For Tier 2A, it is *a priori* unknown whether a low K_{om} is conservative for parent substances because a low K_{om} may lead to more leaching from e.g. the top centimetre of the soil profile, which may reduce the concentration in pore water. For a soil metabolite, the situation is even more complicated because properties of the precursor of the metabolite influence also the exposure assessment. So it is impossible to provide for Tier-2A generic guidance for assessment of conservative values of the K_{om}

and the *DegT50*. Therefore such Tier-2A conservatism assessments have to be based on case-by-case analyses (e.g. calculations could be made with contrasting combinations of extreme values of input parameters). If these would appear to be time consuming, the alternative is to go from Tier 1 to Tier 2B instead (admittedly, going to Tier 2B solves the problem only for parent substances and not for soil metabolites).

7.4. K_{om} in dry soil

In exceptional cases, the all-time high concentration in pore water in the top centimetre of soil as simulated with numerical models in Tiers 2A or 3 may occur when this top centimetre is very dry. The background to this phenomenon is that decreasing moisture content in a closed soil system leads to an increasing concentration in the pore water (see Eqn 7). However, it has been known for decades that the sorption of pesticides to the soil solid phase may increase by about an order of magnitude if the soil becomes so dry that the solid phase is no longer completely covered by a monolayer of water molecules. For example, Hance (1977) showed that sorption of two herbicides increased very strongly when the water content of two soils decreased below that corresponding to about $pF = 4.4$. Therefore the Panel considers it appropriate to include a K_{om} in the simulations with numerical models that increases strongly when the water content decreases below about $pF = 4.4$ in exposure assessments with the numerical models (Tiers 2A and 3).

7.5. Formation fraction of soil metabolites

For the assessment of the formation fraction of soil metabolites, a stepped approach may be followed in all tiers that involve exposure calculations (Tiers 1, 2A, 2B, 2C and 3). The first conservative step is to assume that the formation fraction is 1.0 unless more than one molecule of this metabolite can be formed from one parent molecule. In the latter case, the formation fraction should be set to the number of molecules of this metabolite that can be so formed (e.g. one dazomet molecule which forms two molecules of methyl isothiocyanate in which case the formation fraction should be set to two). The second step is to take the maximum of all relevant formation fractions in the dossier. The third step is to take the arithmetic average of all relevant formation fractions in the dossier, thus also including zero values derived from relevant soil metabolism experiments in which this soil metabolite was not detected. Use of arithmetic means is consistent with the recommendations by FOCUS (2006, p. 235). ‘Relevant’ in this context means that there are no indications that the soil metabolism study in the dossier is invalid for the soil of the selected scenario. If this third step is needed to achieve a conclusion of acceptable risk (i.e. a PEC below the RAC), the Panel recommends checking whether there is correlation between the formation fraction and soil properties such as organic matter, clay and pH. Should such a correlation be found, the Panel recommends going to Tier 2B and to assess the spatial 95th-percentile of the PEC of the soil metabolite including the formation fraction as a substance parameter in the scenario-selection procedure (using Eqns 13 or 14). So for such a case the Panel proposes to base the scenario-selection procedure on the properties of the metabolite. Note that the simple analytical model used in Tier 2B does not include the degradation rate of the metabolite so there is no guarantee that this 95th spatial percentile is accurate (see Chapter 9 for a general discussion of the exposure assessment for metabolites). However, this percentile is considered to be better than available alternative approaches.

7.6. Crop interception of applied substance

Crop interception of applied substance may have a large influence on the exposure in soil of plant protection products that are sprayed onto the crop. This process will be handled differently in the different tiers as described in Table 1: in Tiers 1 and 2B, crop interception will be ignored but it will be included in Tiers 2A, 2C and 3. The guidance described below refers to this latter group of tiers.

Based on the work of FOCUS (2000), Anonymous (2002) provided crop-interception percentages as a function of the BBCH growth stage for a range of crops (BBCH stands for ‘Biologische Bundesanstalt, Bundessortenamt and CHemische Industrie’). The Panel proposes to use these

percentages for all crops except cereals because the Panel considers this to be the best information that is currently available. Van Beinum & Beulke (2010) collected all relevant data on crop interception by cereals and found systematic differences (Figure 17) between the measurements and the relationship proposed by FOCUS (2000). The data shown in Figure 17 are those of van Beinum & Beulke (2010) with one modification: the data shown for a BBCH growth stage of 18 in Figure 17 were reported to be at growth stage 22 by van Beinum & Beulke (2010). These data are from Taylor & Andersen (1987). These authors report the growth stage to range from 14 to 22 and the Panel used the average of this range.

To improve assessment of the crop interception by cereal crops, the Panel divided the measurements reported by van Beinum & Beulke (2010) into classes (Table 11) and calculated the average crop interception for each class. The line based on the average measured value gives a better description than the relationship proposed by FOCUS (2000) (Figure 17), and so the Panel recommends using these averaged values (Table 11).

Table 11: Crop interception as a function of BBCH growth stage for cereals as proposed by FOCUS (2000) and as calculated from the measurements reported by van Beinum & Beulke (2010).

BBCH growth stage	Crop interception (%)	
	FOCUS (2000)	Average of measured values from van Beinum & Beulke (2010)
00-09	0	0
10-19	25	2
20-29	50	22
30-39	70	82
40-69	90	91
70-99	90	81

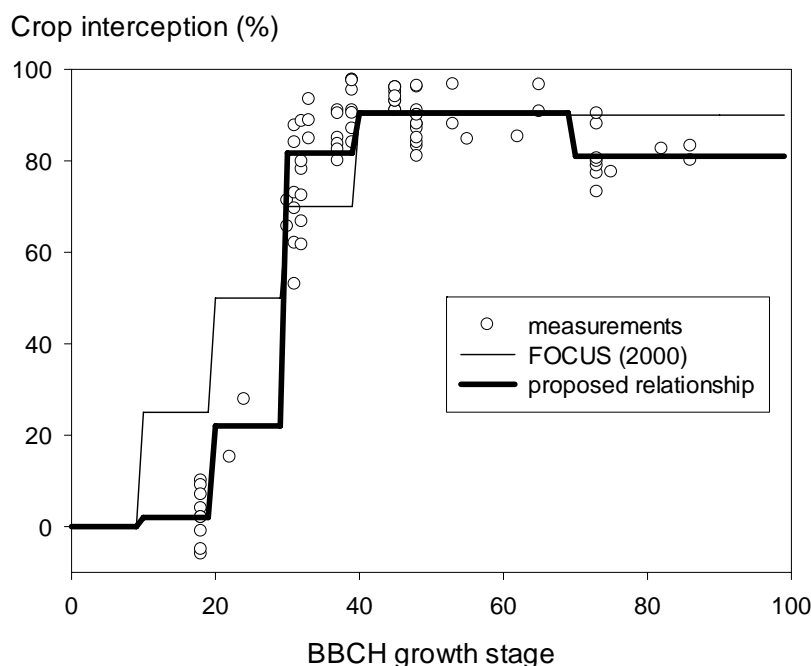


Figure 17: Crop interception as a function of BBCH growth stage for cereals. The measurements are those reported by van Beinum & Beulke (2010) in their Figure 12. The FOCUS-2000 line is the relationship proposed by FOCUS (2000) and the proposed relationship is that of the Panel.

