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EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil

European Food Safety Authority

European Food Safety Authority (EFSA)

This guidance published on 19 October 2017 replaces the earlier version published on 28 April 2015*

Abstract

This EFSA Guidance Document provides guidance for the exposure assessment of soil organisms to plant protection products (PPPs) and their transformation products in accordance with Regulation (EC) No. 1107/2009[1] of the European Parliament and the Council. This guidance was produced by EFSA in response to a question posed by the European Commission according to Article 31 of Regulation (EC) No. 178/2002[2] of the European Parliament and of the Council. Guidance is provided for all types of concentrations that are potentially needed for assessing ecotoxicological effects, i.e. the concentration in total soil and the concentration in pore water, both averaged over various depths and time windows. The current guidance considers both permanent crops and annual crops. The recommended exposure-assessment procedure consists of four tiers. To facilitate efficient use of the tiered approach in regulatory practice, user-friendly software tools have been developed. In higher tiers of the exposure assessment, crop interception and subsequent dissipation at the crop canopy may be included. The models that simulate these processes were harmonised. In addition, easy-to-use tables for the fraction of the dose intercepted by the canopy that is washed off have been developed, which should be used in combination with the simple analytical model. With respect to substance-specific model inputs, this guidance generally follows earlier documents; however, new guidance is included for some specific substance parameters.

Keywords: exposure assessment, soil organisms, exposure scenarios, tiered approaches, guidance, crop interception, fraction reaching soil

Requestor: European Commission

* The guidance was updated and corrected with exposure methodology for permanent crops and crops grown on ridges and with recommendations proposed by stakeholders in the public consultation in 2016 on the draft guidance. The original version of the guidance has been removed from the website, but is available on request.

[1] EC (European Commission), 2009. Regulation (EC) No. 1107/2009 of the European Parliament and of the Council of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC. OJ L 309/1, 24.11.2009, pp. 1–50.

[2] EC (European Commission), 2002. Regulation (EC) No. 178/2002 of the European Parliament and of the Council of 28 January 2002 laying down the general principles and requirements of food law, establishing the European Food Safety Authority and laying down procedures in matters of food safety. OJ L 31, 1.2.2002, pp. 1–22.

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Summary

This European Food Safety Authority (EFSA) Guidance Document provides guidance for the exposure assessment of soil organisms to plant protection products (PPPs) and their transformation products in accordance with Regulation European Commission (EC) No. 1107/2009 of the European Parliament and the Council.[1] This guidance was produced by EFSA in response to a question posed by the EC according to Art. 31 of Regulation (EC) No. 178/2002 of the European Parliament and of the Council.[2] The recommended methodology was developed for the assessment of active substances and metabolites in the context of approval at the European Union (EU) level, and it is expected to be used for the assessment of products at the zonal level as well. This Guidance Document, together with the EFSA Guidance Document on how to obtain *DegT50* values (EFSA, 2014a) and the Forum for Co-ordination of Pesticide Fate Models and their Use (FOCUS) Degradation kinetics report (FOCUS, 2006), is intended to replace the current Directorate-General for Health and Consumer Affairs (DG SANCO) Guidance Document on persistence in soil (SANCO/9188VI/1997 of 12 July 2000) (EC, 2000).

The draft EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil was subject to public consultation from 10 July 2014 to 4 September 2014 and from 3 May 2016 to 10 June 2016. Technical reports have been produced containing the stakeholder comments received during the public consultations and how these comments have been taken into account (EFSA, 2015a; EFSA PPR Panel, 2017).

This Guidance Document is based on the EFSA Opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations of PPPs in soil (EFSA PPR Panel, 2012). The goal is to assess the 90th percentile concentration considering all agricultural fields within a regulatory zone (North–Centre–South) where a PPP is intended to be used. The guidance considers all types of concentrations that are potentially needed for assessing the ecotoxicological effects, i.e. the concentration in total soil (mg/kg) and the concentration in pore water (mg/L), both averaged over various depths and time windows. The guidance also describes how to use older soil ecotoxicological studies in which exposure is expressed in terms of the applied rate (in kg/ha). The current methodology considers annual field crops including field crops grown on ridges and permanent crops.

The recommended exposure-assessment procedure consists of four tiers. To facilitate efficient use of the tiered approach in regulatory practice, user-friendly software tools have been developed for the first three tiers. This includes the new software tool PERSAM (Persistence in Soil Analytical Model) and new versions of the pesticide fate models PEARL (Pesticide Emission At Regional and Local Scales) and PELMO (Pesticide Leaching Model). The software tools generate reports that can be submitted for regulatory purposes. Users of this guidance are advised to use these software tools when performing the exposure assessment. Models other than PEARL or PELMO are currently not supported unless the process descriptions in such numerical models have a similar or higher level of detail than those in PELMO and PEARL (EFSA PPR Panel, 2012). Furthermore, it should be demonstrated that the models give similar results to PEARL and PELMO. This is necessary to guarantee consistency of the tiered approach. If a numerical model is to be used, applicants and rapporteurs are advised to report simulations with at least two numerical models (e.g. PEARL and PELMO) and provide the highest Predicted Environmental Concentration (PEC) for regulatory submissions (this procedure is in line with EC (2014)).

This guidance has changed the tiered assessment scheme given in EFSA PPR Panel (2012) with the goal of simplifying the exposure assessment for regulatory purposes. The exposure assessment starts with simulations for one predefined scenario per regulatory zone, North–Centre–South. At this tier, simulations are carried out with the simple analytical model PERSAM. PERSAM has the advantage that the required number of inputs is very limited and so the documentation requires little effort.

Based on discussions with stakeholders, it was a boundary condition that the exposure assessment can be applied by taking median or average substance properties from the dossiers. Such substance properties are uncertain and inclusion of this uncertainty leads to probability density distributions that show greater spread. Consequently, this boundary condition led to the need to base the exposure-assessment procedure on the spatial 95th percentile concentration instead of the spatial 90th percentile concentration.

A single set of predefined scenarios has been developed for use in Tier-1. These predefined scenarios apply to all permanent and annual crops and are based on the total area of annual crops and permanent crops (excluding permanent grassland) in a regulatory zone. However, the exposure

assessment goal is based on the agricultural area where a PPP is intended to be used. The applicant may therefore wish to perform an exposure assessment for a particular crop. For this purpose, Tier-2 is provided. At this tier, a spatially distributed version of PERSAM is used and the target percentile is directly calculated from the concentration distribution within the area of a given crop. Should the assessment at Tier-2 still indicate an unacceptable risk to soil organisms, the applicant has the option to move to Tier-3A. Tier-3A is also based on the area of a given crop, but uses numerical models (PEARL and PELMO). Tier-3A requires slightly more effort; however, this tier has the advantage that more realistic modelling approaches are used and therefore this tier will deliver less conservative values. At Tier-3A, the same crop- and substance-specific scenarios as selected at Tier-2 are used. Tier-1 is based on the assumption that crop interception of the substance does not occur. In all other tiers, this can be included. To facilitate harmonisation of the regulatory process, canopy processes in PEARL and PELMO were harmonised. This guidance further introduces a table for the default wash-off fraction from the crop canopy that was created based on simulations with PEARL and PELMO. This table should be used at Tier-2. It is considered acceptable to override the default values in this table by values obtained from experiments with the substance and formulation considered and plants under a range of relevant conditions. At Tier-3A, dissipation at the crop canopy and wash-off may be based on simulations with the numerical models. Tier-3B using spatially distributed numerical models is also mentioned. Tier-3B should, however, not be used until agreed software tools and further guidance are available. Post-registration monitoring is proposed as Tier-4.

The predefined scenarios used at Tier-1 are based on the 95th spatial percentile considering the total area of annual crops and permanent crops (excluding permanent grassland) in each regulatory zone. However, the purpose of the exposure assessment is to consider the total area of the crop where the PPP is intended to be applied. Since the 95th spatial percentile of a given crop may be higher, scenario adjustment factors (named crop extrapolation factors in EFSA PPR Panel, 2012) have been included at Tier-1 to ensure that these tiers are more conservative than Tier-2, Tier-3A, and Tier-3B.

The simple analytical model PERSAM is used in lower tiers. Since it cannot be *a priori* guaranteed that the simple analytical model is more conservative than the more realistic numerical models used in Tier-3A and Tier-3B, model adjustment factors have been included in all tiers where the analytical model is used. The model adjustment factors proposed in EFSA PPR Panel (2012) have been reassessed for this Guidance Document and the number of factors has been reduced to ease their use in the regulatory process. Some guidance is given on using Tier-1 predefined scenario definitions for calculating PEC for microbial active substances.

With respect to substance-specific model inputs, this Guidance Document generally follows recommendations given in the FOCUS Degradation kinetics report (FOCUS, 2006), the generic guidance for Tier-1 FOCUS Groundwater assessments (Anonymous, 2014) and the EFSA Guidance Document on how to obtain *DegT50* values (EFSA, 2014a). New guidance is included for (i) the calculation of the rapidly dissipating fraction at the soil surface, (ii) the sorption coefficient in air-dry soil and (iii) the *DegT50* or K_{om} of substances whose properties depend on soil properties such as pH or clay content.

Off-crop exposure (e.g. as a result of spray drift deposition or as a result of storage or disposal of growing media used in horticultural production) is not covered by this EFSA guidance because the current methodology does not describe emissions from the treated field and subsequent deposition of the emitted amounts onto the off-field surface.

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Background as provided by EFSA

During a general consultation of Member States on needs for updating existing guidance documents and developing new ones, a number of European Union Member States (MSs) requested a revision of the SANCO Guidance Document on persistence in soil (SANCO/9188VI/1997 of 12 July 2000) (EC, 2000). The consultation was conducted through the Standing Committee on the Food Chain and Animal Health.

Based on the Member State responses and the Opinion prepared by the PPR Panel (EFSA PPR Panel, 2012), the European Commission tasked the European Food Safety Authority (EFSA) to prepare a Guidance of EFSA for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil in a letter of 31 July 2012. EFSA accepted this task in a letter to the European Commission dated 9 October 2012. The European Commission requests this scientific and technical assistance from EFSA according to Article 31 of Regulation (EC) No 178/2002 of the European Parliament and of the Council.

Following public consultations on the Opinion (EFSA PPR Panel, 2012), Member States and other stakeholders requested 'an *easy to use Guidance Document*' to facilitate the use of the proposed guidance and methodology for the evaluation of PPPs according to Regulation (EC) No 1107/2009.

Once this Guidance Document is delivered, the European Commission will initiate the process for the formal use of the Guidance Documents within an appropriate time frame for applicants and evaluators. It may be noted that guidance on the circumstance under which each individual exposure estimate should be used is still under development.

Terms of reference as provided by the European Commission

EFSA, and in particular the Pesticides Unit, is asked by the European Commission (DG SANTE) to draft an EFSA Guidance Document entitled *'EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil'*. The EFSA Guidance Document should respect the science proposed and methodology developed in the adopted PPR Opinion mentioned in this document (EFSA PPR Panel, 2012).

EFSA proposed to the European Commission (DG SANTE) to include also guidance for permanent crops, crops grown on ridges and annual crops where no tillage is applied into the updated Guidance Document. The European Commission also accepted an extension of the deadline for finalisation of the guidance until end of 2017.

EFSA was requested to organise public consultations on the draft Guidance Document, to ensure the full involvement of Member States and other stakeholders. To support the use of the new guidance, EFSA is requested to organise training of Member State experts, applicants and other relevant stakeholders.

Context of the scientific output

The purpose is to address the Terms of References as provided by the European Commission.

Assessment

1. Introduction

1.1. Aim of this Guidance Document

This document provides guidance for the exposure assessment of soil organisms to plant protection products (PPPs) in the three regulatory zones and in EU MSs in accordance with Regulation (EC) No. 1107/2009 of the European Parliament and the Council (Figure 1). The methodology was developed for the assessment of active substances and metabolites in the context of approval at the European Union (EU) level, and it is expected to be used also for the assessment of products at the zonal level.

The draft EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil was subject to public consultation from 10 July 2014 to 4 September 2014. A technical report has been produced containing the stakeholder comments received during the public consultation and how these comments have been taken into account (EFSA, 2015a).

This Guidance Document presents a brief overview of the recommended procedure and provides the guidance necessary to enable users to carry out the exposure assessment. A comprehensive description of the methodology and the science behind this methodology can be found in EFSA PPR Panel (2010d, 2012), EFSA (2009b, 2010a, 2012), and Beulke et al. (2015). Some further scientific developments have taken place after the publication of these scientific reports with the goal to facilitate and further harmonise the exposure assessment. These scientific developments are described in the Appendices to this Guidance Document.

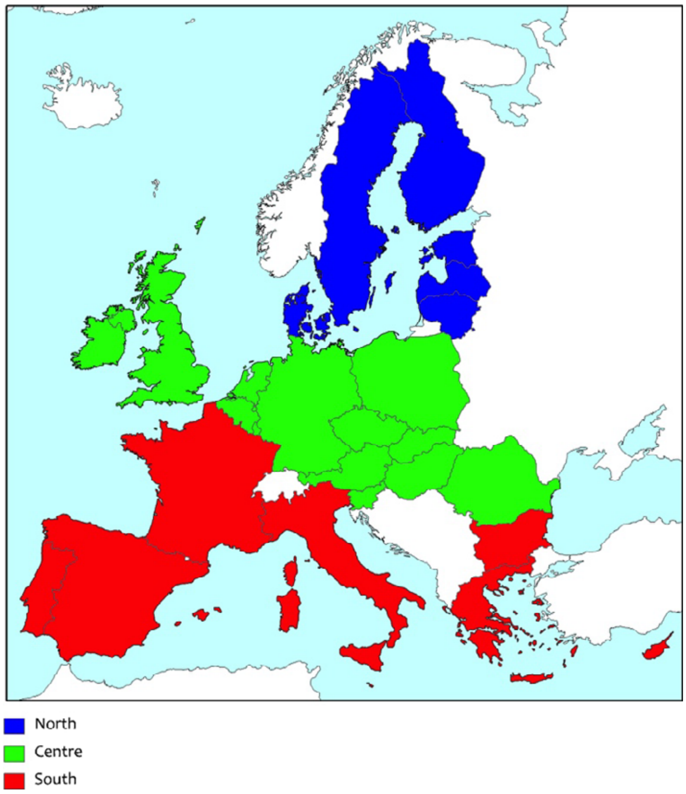

Figure 1: Map of the three regulatory zones according to Regulation (EC) No. 1107/2009 of the European Parliament and the Council. Only those countries that are included in the spatial data set for the PERSAM tool are included in this map

The recommended procedure consists of four tiers (Section 2). The lower tiers are explained in detail. This Guidance Document will also provide brief guidance on spatially distributed modelling with numerical models and post-registration monitoring. The scenarios in this Guidance Document were selected using a procedure that works well for both parent substances and soil metabolites and started with the compilation of a coherent database, which is available for free at the European Soil Data Centre (Panagos et al., 2012).