7.7. Parameters for behaviour on plant surfaces

7.7.1. Introduction

Anonymous (2011) recommends reducing the application rate by the fraction that is intercepted by the crop and to apply this reduced rate to the soil (so making the assumption that substance molecules intercepted by the crop will never reach the soil). As described by EFSA (2010a), the Panel considers this approach not defensible because there is insufficient evidence that wash-off can be ignored under all relevant circumstances (see Section 7.6.3). So the Panel proposes to include simulation of the behaviour of parent substances on plant surfaces in Tiers 2A, 2C and 3, and provides in the next sections guidance proposals for the most important substance parameters for this behaviour.

The Panel notes that the assessment of the exposure of soil organisms to metabolites formed on plant surfaces (e.g. caused by photolysis and subsequent wash off) is impossible because there are no EU data requirements that could identify such metabolites.

7.7.2. Decline on plant surfaces

FOCUS (2001) proposed a default half-life for foliar dissipation of 10 d, acknowledging that higher values (up to 35 d) have been reported. EFSA (2008b) proposed a default half-life of 10 d based on Willis & McDowell (1987). However, EFSA (2010f) proposed a half-life of 30 d referring to USDA (2006), which database shows a number of foliar half-lives in the range between 10 and 30 d. However, the Panel has the impression that these half-lives are based on the decline of the sum of the residue on the plant surface (i.e. the dislodgeable foliar residue, DFR) plus that within the plant. For the soil exposure assessment, the decline of only the DFR (due to plant uptake or due to (photo)degradation at the plant surface) is relevant (volatilisation losses may be simulated separately by the numerical models so these are not included here). Therefore the Panel proposes to use the

default of 10 days recommended by EFSA (2008b). The Panel considers it acceptable that the default value is overruled by experiments with the substance considered and plants under a range of relevant conditions. The Panel recommends the collection and analysis of all relevant literature data on the decline of the DFR of plant protection products in order to further underpin (using also the most recent data) the default value to be used for the half-life of DFR due to degradation on the plant surfaces plus uptake by plants.

7.7.3. *Wash-off from plant surfaces*

Wash-off of plant residues of plant protection products by rainfall is described in most numerical models with:

$$R_w = w q m_a \quad (31)$$

where R_w is the rate of wash off of mass of substance per field area ($\text{mg dm}^{-2} \text{ d}^{-1}$), w is the wash-off factor (mm^{-1}), q is the rainfall rate (mm d^{-1}), and m_a is the mass of substance per field area on the plant surface (mg dm^{-2}). If no other loss processes of substance occur on the plant surface, it can be derived from Eqn 31 that the decline of m_a after a single application can be described with:

$$m_a = m_{a,0} \exp(-w Q) \quad (32)$$

where $m_{a,0}$ is m_a immediately after application and Q is cumulative rainfall (mm) after application.

FOCUS (2001, p. 202) proposed to use as a first step a default value for w of 0.05 mm^{-1} . As a second step, FOCUS (2001) proposed the following empirical relationship between the wash-off factor and the water solubility of the substance:

$$w = 0.0016 S^{0.3832} \quad (33)$$

where S is the water solubility (mg L^{-1}); note that FOCUS (2001) used 0.016 as proportionality factor based on cm^{-1} as unit for w whereas here the unit mm^{-1} is used. Figure 18 shows that Eqn 33 predicts that w is less than 0.001 mm^{-1} when the water solubility is below 0.1 mg L^{-1} . This implies that in the order of 1000 mm of rainfall would be needed to wash off most of the dosage for substances with such a low solubility.

Leistra (2005) compiled literature data on experiments of wash-off of plant protection products. He reported combinations of wash-off percentages and cumulative rainfall for 32 experiments with 12 plant protection products. These included substances such as the pyrethroids permethrin, cypermethrin and fenvalerate which have a water solubility of less than 0.01 mg L^{-1} . Eqn 32 can be used to assess the wash-off factor from experiments where the substance is applied to plant surfaces and the fraction of the dose washed off is measured after a certain amount of cumulative rainfall. It can be shown that:

$$w = -\frac{\ln(1-\omega)}{Q} \quad (34)$$

where ω is the fraction of the dose washed off (i.e. $1 - m_a / m_{a,0}$). The Panel calculated the wash-off factors with Eqn 34 from the 32 reported combinations of wash-off and rainfall and plotted these as a function of the time between application and rainfall. This was done because Leistra (2005) concluded that the ease of wash-off decreases with time after application. There was considerable variation in the wash-off factors (Figure 19) but those found after 6 days were generally lower than those found shortly after application. For six substances, measurements were available both for rainfall a few hours

after application and 6 days after application, and for all these substances the wash-off factor decreased considerably with time: the wash-off factor after 6 days was 0.2 to 0.5 times the value found at a few hours after application for fenvalerate; for parathion-methyl this value was 0.002 to 0.04, for permethrin and azinphos-methyl it was 0.2 and for sulprofos it was 0.3. For chlorothalonil, the wash-off factor was 0.11 mm^{-1} for rain 3 h after application and it decreased to 0.08 and 0.04 mm^{-1} for rain at 1 and 7 days after application, respectively.

For lipophilic substances such as the aforementioned pyrethroids, Eqn 33 predicts wash-off factors of the order of magnitude of 0.001 mm^{-1} or less (Figure 18). However, Figure 19 shows much higher measured values. This difference is probably caused by formulation additives which may lead to wash-off of concentrations that are much higher than the water solubility. For example, Leistra (2005) mentions reported permethrin concentrations in the wash-off water in the order of 10 mg L^{-1} whereas its water solubility is only 0.006 mg L^{-1} .

Most of the wash-off factors derived from measurements with rainfall after six days were based on the assumption that no other loss processes (e.g. plant uptake) occurred in these six days. This may have caused underestimation of part of the w values as reported for six days in Figure 19 because ω in Eqn 34 was underestimated. This can be illustrated with the following example. Let us consider an experiment in which 1.0 mg of substance is on the plant surface at the start. Assuming a half-life of 10 d (i.e. the recommended default value) gives 0.66 mg left after 6 days. Let us further assume that the wash-off measurement shows that 0.30 mg is washed off by 25 mm rainfall after 6 days. In this case the true value of ω is $0.30/0.66 = 0.45$ whereas the assumed ω value is $0.30/1 = 0.30$. The true value of w (Eqn 34) is 0.024 mm^{-1} whereas the assumed w value is 0.014 mm^{-1} . So using the default half-life of 10 d resulted in this example in an underestimation of the wash-off factor by 68%.

Based on the above analysis, the Panel considers use of Eqn 33 to assess the wash-off factor not defensible. Instead the Panel proposes to use as a conservative default $w = 0.1 \text{ mm}^{-1}$ which is close to the maximum of 0.2 mm^{-1} in Figure 19 found for rainfall within a few hours after application. The Panel does not propose to use this maximum of 0.2 mm^{-1} because this maximum value was only found for rainfall 1 hour after application and because rainfall so shortly after application is very unlikely. This default value can be refined by wash-off experiments with the plant protection product considered. These experiments should not be carried out with the pure active ingredient but with relevant formulated products. This default $w = 0.1 \text{ mm}^{-1}$ is twice that of the default of 0.05 mm^{-1} proposed by FOCUS (2001).

The recommendation to replace Eqn 33 with the default $w = 0.1 \text{ mm}^{-1}$ applies of course not only to the soil exposure scenarios but also to the FOCUS surface-water scenarios. It is also recommended to use crop interception routines and the wash-off estimated using this default factor in FOCUS groundwater leaching assessments. The effect of these recommendations on the PEC in groundwater and surface water will vary from case to case. For the PEC in groundwater, the new default will lead to wash-off of most of the intercepted substance molecules when heavy rain falls shortly after application. As there is a more or less linear relationship between PEC and the soil load for leaching scenarios, one may assume as a first indication that the PEC will be increased by a factor of up to $1/(1-I)$ where I is the intercepted fraction (so if 90% was intercepted, the PEC is likely to become up to ten times higher). For the PEC in surface water, the effects of these recommendations are difficult to quantify.

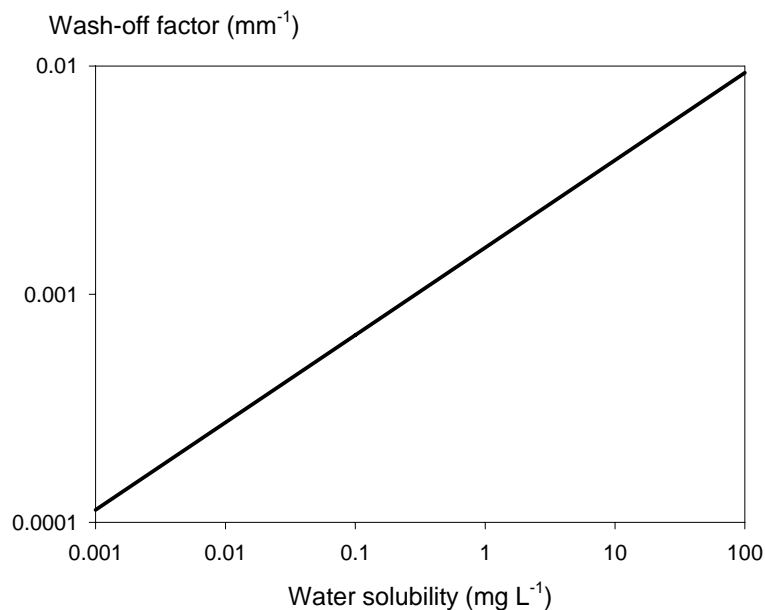


Figure 18: Wash-off factor as a function of water solubility as calculated with Eqn 33 (as proposed by FOCUS, 2001).

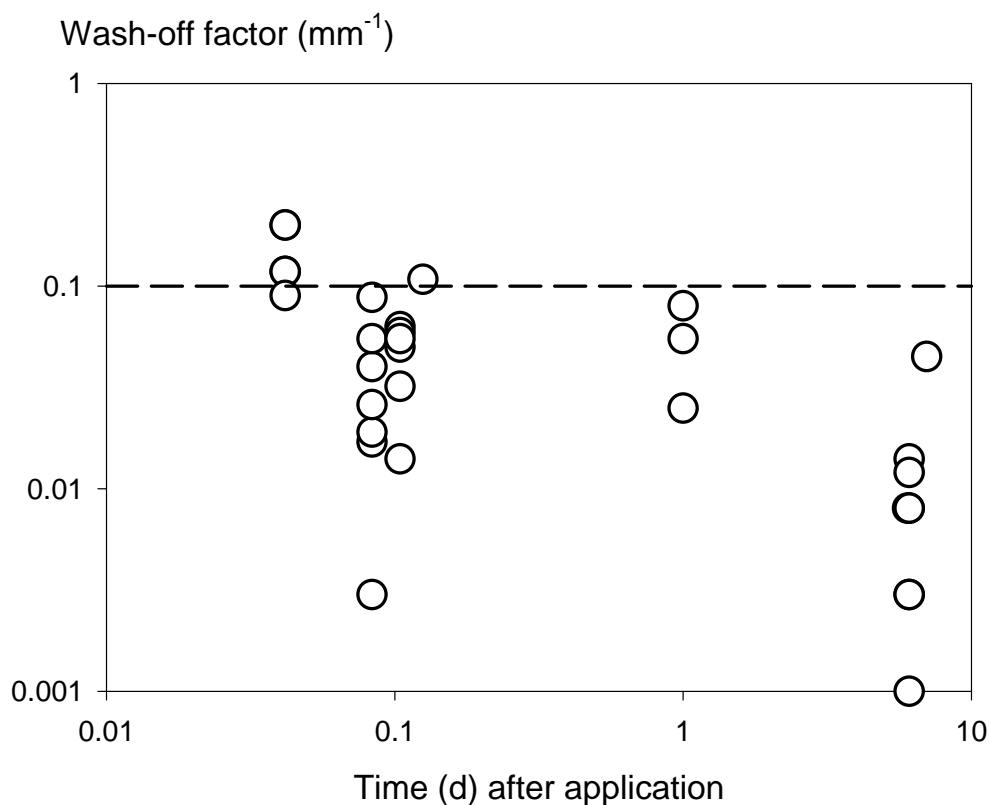


Figure 19: Wash-off factor as a function of the time between rainfall and application of the substance. The points were calculated from the measurements for 12 substances reported in the review by Leistra (2005) using Eqn 34. The dashed line is 0.10 mm⁻¹.