The PERSAM tool can also be used for Tier-1 and Tier-2 exposure assessments of plant protection products at the national level in EU MSs in accordance with Regulation (EC) No. 1107/2009.[3] The guidance can also be used for selection of scenarios at Tier-2 and Tier-3 for individual EU MSs. This implies that, for these tiers, the guidance can be used without modification for the exposure assessment within the territory of an EU Member State. The scenarios at Tier-1 apply to the zonal level. Tier-1 is assumed also to be conservative enough for use at the national level due to the relatively high assessment factors used at Tier-1.

[3] Croatia and Norway are currently not included in the PERSAM software as some data layers were not available for these countries at the time of publication of this guidance.

1.2. The exposure-assessment goal

As described in EFSA PPR Panel (2012), the methodology is based on the goal to assess the 90th percentile concentration considering all agricultural fields within a regulatory zone (North–Centre–South) where the particular PPP is intended to be used. The agricultural area of use is represented by the crop in which the pesticide is intended to be used, e.g. for a pesticide that is to be applied in maize, the area is defined as all fields growing maize in a regulatory zone. By defining the total area as the regulatory zones within the EU, considerably fewer scenarios were distinguished here than in earlier guidance, which used climatic and paedological data to identify scenarios (e.g. Forum for Co-ordination of Pesticide Fate Models and their Use (FOCUS) Groundwater reports of 2000 and EC (2014), in which nine scenarios were distinguished). This step was implemented to keep the regulatory process as simple as possible. In general, exposure estimates for all three zones should be evaluated for review of substances at the EU level. For zonal evaluations of PPPs it would be sufficient to consider only the exposure estimates for the particular zone in question.

The exposure assessment is part of the terrestrial effect assessment. This Guidance Document therefore considers all types of concentrations that are potentially needed to assess the ecotoxicological effects. Please note that guidance on the circumstance under which each individual exposure estimate should be used still needs to be developed. EFSA (2009a) indicated that the following types of concentrations are needed:

- The concentration in total soil (mg/kg) averaged over the top 1–20 cm of soil for various time windows: peak and time-weighted averages (TWAs) for 7–56 days.
- The concentration in pore water (mg/L) averaged over the top 1–20 cm of soil for the same time windows.

Until EFSA guidance on the risk assessment for in-soil organisms is prepared, this exposure guidance proposes to use the assessment depths of 5 cm and 20 cm (the latter in case of soil incorporation) in line with the currently applied procedure (FOCUS, 1997).

As indicated in EFSA PPR Panel (2012), the peak concentration is approximated by the maximum concentration of time series of 20 years (application each year), 40 years (application every 2 years) or 60 years (application every 3 years). The TWA concentrations are calculated for periods over a maximum of 56 days after the occurrence of the peak concentration.

Older soil ecotoxicological studies sometimes expressed exposure in terms of only the applied rate (in kg/ha). This Guidance Document therefore also briefly describes how to express exposure in kg/ha.

Presently, pore water concentrations are not used in standard risk assessments for soil organisms; however, the pore water concentrations were included in the methodology in case the standard approach would be revised in the future (as recommended by EFSA (2009b, 2009a), ECHA (2016) and EFSA PPR Panel (2017)). However, currently, until new in soil effect guidance is available, the uniform principles (Regulation EU No. 546/2011) propose that effect concentrations are to be expressed in mg/kg dry weight soil.

Based on discussions with stakeholders, it was a boundary condition that the exposure-assessment methodology could be applied by taking median or average substance properties from the dossiers (so neither high or low percentile values nor worst-case substance properties should be used). Such substance properties are uncertain and inclusion of this uncertainty leads to probability density functions that show greater spread. Therefore, this boundary condition led to the need to base the exposure-assessment procedure on the spatial 95th percentile concentration instead of the 90th percentile spatial concentration (see Section 4.2.5 of EFSA PPR Panel (2012) for details). This was combined with the conservative approach of taking the 97.5th percentile in time of the numerical models (as described by EFSA, 2012, there were usually only small differences between the 72.5th and 97.5th temporal percentiles, so the effect of this conservative assumption is usually small).

1.3. Cropping and applications systems covered by this guidance

The methodology covers a wide range of different cropping and application systems (Figure 2). The exposure assessment for annual crops differs from that for permanent crops because the distribution of organic matter with depth in permanent crops differs from that in annual crops. For this reason, the exposure assessment scheme makes a distinction between annual crops (left-hand side of Figure 2) and permanent crops right-hand side of Figure 2).

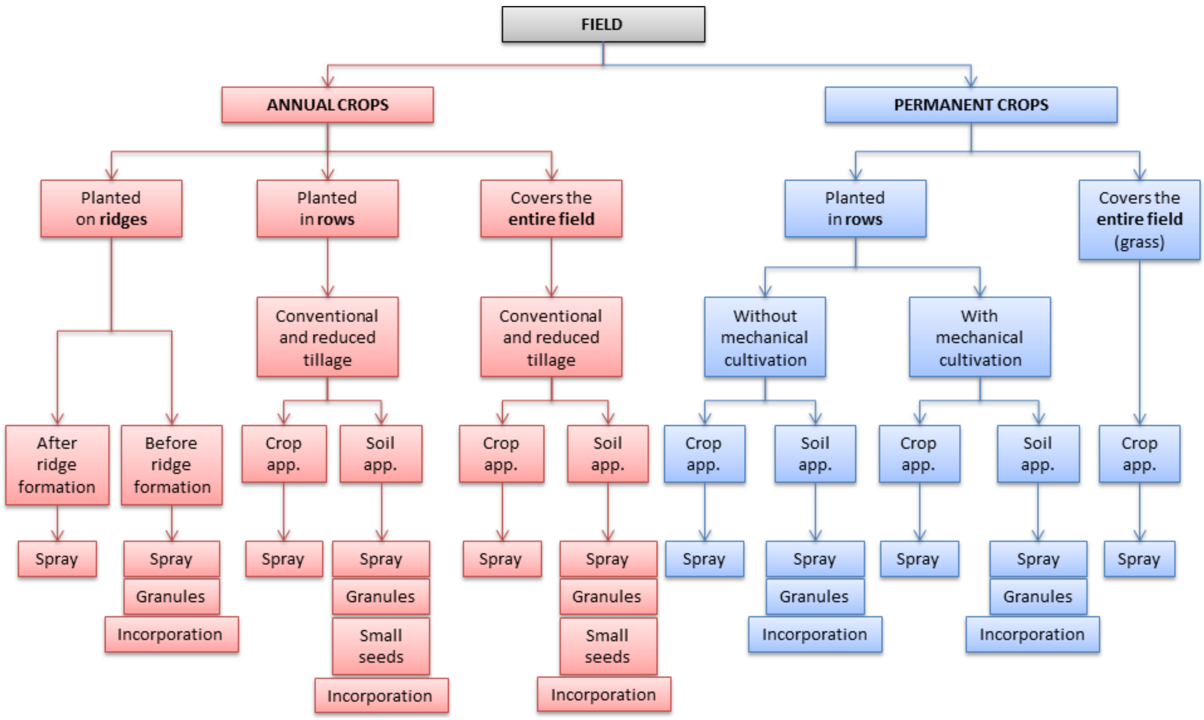

Figure 2: Cropping and application systems covered by this guidance

As indicated in Figure 2, incorporated applications are covered by the guidance. In this context, incorporation can include either placement at a certain soil depth (i.e. precision drilling treated seeds, placing granules in a furrow at drilling or injection of a liquid or gas) or application at the soil surface (by spraying, broadcasting granules, broadcasting treated seed) followed immediately by a cultivation method that both incorporates and mixes materials (including the active substance) more evenly between the soil surface and the mixing depth resulting from the cultivation technique.