8. ASSESSMENT OF UNCERTAINTY IN EXPOSURE RESULTING FROM UNCERTAINTY IN SUBSTANCE PROPERTIES AS DERIVED FROM REGULATORY DOSSIERS (*DegT50* AND *K_{om}*)

The proposed tiered exposure-assessment procedure (Chapters 2 to 6) does not consider the uncertainty in substance properties as derived from regulatory dossiers. For example, the uncertainty in *DegT50* and *K_{om}* considered in Section 4.2.5 (leading to the shift from the 90th to the 95th spatial percentile) dealt with the effect of the expected spatial variability of these properties within each of the three regulatory zones, assuming that the probability density functions of *DegT50* and *K_{om}* within each of these zones were exactly known. However, this is of course not the case for any particular substance. Guidance to prevent systematic errors in substance properties, or to ensure that they are conservative, was given in Chapter 7 and in the guidance documents to which this Chapter refers. Now we consider the effect of random uncertainty in spatially variable substance properties resulting from the limitations of the sample size of the measurements of such properties in the regulatory dossiers. This uncertainty does not exist for molecular properties such as the water solubility and the saturated vapour pressure but it exists for all soil-substance and plant-substance properties (for example, the Freundlich sorption exponent, the formation fraction of a metabolite, the wash-off factor). The Panel considers the *DegT50* and *K_{om}* to be the substance properties that may lead to most uncertainty (they are also the only soil-substance properties in the simple analytical model) and therefore limited the assessment to these properties.

As described in Section 4.2.5, the selection procedure for the Tier-2A scenarios was based on the assumption that geomean *DegT50* and *K_{om}* values will be used in the scenario calculations. As described by EFSA (2010d, p. 36), the geomean of the statistical population of a parameter is needed for that purpose and this may differ from the geomean of the sample population. In general, the uncertainty of the estimated geomean decreases with increasing sample size (see Figure 13 of EFSA, 2010d).

To illustrate this possible effect of this uncertainty, calculations were made for a substance whose arithmetic mean *DegT50* and *K_{om}* values were equal to those of substance P3 in Table 2 (*DegT50* = 200 d and *K_{om}* = 1000 L kg⁻¹). It was assumed that both *DegT50* and *K_{om}* were lognormally distributed with a CV of 0.5 (see Section 4.2.5 for justification of this CV value). The geometric mean of the population of *DegT50* and *K_{om}* was thus 179 d and 894 L kg⁻¹, respectively (calculated from the arithmetic mean and the CV using the properties of a lognormal distribution). It was furthermore assumed that four *DegT50* values and four *K_{om}* values were available in the dossier. A set of four values of *DegT50* and four values of *K_{om}* were randomly sampled from the population of *DegT50* and *K_{om}* values. From these sampled sets, the sample geometric means of *DegT50* and *K_{om}* were calculated. The spatial probability density function of the concentration in the pore water (for an annual dose of 1.0 kg ha⁻¹, *z_{eco}* = 20 cm and *z_{til}* = 20 cm) was calculated with the simple analytical model for the EU-15 map of agricultural land as described by Tiktak *et al.* (2004). To calculate the probability density function, it was assumed that the *DegT50* and the *K_{om}* were lognormally distributed stochastic variables (using again a CV of 0.5). The calculation of spatial probability density function was repeated several thousand times for different sample geomeans that were derived from sets of four sampled *DegT50* and *K_{om}* values (thus simulating several thousand possible dossiers).

To interpret the results (Figure 20), let us assume that we are interested in the 90th spatial percentile. This is the horizontal line at cumulative probability density of 0.90. The graph then shows that this PEC has a 5th percentile of about 0.04 mg L⁻¹, a 50th percentile of about 0.07 and a 95th percentile of about 0.105 mg L⁻¹. So the 5th percentile was about 40% lower than the 50th percentile and the 95th percentile was about 60% higher. The 50th-percentile line is that calculated without considering this uncertainty. This line is between the lines for the south and centre zones in Figure 12 (bottom right graph). An effect of 40-60% on the 90th percentile in Figure 12 is larger than the differences between the 90th percentiles of the three zones in Figure 12. This shows that the effect of the uncertainty in the dossier information on the concentration in the pore water may be considerable if only four *DegT50* values and four *K_{om}* values are available.

Further calculations showed that the effect of uncertainty in these dossier parameters on the PEC (i) was larger for the concentration in the pore water than for the concentration in total soil, (ii) increased in the sequence P1-P2-P3, (iii) was larger for $z_{eco} = 20$ cm than for $z_{eco} = 1$ cm for the concentration in total soil, and (iv) was about equal for $z_{eco} = 20$ cm and $z_{eco} = 1$ cm for the concentration in the liquid phase. The effect ranged from negligibly small to the one shown in Figure 20.

The Panel considered also an alternative simplified calculation procedure. First the location where the 95th percentile was located was selected assuming no stochastic spatial variability of *DegT50* and K_{om} and assuming that these parameters were equal to the geomean of the statistical population. Then the distribution of the concentration was calculated at this location considering the uncertainty of the geomean values of *DegT50* and K_{om} . It appeared that this simplified procedure resulted in cumulative probability density functions that were very close to the original procedure for all cases considered. As a consequence, the Panel considers it defensible to assess the effect of the uncertainty in substance properties as derived from regulatory dossiers by calculations with Tier-2A scenarios. These are the spatial 95th percentile of the locations and so, based on the experience from the preceding paragraph, it may be expected that the resulting distributions of the concentration will resemble those that would have been calculated with these models for all pixels (the latter calculations are of course impossible because the numerical models are parameterised only for one pixel in each regulatory zone).