The guidance does not cover all cropping and application systems. Applications by drip irrigation or dipping and drenching are, for example, not covered. Furthermore, use of this guidance for soil injection of gaseous substances should be done with caution. For uses that are not covered by this guidance, the applicant should describe how the Guidance Document is implemented and justify its applicability.

Off-crop exposure (e.g. as a result of spray drift deposition or as a result of storage or disposal of growing media used in horticultural production) is not covered by this EFSA guidance because the current methodology does not describe emissions from the treated field and subsequent deposition of the emitted amounts onto the off-field surface. EFSA PPR Panel Opinion (2017) provides some considerations; however, appropriate off-crop exposure scenarios that apply to a given percentile of the concentration distribution still need to be developed.

1.3.1. Annual crops

The exposure assessment was originally developed for spray applications in annual crops covering the entire field (EFSA PPR Panel, 2010d) and this has been implemented as the default assumption in this Guidance Document. However, additional work revealed that, with small modifications, the methodology could also be used for non-uniform applications for in-row crops and crops grown on ridges and for band applications, strip applications and spot applications (second row in Figure 2). If such non-uniform treatments are applied, this should be indicated in the Good Agricultural Practice (GAP) table including the fraction of the soil surface area treated.

It was further proposed to make a distinction between conventional/reduced tillage systems and no-tillage systems (EFSA PPR Panel, 2010d) because annual ploughing has a large diluting effect on the concentration in the topsoil, which does not occur in no-tillage systems. However, the GAP tables included in regulatory submissions do not include information on whether the substance is applied in no-tillage systems. Furthermore, the area of soil with no-tillage systems is relatively small in many EU countries. For these reasons, no specific guidance was developed for no-tillage systems (see

Section 2.10 for additional considerations). Until guidance for no-tillage systems is developed, it is recommended to use the guidance for tilled systems for annual crops.

This guidance covers spray applications, applications of granular products (to the soil surface, incorporated or placed at a certain soil depth) and treated small seeds (typically placed at a certain soil depth if incorporated). Guidance for spray applications is given in Section 3. For granules and small seeds, the same guidance is to be used; however, the additional considerations in Section 4 should be taken into account. This guidance does not cover large treated seeds; please refer to the SANCO draft guidance on seed treatment (EC, in preparation; SANCO/10553/2012) for guidance on large treated seeds. However, in view of the simple PEC_{sphere} concept given in the SANCO draft guidance, it is recommended to replace the default soil density of 1.5 dm^3/kg stated there with more realistic worst-case soil density values, e.g. as given for the Tier-1 scenarios. In the SANCO draft guidance on seed treatments, large seeds are defined as seeds with a diameter $>$ 0.5 cm and small seeds are defined as seeds with a diameter $\leq$ 0.5 cm. For the EFSA guidance, it is proposed to handle maize seeds and pelleted seeds as small seeds. When it is intended that cultivation practices result in soil incorporation at the time of application, this point should be clearly indicated in the GAP table included in the regulatory submission.

1.3.2. Permanent crops

Also, in the case of permanent crops, a distinction is made between crops grown in rows (e.g. fruits, vines and olives) and crops that cover the entire field (mainly permanent grassland). In permanent crops grown in rows, mechanical cultivation can be carried out in or between the crop rows. Based on Beulke et al. (2015), mechanical cultivation is assumed between the rows in citrus, vines, olives and hops. In olives, mechanical cultivation is also assumed in the crop rows. In all other permanent crop situations, no mechanical cultivation is assumed. When mechanical cultivation is carried out, the mixing depth is assumed to be 5 cm. The mixing depth of 5 cm is consistent with the depth distribution of organic matter in situations with mechanical mixing. Note that the mixing depth in permanent crops is considerably less than the tillage depth in annual crops (20 cm).

For permanent crops grown in rows, pesticides can be applied to the crop canopy (air blast applications) or to the soil (ground spray applications or granular applications to the soil surface with or without immediate subsequent cultivation to mix substance over the assumed 5 cm mixing depth) (Figure 3). Application to the soil can be in the crop row ('in-row treatment') or between the crop rows ('between-row treatment'). In the case of air blast applications, exposure of soil organisms will occur both in and between the crop rows. In the case of in-row soil treatments, exposure is considered relevant in-row only and in the case of between-row soil treatments, exposure is considered between the rows only. The same set of predefined scenarios is used for all combinations; however, the calculation procedure differs between the various application types. The application types to be considered should be clearly indicated in the GAP table included in the regulatory submission. When it is intended that cultivation practices result in soil incorporation at the time of application, this point should also be clearly indicated in the GAP table.

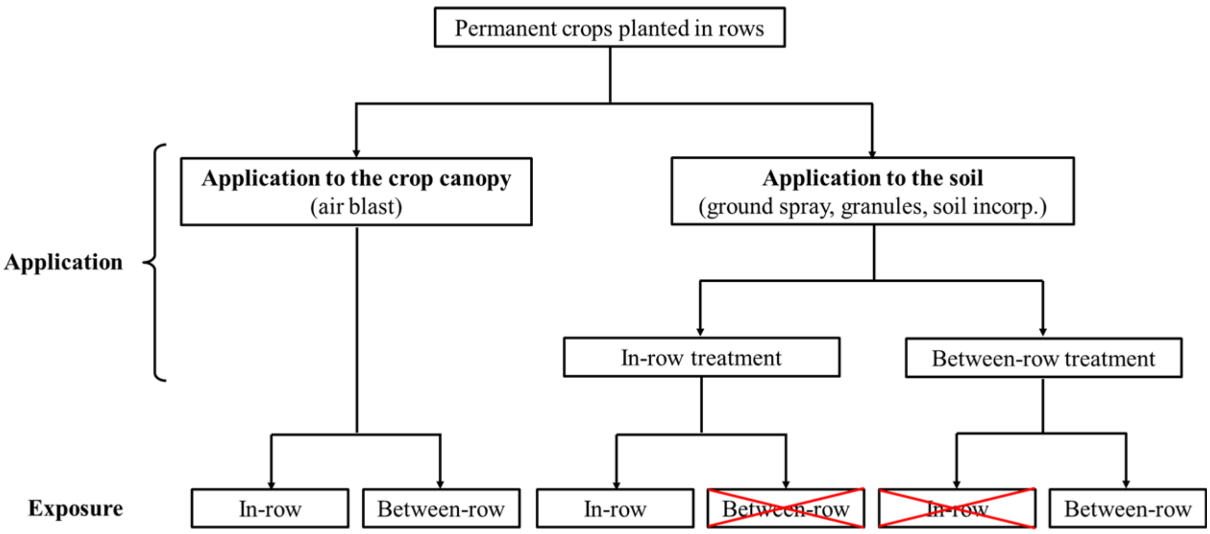

Figure 3: Application systems in permanent crops grown in rows covered by this guidance

1.3.3. Protected crops

When the uses being assessed includes a crop that can be grown under protection (greenhouses and crops grown under cover) and soil has not been precluded as being a possible growing substrate, soil exposure calculations for these uses have to be calculated following the procedures outlined in this guidance (see Section 3.2 of EFSA, 2014b for details). The only exception is when the applicant specifies that they wish use to be restricted to high technology greenhouses that are permanent structures, the changes to the soil parameters and the soil organism community can be considered such that a risk assessment for soil organisms is not relevant (EFSA, 2014b). However, for persistent substances (*DegT90* > 1 year; uniform principles (Regulation EU No. 546/2011)[4]), an assessment as it is for open field is required with regard to their residues, to account for possible change of destination of the soil within the structure in the longer term (e.g. if the soil is removed and used outside and/or the structure is removed).

1.4. Software tools

To facilitate efficient use of the tiered approach in regulatory practice, user-friendly software tools have been developed. This development includes the software tool PERSAM (Persistence in Soil Analytical Model) (Decorte et al., 2016a; updated version in preparation); based on EFSA (2015b) and Tiktak et al. (2013) and new versions of the pesticide fate models PEARL (Pesticide Emission At Regional and Local Scales) (Tiktak et al., 2000; Van den Berg et al., 2016) and PELMO (Pesticide Leaching Model) (Klein, 2011) that have been adapted to deliver the appropriate soil exposure concentrations. Applicants are advised to use these software tools when performing the exposure assessment. However, applicants might want to use the analytical model outside the PERSAM software (see the listing of the model in Appendix A). This use must be performed in combination with the EFSA spatial data set (version 1.1) as available at the Joint Research Centre (JRC) website. Applicants should demonstrate that their own software reproduces an identical output to that of the PERSAM tool, e.g. by comparison of the predefined scenarios.

For higher-tier assessments, models other than PEARL or PELMO are not currently supported. The reason is that consistency of the tiered approach cannot be guaranteed when using different models. If applicants chose to use another model, other than PERSAM, PEARL or PELMO, they should demonstrate that their model produces the same output (identical output) (see Section 3.1 for more details). If a numerical model is to be used, applicants and rapporteurs are advised to report simulations with at least two numerical models (e.g. PEARL and PELMO) and provide the highest Predicted Environmental Concentration (PEC) for regulatory submissions (this procedure is in line with EC (2014)). For complex assessments using other models and modelling approaches, it is recommended to agree the approach with the competent authority before submission.

The currently available version of the PERSAM model is not applicable for permanent crops for all evaluation depths because it assumes mixing of the top 20 cm of the soil before each application and ignores leaching from the evaluation layer. For these two reasons, a new version of PERSAM has been developed that is described in Appendix A. For consistency reasons, this new version of the analytical model is also being used for annual crops. Notice that at the time of publication of this Guidance Document, the software tools have not been fully aligned with the Guidance Document. However, an update of the tools is foreseen before the Guidance will be notified for use in regulatory submissions.

1.5. Structure of this Guidance Document

Section 2 gives an overview of the tiered approach and highlights some new developments that have taken place since the publication of the scientific Opinion (EFSA PPR Panel, 2012) on which this Guidance Document is based. Section 3 provides practical guidance on how to perform exposure assessments in soil for active substances of PPPs and for the metabolites of these active substances. Section 3 is applicable to spray applications in crops covering the entire field. The guidance also applies to crops grown on ridges and crops grown in rows; however, additional guidance in Section 4 needs to be considered. Section 4 also gives additional guidance for other application types (small seed treatments and granules). Section 5 briefly describes documentation requirements. Scientific backgrounds to the new developments, desirable future developments and practical examples are given in the Appendices.

[4] Regulation (EU) No. 546/2009 of the European Parliament and of the Council as regards uniform principles for evaluation and authorisation of plant protection products.

2. Overview of the tiered approach and new developments

This section provides a general overview of the tiered approach and highlights some new developments that have taken place since the publication of the scientific Opinion on which this Guidance Document is based.

2.1. General overview

EFSA's PPR Panel (2012) proposed a tiered assessment scheme for the exposure assessment of soil organisms in annual crops. This guidance has changed the tiered assessment scheme with the goal to simplify the exposure assessment for regulatory purposes. Moreover, this guidance extends the use of the tiered assessment scheme to permanent crops and crops grown on ridges. The revised scheme can be found in Figure 4. The lower tiers are more conservative and less sophisticated than the higher tiers, but all tiers aim to address the same exposure assessment goal (i.e. the 90th percentile concentration within the area of intended use of a PPP). This principle allows direct movement to higher tiers without performing assessments for all lower tiers (an applicant may, for example, directly go to higher tiers without first performing a Tier-1 assessment).

The exposure assessment starts with simulations for one predefined scenario per regulatory zone, North–Centre–South. Simulations are carried out with PERSAM at Tier-1. PERSAM has the advantage that the required number of inputs is very limited and so the documentation requires little effort. As mentioned in Section 1.4, a new version of PERSAM has been developed that is also applicable to permanent crops (Appendix A).

The predefined scenarios in Tier-1 are based on the total area of annual and permanent crops (excluding permanent grassland) in a regulatory zone. However, the exposure assessment for annual crops differs from that for permanent crops (e.g. the distribution of organic matter with depth in permanent crops differs from that in annual crops). This difference is considered in the parameterisation of the scenarios. The exposure-assessment goal is based on the agricultural area where a substance is intended to be used. The applicant may therefore want to perform an exposure assessment for a particular crop. For this purpose, Tier-2 is provided. At this tier, PERSAM is used to directly calculate the target percentile from the concentration distribution within the area of a given crop.

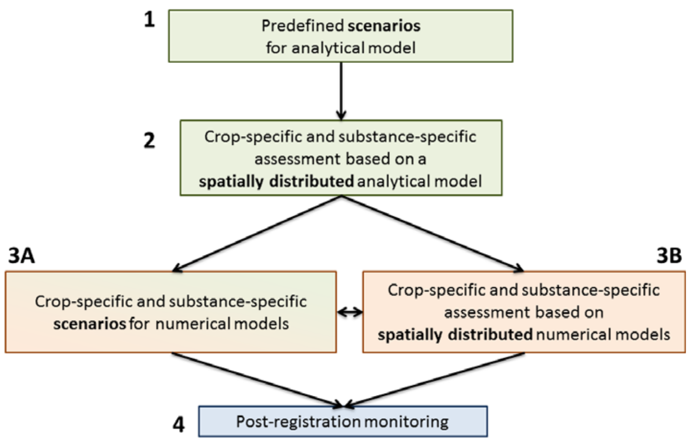

Figure 4: Tiered scheme for the exposure assessment of soil organisms in annual crops and in permanent crops. The scheme applies to both the concentration in total soil and the concentration in pore water. Tier-1, Tier-2 and Tier-3 are all based on one PEC for each of the regulatory zones, North, Centre and South, and allow for one or multiple applications every 1, 2 or 3 years. At Tier-1 and Tier-2, the analytical model in the software tool PERSAM is used. At Tier-3A and Tier-3B, modelling is carried out with numerical models

The predefined scenarios at Tier-1 are not designed for substances whose properties depend on soil properties such as pH or clay. For such substances, the applicant should therefore go to Tier-2 or Tier-3 directly. These tiers offer the option to include relationships between substance properties (*DegT50* and K_{om} or K_{oc}) and soil properties such as pH or clay.

Tier-1 is based on the assumption that crop interception of the substance does not occur. In all other tiers, crop interception and subsequent loss processes at the plant canopy can be included. This assessment can be carried out by simulations with the numerical models at Tier-3A or Tier-3B, or by using a table with default wash-off fractions from the crop canopy depending on crop development (Tables 9 and 10) at Tier-2. Refer to Section 2.5 for details on crop canopy processes.