To illustrate the effect of the uncertainty in substance properties as derived from regulatory dossiers, Tier-2A calculations were made for a substance whose median *DegT50* and K_{om} values were equal to those of substance P3 in Table 2 (*DegT50* = 200 d and K_{om} = 1000 L kg⁻¹). It was assumed that both *DegT50* and K_{om} were lognormally distributed with a standard deviation of the logarithm of 0.5 (corresponding to a CV of 0.53) and that the geomean of four values available in the dossier was used for each. The substance was applied to winter wheat at a rate of 1.0 kg ha⁻¹ one day before emergence. Cumulative probability density functions were based on 400 runs (each using different *DegT50* - K_{om} geomean combinations). The concentrations follow the expected sequences: North > Centre > South for the concentration in total soil and South > Centre > North for the pore-water concentration (Figure 21). The uncertainty from having only four *DegT50* and K_{om} values is for the concentration in total soil highest for the North scenario: the 5th percentile is about 1.5 mg kg⁻¹ and the 95th percentile is about 2.7 mg kg⁻¹, and so about a factor two difference between these percentiles. For the concentration in the pore water, the uncertainty is largest for the South scenario: the 5th and 95th percentiles range from about 0.04 to 0.12 mg L⁻¹, so differing by a factor of three. Using the above procedure, calculations on the uncertainty resulting from the available number of *DegT50* and K_{om} values in the dossier could be included on a routine basis in the soil exposure assessment if deemed necessary by the SCFCAH (the Standing Committee on Food Chain and Animal Health). This procedure could also be applied on a routine basis in the assessment of leaching to groundwater and exposure of aquatic organisms.

Cumulative probability density (-)

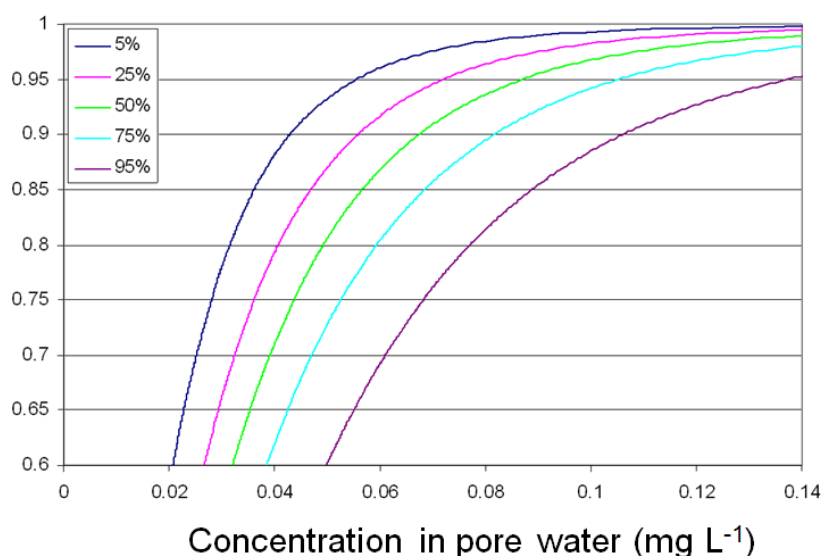


Figure 20: Cumulative probability density⁸ as a function of the concentration in the pore water of substance P3. The lines indicate the 5th to 95th percentiles resulting from the uncertainty in the values of *DegT50* and *K_{om}* in the dossier (taking the geomean of four dossier values for both). Calculations were made with the simple analytical model for EU-15 map (based on 1051 scenarios) described by Tiktak *et al.* (2004) using an annual dose of 1.0 kg ha⁻¹, *z_{eco}* = 20 cm and *z_{til}* = 20 cm. Note that the vertical axis starts at 0.60.

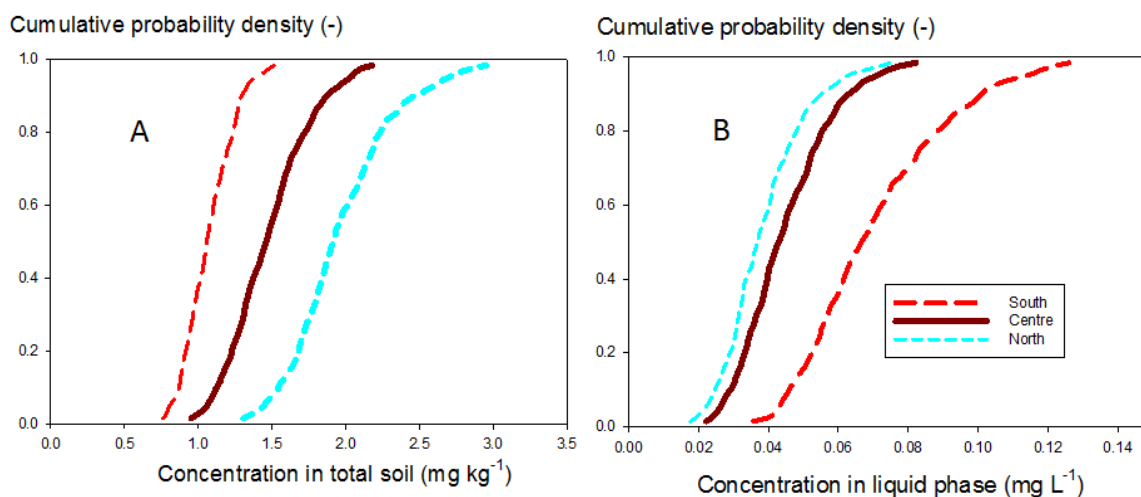


Figure 21: Cumulative probability density functions of the concentration in total soil (part A) and the concentration in pore water (part B) as calculated for the Tier-2A scenarios with the PEARL model assuming that *DegT50* and *K_{om}* are the geomean of four values available in the dossier and that these values in the dossier were lognormally distributed with a standard deviation of the logarithm of 0.5 and with median values equal to those of P3 (*DegT50* = 200 d and *K_{om}* = 1000 L kg⁻¹). Calculations were for application of 1.0 kg ha⁻¹ one day before emergence in winter wheat.

⁸ The ‘(-)’ in the legend of the vertical axis indicates that the cumulative probability density has no unit because it is a dimensionless quantity.