Should the assessment at Tier-2 still indicate an unacceptable risk to soil organisms, the applicant has the option to move to Tier-3A, which uses the same crop- and substance-specific scenarios as selected in Tier-2. In Tier-3A, the scenario is first identified in the PERSAM software. PERSAM then generates a transfer file containing the geographical coordinates as well as the soil and climate properties of the scenario. This file is used by PEARL or PELMO to generate automatically the input files for the Tier-3A scenarios.

The scheme also contains a Tier-3B, which is a spatially distributed modelling approach based on calculations with the numerical models for many scenarios for each of the zones. Spatially distributed modelling with PEARL or PELMO has the advantage that the spatial 95th percentile of the PEC for all types of concentration of either the parent substance or any soil metabolite can be derived by statistical analysis of the output of the model runs. It can, however, not *a priori* be guaranteed that spatially distributed modelling delivers lower concentrations than Tier-3A. For this reason, spatially distributed modelling is not considered a tier higher than Tier-3A. Brief guidance on how to establish Tier-3B is given in Section 3.5. However, it is recommended not to use Tier-3B until agreed software tools are made available.

Tier-4 is a post-registration monitoring approach, which is described in Section 3.6.

2.2. Properties of the predefined soil exposure scenarios

As described in the previous section, Tier-1 is based on one predefined scenario per regulatory zone (North–Centre–South) for each of the two types of Ecotoxicological Relevant Concentration (ERC), namely the concentration in total soil and the concentration in pore water. These scenarios are briefly described in the sections below; a comprehensive description of the scenarios is given in Appendix B.

The predefined scenarios are based on the total area of annual and permanent crops (excluding permanent grassland) in a regulatory zone (EFSA PPR Panel, 2012). The properties of these scenarios are summarised in Tables 1 and 2 and their position is shown in Figure 5. Soil properties in Table 1 and Table 2 are averages over the top 30 cm. The FOCUS climatic zone as defined in EC (2014) is included because the FOCUS zone plays an important role in the parameterisation of the scenario (please refer to Appendix B for details).

Annual crops are assumed to be tilled annually and therefore these averages apply to the entire soil layer. However, in permanent crops, organic matter cannot be assumed to be uniformly distributed within this top 30 cm soil layer. Beulke et al. (2015) introduced correction factors for calculating the depth distribution of organic matter in the top 30 cm (Table 3). Notice that they made a distinction between situations with and situations without mechanical cultivation depending on the crop type. In situations without mechanical cultivation, it is assumed that organic matter decreases sharply with depth. In situations with mechanical cultivation (typically between the rows only), a depth gradient can still be observed, but less pronounced than in situations without mechanical cultivations. Averaged over the top 30 cm the organic-matter content is the same for both situations.

Table 1: Properties of the predefined scenarios for annual crops and permanent crops used at Tier-1 for the concentration in total soil

Zone	Code	FOCUS zone	Member state	T_{arit}[(a)] (°C)	T_{arr}[(b)] (°C)	P[(c)] (mm)	f_{om}[(d)] (–)	Texture class	θ_{fc}[(e)] (m^3/m^3)	ρ[(f)] (kg/dm^3)
North	CTN	Hamburg	Estonia	5.7	7.6	639	0.220	Coarse	0.244	0.707
Centre	CTC	Hamburg	Poland	7.4	9.3	617	0.122	Coarse	0.244	0.934
South	CTS	Hamburg	France	10.2	11.7	667	0.070	Medium	0.349	1.117

Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to Appendix B.
CTC: scenario for the total concentration in the Centre Zone; CTN: scenario for the total concentration in the North Zone; CTS: scenario for the total concentration in the South Zone. Geographical coordinates of the scenarios are:
CTN – 5141/3991, CTC – 5281/3111, CTS – 3898/2932.
(a): T_{arit} is the arithmetic mean annual temperature.
(b): T_{arr} is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012).
(c): P is the annual mean precipitation (mm).
(d): f_{om} (–) is the organic-matter content averaged over the top 30 cm.
(e): θ_{fc} (m^3/m^3) is the water content at field capacity.
(f): ρ (kg/dm^3) is the dry bulk density of the soil.

Table 2: Properties of the selected predefined scenarios for annual crops and permanent crops used at Tier-1 for the concentration in pore water

Zone	Code	FOCUS zone	Member state	T_{arit}[(a)] (°C)	T_{arr}[(b)] (°C)	P[(c)] (mm)	f_{om}[(d)] (–)	Texture class	θ_{fc}[(e)] (m^3/m^3)	ρ[(f)] (kg/dm^3)
North	CLN	Hamburg	Denmark	8.0	9.2	602	0.025	Medium	0.349	1.371
Centre	CLC	Châteaudun	Austria	9.3	11.3	589	0.018	Medium	0.349	1.432
South	CLS	Sevilla	Spain	15.4	16.7	526	0.010	Medium	0.349	1.521

Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to Appendix B.
CLC: scenario for the concentration in pore water for the Centre Zone; CLN: scenario for the concentration in pore water for the North Zone; CLS: scenario for the concentration in pore water for the South Zone. Geographical coordinates of the scenarios are: CLN – 4422/3645, CLC – 4806/2872, CLS – 3490/1974.
(a): T_{arit} is the arithmetic mean annual temperature.
(b): T_{arr} is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012).
(c): P is the annual mean precipitation (mm).
(d): f_{om} (–) is the organic-matter content averaged over the top 30 cm.
(e): θ_{fc} (m^3/m^3) is the water content at field capacity.
(f): ρ (kg/dm^3) is the dry bulk density of the soil.

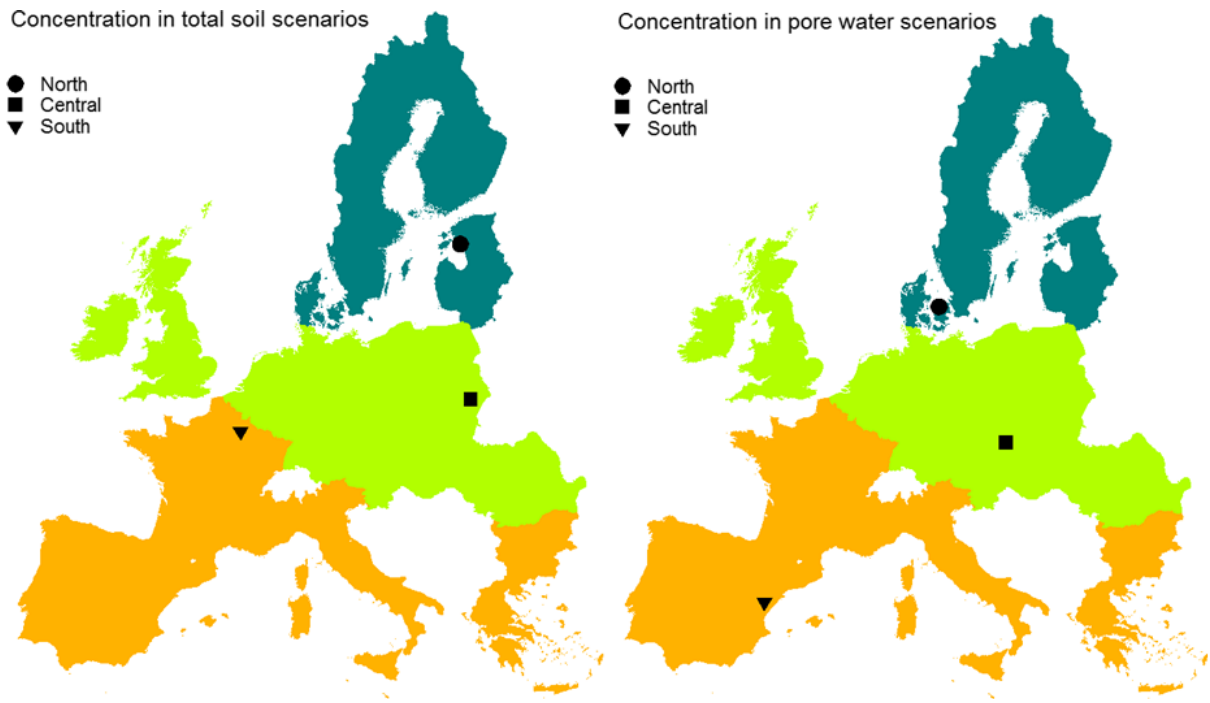

Figure 5: Position of the six predefined scenarios for carrying out Tier-1 soil exposure assessments. The colours indicate the regulatory zones North, Centre and South