9. EXPOSURE ASSESSMENT FOR SOIL METABOLITES

As follows from Chapters 3 to 6, soil metabolites are not included in any of the scenario-selection procedures. One reason for this is that the simple analytical model was developed for parent substances and no equivalent simple analytical model is available for soil metabolites. However, this could have been overcome by using another type of simple model that could include soil metabolites (e.g. a parent-metabolite model based on the differential equations for degradation and formation). However, the Panel did not follow that path because use of such a model would probably have shown that the relationships between scenario properties and vulnerability are too complex to justify use of only a single scenario for each regulatory zone for the concentration in total soil or that in pore water for parent substances and metabolites.

The only straightforward solution to this scenario-selection problem for all types of soil metabolites is to develop Tier 4 (the spatially distributed modelling with numerical models) as described in Section 6.4. As long as spatially distributed modelling with numerical models is not yet possible at the EU level, the Panel proposes to use the tiered approach of Figure 6 also for soil metabolites. However, risk managers should be aware that the exposure assessment for soil metabolites is not based on the exposure-assessment goals as specified in Section 1.4.

10. CONCLUSIONS AND RECOMMENDATIONS

CONCLUSIONS

1. Development of scientific methodology for assessment of exposure of organisms to plant protection products and their soil metabolites requires a detailed definition of the exposure-assessment goal. This definition is a risk-management decision. The proposed methodology is provisionally based on the goal to assess the 90th-percentile concentration considering all agricultural fields within a regulatory zone where the particular active ingredient is applied. This goal is considerably less differentiated in space than those for the current EU exposure-assessment methodologies for leaching to groundwater and exposure of aquatic organisms. This was done to keep the regulatory approach for exposure of organisms in soil as simple as possible.
2. The proposed exposure-assessment methodology is restricted to spray applications to annual crops under conventional or reduced tillage (excluding tillage systems with ridges and furrows). The Panel proposes to base this methodology on a tiered approach. Tier 1 is based on a simple analytical model. Tier 2A is based on simulations with numerical models. To keep the approach as simple as possible, the Panel based Tiers 1 and 2A for each regulatory zone on only one scenario for the concentration in total soil and on only one scenario for the concentration in pore water. These scenarios are to be used for all these annual crops and for all plant protection products in each regulatory zone. Tiers 2B and 2C are based again on the simple analytical model but in these tiers a specific crop or crop group and a specific plant protection product are considered. Tier 3 is based on simulations with numerical models but, as in Tiers 2B and 2C, a specific crop or crop group and a specific plant protection product are considered. All tiers aim to assess the same exposure endpoint, i.e. the 90th percentile of a certain type of concentration considering all agricultural fields within a regulatory zone where the particular active ingredient is applied.
3. Based on discussions at the IRIS workshop (attended by Member States and stakeholders), it was a boundary condition that the proposed exposure-assessment methodology can be applied by taking median or average substance properties (such as the degradation half-life in soil and the sorption coefficient) from the dossiers. Such substance properties are uncertain and inclusion of this uncertainty leads to probability density functions of concentrations that show more spread. As a consequence, this boundary condition led to the need to base the scenario selection procedure on the 95th-percentile concentration instead of the 90th-percentile concentration.
4. There appeared to be distinct differences between the properties of the scenarios selected for (i) the concentration in total soil and (ii) the concentration in pore water. So it was necessary to use different scenarios for these different types of concentration.
5. Peak concentrations in total soil and in pore water were calculated with numerical models for the Tier-2A scenarios. The calculations were carried out for applications to bare soil in sugar beet and winter wheat and for a number of example substances. The differences in concentration amongst the three regulatory zones appeared to be no more than a factor of two. These differences are comparatively small in view of the considerable differences in climate and soil properties between the three regulatory zones. The concentration in total soil decreased in the order North-Centre-South whereas the concentration in pore water usually decreased in the order South-Centre-North.
6. The area of the crop within a regulatory zone appeared to have a distinct effect on the 95th-percentile concentration. Therefore in the Tier-1 and Tier-2A assessments (which are based on the total area of annual crops in a zone), the concentrations have to be multiplied

with a so-called ‘crop extrapolation factor’ to ensure that these assessments are conservative enough. This crop extrapolation factor depends on the type of concentration, the regulatory zone and the area of the crop. The Panel assessed this factor for 12 crops using maps of their density at a resolution of $1 \times 1 \text{ km}^2$ for the whole EU and found the required factor to range from 1.02 to 1.79. If no map of the density of the particular crop is available, the crop factor has to be based on the 100th-percentile concentration considering the whole area of annual crops in a regulatory zone. The range of crop factors based on this 100th percentile was from 1.3 to 3.2. These results indicate that the effect of the area of the crop on the exposure endpoint may be in the same range as the differences between the regulatory zones.

7. Tier-2A calculations of concentrations for example substances, using the numerical models PEARL and PELMO, showed distinct differences between these models. So in tiers based on calculations with numerical models (Tiers 2A and 3), the choice of the model is also a source of uncertainty. If the margin of safety for the assessment of effects on organisms in soil is less than a factor of two, risk managers could consider the necessity of performing calculations with both PELMO and PEARL and of using the highest exposure concentration of the two models.
8. The Panel notes that certain models other than PELMO and PEARL are equally adequate, and encourages the parameterising of the scenarios for such additional numerical models. The only requirement is that the process descriptions in these models have a level of detail similar to or higher than those in PELMO and PEARL (PRZM and MACRO fulfil this requirement).
9. Registration dossiers contain at least four studies on the degradation half-life in soil and the sorption coefficient. The exposure-assessment methodology is based on the use of the geomean of the relevant statistical population of these substance properties which may differ from the geomean of the sample population derived from the data in the dossier. The Panel developed a procedure to assess the uncertainty in the soil exposure concentrations resulting from the limited number of studies on the degradation half-life in soil and the sorption coefficient in the dossiers. Preliminary calculations showed that this uncertainty depends strongly on (i) the type of concentration, (ii) the substance properties, and (iii) the ecotoxicological averaging depth. In these calculations, it was assumed that only four studies were available for the degradation half-life in soil and the sorption coefficient and the uncertainty ranged from negligibly small to about 50% higher or lower concentrations. Using the above procedure, calculations on the uncertainty resulting from the available number of *DegT50* and *K_{om}* values in the dossier could be included on a routine basis in the exposure assessment if deemed necessary by the SCFAH.
10. The organic-matter content of topsoil plays an important role in the exposure assessment; this content has been derived from the EU map of soil organic-carbon contents (the OCTOP map). However, the OCTOP map is likely to overestimate the organic-matter content for arable soils with higher organic-matter content in northern Europe; such overestimation leads to underestimation of the soil bulk density and hence the exposure assessment is expected to overestimate the 90th-percentile concentration in total soil. For southern Europe, the OCTOP map is likely to underestimate the organic-matter content for arable soils with lower organic-matter content; such underestimation leads to underestimation of sorption and hence the exposure assessment is expected to overestimate the 90th-percentile concentration in pore water. These systematic biases occur because the map was not specifically developed for the area of annual crops, and so organic-matter contents associated with other land uses also influenced the map.