Table 3: Correction factors for estimating the distribution of organic matter within the top 30 cm of the soil in permanent crops. The organic-matter content of a layer is calculated by multiplying the correction factor below with the organic-matter content in Tables 1 and 2, respectively

Depth (cm)	Correction factor for situations without mechanical cultivation (–)	Correction factor for situations with mechanical cultivation (–)
0–5	1.95	1.50
5–10	1.30	1.20
10–20	0.76	0.90
20–30	0.62	0.75

2.2.1. Dealing with litter in permanent crops

According to Beulke et al. (2015), data on the litter layer are scarce and it is suggested that no litter layer is present in the majority of the permanent crops. Furthermore, the current exposure models are not capable of simulating exposure in the litter layer. For these reasons, no litter layer is accounted for in the present Guidance Document. However, litter might become more important in the future as good soil-management practices are promoting the presence of organic matter on the soil, so there may be a shift to a more sustainable management of this litter layer (EFSA PPR Panel, 2017). Should there be a need for estimating exposure in litter; a simple estimation of the peak concentration could be based on the current scenarios for permanent crops considering the application rate, the crop interception at the time of application, and a bulk density of litter assuming an organic-matter content of 100% (i.e. 0.126 kg/L). Nevertheless, the development of more advanced computer models that also consider additional processes (e.g. the uptake of pesticide *via* the plant roots) would be necessary to describe this exposure completely.

2.3. Scenario adjustment factors

The scenarios in Tables 1 and 2 are based on the 95th spatial percentile concentration considering the total area of annual and permanent crops in each regulatory zone. However, the purpose of the exposure assessment is to consider the total area of the crop where the PPP is intended to be applied. For any specific crop assessed, the spatial statistical distribution of the exposure concentrations would be different. Therefore, in Tier-1 default scenario adjustment factors are applied because the 95th percentile scenario for a specific crop could differ from the 95th percentile scenario for all arable land (see Table 4 for an overview of tiers where scenario adjustment factors are needed).

Table 4: Overview of inclusion of canopy processes, scenario adjustment factors, and model adjustment factors in the different modelling tiers of Figure 4. '+' indicates that the process or factor is included, '–' indicates that it is not included. Notice that the adjustment factors are automatically applied by the models

Tier	Canopy processes	Scenario adjustment factors	Model adjustment factors
1	–	+	+
2	+	–	+
3A	+	–	–
3B	+	–	–

The default scenario adjustment factors are listed in Table 5. For substantial future changes to spatial data sets, a revision of the scenarios and the adjustment factors might again be needed. However, this is not expected to happen very often.

Table 5: Default scenario adjustment factors (f_s) used when performing an assessment for one of the predefined scenarios at Tier-1 for the three regulatory zones and for the concentration in total soil and for the concentration in pore water. Refer to Appendix C for background information

Regulatory zone	Default scenario adjustment factors to be used for the	
	Concentration in total soil	Concentration in pore water
North–Centre–South	1.4	1.6

2.4. Crop selection at Tier-2, Tier-3A and Tier-3B

With the exception of Tier-1, an assessment is always performed for a specific crop. The starting point is the list of crops described in EC (2014), hereafter referred to as 'FOCUS crops'. These crops should be specified at Tier-2 (PERSAM), Tier-3A and Tier-3B (numerical models). In case of annual crops, one Common Agricultural Policy Regionalised Impact (CAPRI) crop or crop group is linked to the FOCUS crop (Table 6). As described in EFSA PPR Panel (2012), PERSAM uses these so-called CAPRI crops or crop groups (Leip et al., 2008) as a proxy of the area of potential use of the PPP. EU crop maps for CAPRI crops are available at a scale of 1×1 km^2. Contrary, the area for permanent crops in PERSAM is based on the CORINE Land Cover database and EUROSTAT data sets (Beulke et al., 2015).

Table 6 give the link between the FOCUS and the CAPRI crop lists for annual crops. As an example, if the user wants to carry out an assessment for the FOCUS crop 'cabbage', the CAPRI crop 'other fresh vegetables' is selected in PERSAM as an estimate of the 'cabbage' cropping area. The link between the FOCUS crop and the crop in PERSAM for permanent crops is given in Table 7. Note that for permanent crops the user also has to specify the exposure type (in-row or between-row exposure) for which the assessment should be carried out.

When a crop is not specified in Tables 6 and 7, the notifier should use the crop in PERSAM with the highest scenario adjustment factor (see Tables C.1–C.4 for their values) unless it can be justified that the crop under consideration should be assigned a different crop. Only if a well-documented crop map is available, it is acceptable to use Tier-2 or Tier-3A to calculate the 95th spatial percentile of the PEC using this crop map. 'Well documented' implies that the methodology for deriving this crop map should be described preferably by referring to a scientific background report and/or paper. The methodology should be reproducible and be based on generally accepted procedures. Further considerations on data quality are given in EFSA's scientific Opinion on Good Modelling Practice (EFSA PPR Panel, 2014).

Table 6: Link between FOCUS and CAPRI crops for annual crops. The table further shows which FOCUS scenario (dominant FOCUS zone) is used to build the Tier-3A scenario

FOCUS crop	CAPRI crop[d]	North	Centre	South
Beans (field- and vegetable beans)[c]	Pulses	HA	CH	HA
Cabbage	Other fresh vegetables	HA	CH	SE
Carrots	Other fresh vegetables	HA	CH	SE
Cotton	Texture crops	–	HA	TH
Linseed	Texture crops	HA	HA	SE
Maize	Maize	HA	CH	HA
No crops (= fallow)	Fallow	HA	HA	SE
Oil seed rape (summer)	Oilseed rapes	HA	HA	HA
Oil seed rape (winter)	Oilseed rapes	HA	HA	HA
Onions[a]	Other fresh vegetables	HA	HA	SE
Peas (animal)	Pulses	HA	CH	HA
Potatoes	Potatoes	HA	HA	HA
Soybean	Soya beans	–	CH	TH
Spring cereals	Cereals[b]	HA	CH	HA
Strawberries	Other fresh vegetables	HA	CH	SE
Sugar beets	Sugar beets	HA	HA	HA
Sunflower	Sunflower	–	CH	HA
Tobacco	Tobacco	–	CH	TH
Tomatoes	Other fresh vegetables	HA	CH	SE
Winter cereals	Cereals[b]	HA	CH	HA

CH: Châteaudun; HA: Hamburg; JO: Jokioinen; KR: Kremsmünster; OK: Okehampton; PI: Piacenza; PO: Porto; SE: Seville; TH: Thiva. See EC (2014) for further details.
(a): Also to be used for flower bulbs because there is no such crop in FOCUS.
(b): Barley, common wheat, durum wheat, oats and rye.
(c): Field beans in North and Centre; vegetable beans in South.
(d): Used as a proxy of the area of potential use of the PPP.