RECOMMENDATIONS

1. The proposed exposure-assessment methodology is based on the population of all agricultural fields within a regulatory zone grown with the crop or group of crops that are considered for the plant protection product within the EU registration procedure. So to apply the exposure-assessment methodology for EU registration, a list of possible annual crops for this registration has to be defined. This definition is a risk-management decision. The Panel recommends that the SCFCAH makes a decision regarding this list of crops, after which it would be advisable to develop maps for as many of those crops as possible (if not yet available as a CAPRI crop), using the CAPRI methodology. It is recommended to do this at the same $1 \times 1 \text{ km}^2$ scale as used for this guidance development in order to facilitate the use of these maps in higher tiers of the proposed methodology (these maps are also likely to be useful in other exposure-assessment methodologies).
2. The tiered approach contains many tiers and the procedures to be followed in each tier are complicated. Thus efficient use of the approach in regulatory practice is impossible without appropriate software tools. Therefore the Panel recommends developing user-friendly versions of numerical models that can calculate exposure concentrations for the six Tier-2A scenarios. Furthermore, the Panel recommends developing a single user-friendly software tool that can perform the following tasks: (i) calculation of the Tier-1 PECs, (ii) calculation of the Tier-2B 95th-percentile PECs, (iii) calculation of the Tier-2C 95th-percentile PECs using output from Tier-2A simulations for the soil load including wash-off, and (iv) selection of the grid cell corresponding to the 95th-percentile PEC as needed for the scenario development of Tier 3. After this tool has become available, the Panel recommends checking iteratively the consistency of the tiered flow chart considering the three regulatory zones, all types of concentration, all relevant crops and the range of substance properties.
3. The Panel recommends checking (using again this user-friendly tool) whether the proposed shift from the 90th to the 95th spatial percentile to account for the uncertainty in *DegT50* and *K_{om}* is appropriate considering the three regulatory zones, all types of concentration, all relevant crops and the range of substance properties.
4. The development of the exposure-assessment methodology would have been much easier and much more straightforward if appropriate tools for spatially distributed modelling with numerical models had been available. Because this was not the case, the proposed methodology had to be based on a number of simplifying assumptions. The development of such tools has now become feasible since maps of relevant data have now become available for the whole EU at a resolution of $1 \times 1 \text{ km}^2$. Therefore the Panel recommends developing such tools.
5. The tiered approach to assess 90th-percentile concentrations was developed considering only parent substances because developing a methodology that also included soil metabolites was considered too complex as long as appropriate tools for spatially distributed modelling with numerical models are not yet available. Nevertheless, the Panel recommends using this tiered approach also for soil metabolites in the absence of a better alternative. However, risk managers should be aware that there is no guarantee that exposure endpoints for soil metabolites are close to the 90th percentile.
6. The half-life for decline of the dislodgeable foliar residue (DFR) on plants, resulting from both degradation on plant surfaces and uptake by plants (but not considering losses due to volatilisation), is an input parameter for the numerical models that may have a large effect on soil exposure concentrations of substances sprayed on full-grown crops. This half-life is not part of the EU data requirements and therefore is usually not available in dossiers. Thus a default half-life is needed. The Panel recommends using a default half-life of 10 d (based on a

previous EFSA Opinion). The Panel recommends the collection and analysis of all relevant literature data on the decline of the DFR in order to further underpin the default value of the DFR half-life.

7. In view of the perceived likely systematic bias in the use of the OCTOP map for arable soils, the Panel recommends that a revised OCTOP map is generated that considers only the area of annual crops; the data needed to generate such a map is only available at the Joint Research Centre (JRC). For development of other exposure-assessment methodologies, it may be useful to generate also OCTOP maps that consider only the area of pasture and only the area of permanent crops.
8. The Panel recommends using an estimator of the median K_{om} for all exposure assessments (e.g. soil and aquatic organisms, leaching to groundwater) and using for that purpose either a bias-corrected geomean estimator or the conventional geomean.

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GLOSSARY AND ABBREVIATIONS

BBCH code	Biologische <u>B</u> undesanstalt, <u>B</u> undessortenamt and <u>C</u> hemische industrie code: decimal code to characterise crop development stage
CAPRI	<u>C</u> ommon <u>A</u> gricultural <u>P</u> olicy <u>R</u> egional <u>I</u> mpact assessment model
<i>DegT50</i>	half-life resulting from transformation of substance in the soil matrix
DFR	<u>D</u> islodgeable <u>F</u> oliar <u>R</u> esidue
ERC	<u>E</u> cotoxicologically <u>R</u> elevant <u>C</u> oncentration
FOCUS	<u>F</u> orum for <u>C</u> o-ordination of pesticide fate models and their <u>U</u> se
IRIS	Acronym for EFSA workshop organised May 2009 (<u>I</u> mproved <u>R</u> ealism <u>I</u> n <u>S</u> oil risk assessment)
K_{om}	organic-carbon/water partition coefficient
MACRO	numerical model for behaviour of plant protection products and their soil metabolites
metabolite	any metabolite or a degradation product of an active substance, safener or synergist, formed either in organisms or in the environment (thus including also oxidation products which may have a larger molecular mass than the parent substance)
OCTOP map	map with resolution of 1×1 km ² describing the <u>O</u> rganic <u>C</u> arbon in the <u>T</u> OP 30 cm of soil for the whole EU
PBT	<u>P</u> ersistence <u>B</u> ioaccumulation <u>T</u> oxicity
PEARL	numerical model for behaviour of plant protection products and their soil metabolites
PEC	<u>P</u> redicted <u>E</u> nvironmental <u>C</u> oncentration
PEC _{SOIL}	<u>P</u> redicted <u>E</u> nvironmental <u>C</u> oncentration in soil
PELMO	numerical model for behaviour of plant protection products and their soil metabolites
PPP	<u>P</u> lant <u>P</u> rotection <u>P</u> roduct
PPR Panel	Scientific Panel on <u>P</u> lant <u>P</u> rotection Products and their <u>R</u> esidues
PRZM	numerical model for behaviour of plant protection products and their soil metabolites
RAC	<u>R</u> egulatory <u>A</u> cceptable <u>C</u> oncentration
type of concentration	the concentration scenario considered in the risk assessment, e.g. the concentration in total soil averaged over the top 5 cm or the concentration in the pore water averaged over the top 20 cm
TWA	<u>T</u> ime- <u>W</u> eighted <u>A</u> verage

APPENDIX I. EXPOSURE ASSESSMENT BASED ON THE TOTAL AMOUNT IN SOIL

Older soil ecotoxicological studies often expressed exposure only in terms of the applied rate (in kg ha^{-1}). The Panel has reservations whether this is an appropriate procedure for linking exposure to effects. However, if such studies have to be used, the Panel proposes performing the exposure assessment on the basis of the concentration in the top 20 cm of soil. Only the scenarios for the concentration in total soil are relevant for such cases and the amount in the top soil is calculated from this concentration as given below.

The total amount in soil, Z (kg ha^{-1}) can be calculated from the PEC in total soil (in mg kg^{-1}) for an ecotoxicological averaging depth (z_{eco}) of 20 cm and the dry bulk density ρ (in kg L^{-1}) with:

$$Z = a \rho PEC$$

with $a = 2 \text{ kg L ha}^{-1} \text{ mg}^{-1}$ (a is needed to convert the concentration in the top 20 cm into the total amount in kg ha^{-1}). So if $\rho = 1.05 \text{ kg L}^{-1}$ and the PEC is 1 mg kg^{-1} then $Z = 2 \times 1.05 \times 1 = 2.1 \text{ kg ha}^{-1}$. The Panel proposes to take the total amount in the top 20 cm because this is the largest value for the ecotoxicological averaging depth (Section 1.4.1) which is a conservative approach for calculating Z .

APPENDIX II: PRELIMINARY PROPOSAL FOR LIST OF ANNUAL CROPS FOR WHICH REGISTRATION OF A PLANT PROTECTION PRODUCT MAY BE PROVIDED AT EU LEVEL (BASED ON THE LIST USED IN UK REGISTRATION; CRD, 2006)⁹

Primary group	Crop	Primary group	Crop
Cereals	Barley	Stem vegetables	Asparagus
	Forage maize		Celery
	Grain maize		Chicory
	Millet		Florence fennel
	Oats		Globe artichoke
	Rye		Leek
	Sorghum		Rhubarb
	Triticale		Seakale
	Soft wheat	Bulb vegetables	Garlic
	Durum wheat		Bulb onion
Oil seeds	Evening primrose		Shallot
	Honesty		Salad onion
	Linseed	Fruiting vegetables	Aubergine
	Oilseed rape		Chilli
	Sunflower		Tomato
	Borage		Pepper
	Canary flower		Courgette
	Crambe		Cucumber
	Mustard		Marrow
Vegetable brassicas	Kohlrabi		Melon
	Brussels sprouts		Watermelon
	Cabbage		Winter squash and pumpkin
	Broccoli/calabrese		Summer squash and other edible skin varieties
	Cauliflower		Sweetcorn
	Choi sum	Root & tuber crops	Carrot
	Chinese cabbage		Celeriac
	Collard		Chicory root
	Fodder rape		Parsley root
	Kale		Potato
	Komatsuna		Salsify
	Salad greens		Parsnip
	Pak choi		Fodder beet
Legumes	Lentil		Red beet
	Lupin		Mangel
	Broad bean		Sugar beet
	Combining pea		Horseradish
	Dwarf French bean		Mooli
	Edible podded pea		Radish
	Field bean		Swede
	Runner bean		Turnip
	Soya bean	Herbs	See list of about 60 herbs in CRD (2006)
	Vining pea		
Leafy vegetables	Burnet		
	Endive		
	Cress	Agricultural herbage	Vetch
	Orache		Lucerne
	Land cress		Sainfoin
	Lambs lettuce		Red clover
	Lettuce		White clover
	Rocket	Other crops	Hops
	Spinach		Quinoa
	Spinach beet		Canary grass
Leafy vegetables	Watercress	Industrial crops	Miscanthus
			Hemp
			Woad

⁹ The column 'primary group' is not part of the list; it is only given to increase the readability and accessibility of the list. See CRD (2006) for the definitions of the crops.

APPENDIX III: PROPERTIES OF THE EXAMPLE SUBSTANCES.

Number of example substance	$DegT50$ (d) at 20°C and pF = 2	K_{om} (L kg ⁻¹)
1	10	10
2	31	10
3	10	31
4	31	31
5	100	31
6	10	100
7	31	100
8	100	100
9	316	100
10	10	316
11	31	316
12	100	316
13	316	316
14	1000	316
15	10	1000
16	31	1000
17	100	1000
18	316	1000
19	1000	1000

APPENDIX IV: MONTHLY TEMPERATURES (°C) OF THE GROUNDWATER SCENARIOS AS DESCRIBED BY FOCUS (2009)

	1	2	3	4	5	6	7	8	9	10	11	12
Châteaudun	3.90	4.55	7.58	9.68	13.61	16.78	19.42	19.10	16.18	12.14	7.19	4.92
Hamburg	1.22	1.01	4.49	7.58	12.34	15.12	17.29	17.05	13.79	9.75	5.23	2.57
Jokioinen	-7.55	-7.46	-2.51	2.79	9.29	13.46	15.84	14.66	9.49	4.93	0.08	-4.90
Kremsmünster	-1.01	-0.15	4.71	7.81	12.79	15.73	18.00	17.64	14.22	9.24	3.39	0.26
Okehampton	3.40	3.33	6.49	8.57	12.53	15.25	17.66	17.50	14.91	11.32	6.91	4.63
Piacenza	2.64	4.49	8.96	12.11	17.00	20.91	23.87	23.38	19.67	14.08	7.50	3.65
Porto	9.25	10.3	11.73	12.96	15.14	18.57	20.48	20.52	19.45	15.80	12.48	10.50
Sevilla	10.74	11.92	13.88	15.3	18.33	22.46	26.00	26.33	24.05	18.96	14.59	12.11
Thiva	8.64	9.05	10.98	13.99	18.02	22.33	24.47	24.43	21.72	17.70	12.89	9.87