The numerical models at Tier-3A not only need the crop type but also detailed information about crop development, weather and irrigation data. This information is derived from FOCUS Groundwater input files (EC, 2014). Tables 6 and 7 show the FOCUS information used to build the Tier-3A scenario. This selection is based on the dominant FOCUS zone within each regulatory zone. (The dominant zone is the zone with the highest crop area within a regulatory zone.) Notice that in some cases the dominant FOCUS scenario cannot be linked to a FOCUS crop. In those cases, a second-best alternative was chosen; please refer to Table B.5 in Appendix B for details.

Table 7: Link between FOCUS crops and permanent crops. The table further shows which FOCUS scenario (dominant FOCUS zone) is used to build the Tier-3A scenario. Note that in permanent crops grown in rows there is a distinction between in-row and between-row exposure

FOCUS crop	Permanent crop[(d)]	North	Centre	South	Exposure type
Apples	Apples[(e)]	HA	HA	SE	In-row (apples)
					Between-row (grass cover)
Bush berries[(a)]	Bush berries	HA	CH	SE	In-row (bush berries)
					Between-row (grass cover)
Citrus	Citrus	–	–	SE	In-row (citrus)
					Between-row (bare soil)
Grass	Permanent grass	HA	HA	HA	Not relevant
Hops[(b)]	Hops	–	HA	HA	In-row (hops)
					Between-row (bare soil)
Olives[(c)]	Olives	–	–	SE	In-row (olives)
					Between-row (bare soil)
Vines	Vines	–	CH	SE	In-row (vines)
					Between-row (bare soil)

CH: Châteaudun; HA: Hamburg; JO: Jokioinen; KR: Kremsmünster; OK: Okehampton; PI: Piacenza; PO: Porto; SE: Seville. See EC (2014) for further details.
(a): Development stages set to those for FOCUS apples; all other crop parameters from FOCUS bush berries (Jokioinen only; Beulke et al., 2015).
(b): Not a FOCUS GW crop; citrus crop parameter used; max. Leaf Area Index (LAI) set to 5 m/m^3 (Beulke et al., 2015).
(c): Not a FOCUS GW crop; development stages, rooting depth and max. LAI taken from Beulke et al. (2015).
(d): Used as a proxy of the area of potential use of the PPP.
(e): Pome and stone fruits.

2.5. Model adjustment factors

The simple analytical model is used in lower tiers. As it cannot be *a priori* guaranteed that the simple analytical model is conservative enough when compared with the more realistic numerical models used in Tier-3A and Tier-3B, model adjustment factors are needed in all the tiers that use the analytical model (Table 4). The model adjustment factors proposed in EFSA (2010a) have been reassessed to incorporate the effect of changing model parameters other than *DegT50* and K_{om}. Since not all possible combinations of model parameters could be studied, the model adjustment factors were rounded up for the sake of simplicity. The revised model adjustment factors are listed in Table 8.

The model adjustment factors used in the tiered approach have been calculated using PEARL and PELMO, so consistency of the tiered approach cannot be guaranteed when using different models. The use of models other than PEARL and PELMO is therefore not currently supported. However, EFSA PPR Panel (2012) encourages parameterising the scenarios for other numerical models, 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. Furthermore, applicants should demonstrate that their own software reproduces the same output (identical output) as PERSAM, PEARL and PELMO, e.g. by comparison for scenarios in Appendix H (see Section 1.4).

Table 8: Model adjustment factors (f_M) used when performing an assessment with the analytical model. Refer to Appendix C for background information

Zone	Model adjustment factors to be used for the	
	Concentration in total soil	Concentration in pore water
North–Centre–South	3.0	4.0

In case of multiple applications in December, January and February, the model adjustment factor may not be entirely sufficient to cover differences between the analytical and the numerical model (for details please refer to Appendix C.2). In these cases, the applicant should therefore directly move to Tier-3A and use the Tier-2 software only for scenario selection.

2.6. Crop canopy processes

Tier-1 is based on the assumption that crop interception of the substance does not occur. In all other tiers, this may be included (Table 4). Since the introduction of the FOCUS groundwater scenarios, it has been common practice to reduce the application rate by the fraction that is intercepted by the crop canopy and to apply this reduced fraction to the soil (Anonymous, 2014). As described by EFSA PPR Panel (2010d), this approach is not considered defensible because there is insufficient evidence that wash-off from the crop canopy can be ignored. Therefore, the effect of dissipation at the crop canopy and foliar wash-off should be included when the substance is applied to the crop canopy.

Crop canopy processes and foliar wash-off can be simulated by PEARL and PELMO in Tier-3A and Tier-3B. However, Reinken et al. (2013) identified serious differences between PEARL and PELMO with respect to the parameterisation of wash-off calculations. The working group concluded that these differences were primarily caused by differences in the calculation of the crop cover fraction and crop development. After harmonisation of crop development and the calculation of the crop cover fraction, differences between PEARL and PELMO were, generally, small (median deviation is 4%).

The analytical model used at Tier-2 cannot simulate plant processes. For this reason, tables of default wash-off fractions from the canopy depending on the crop development stage were created based on simulations with PEARL and PELMO (Tables 9 and 10). At Tier-2, these tables are used by PERSAM to calculate the fraction of the dose reaching the soil for each individual application depending on the crop and the BBCH code specified by the user.

The fraction of the dose reaching the soil is defined as the sum of the fraction of the dose washed off and the fraction of the dose that directly reaches the soil (see also Figure 7):

$$f_{soil} = (1 - f_i) + f_i f_w \tag{1}$$

where f_{soil} is the fraction of the dose reaching the soil, f_i is the fraction of the dose intercepted and f_w is the default wash-off fraction of the dose intercepted by the crop canopy. Notice that the fraction of the dose intercepted is based on EFSA (2014a) at all tiers. Further details on the development of the tables are given in Appendix D. Note that this guidance uses the fraction of the dose reaching the soil (f_{soil}) based on average fractions washed off instead the maximum fraction washed off ($F_{soil,max}$), which was used in EFSA PPR Panel (2012). The background for this is that using the maximum value in the wash-off tables would lead to considerable overestimation of the exposure concentration, which is the result of assuming that the maximum wash-off occurs every year (Appendix D.2).

Crop interception should not be included in calculations for row, band, strip or spot treatments, and crops grown on ridges unless the spray is targeted on just the crop canopy or the crop canopy has closed between the rows or ridges.

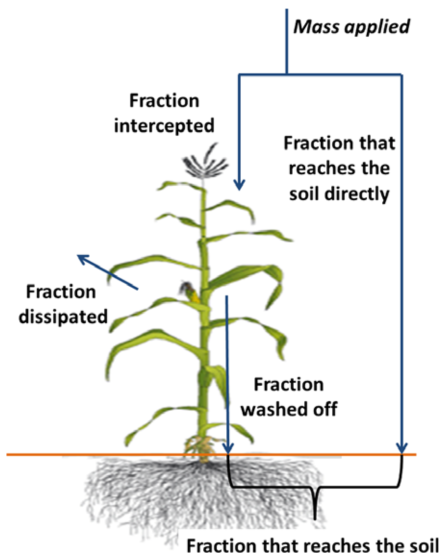

Figure 6: Schematic overview of the processes occurring at the crop canopy. The fraction of the dose reaching the soil is the sum of wash-off from the canopy and the fraction of the dose that reaches the soil directly

Table 9: Default foliar wash-off fractions (f_w) of the dose intercepted by the canopy in annual crops used at Tier-2 considering canopy processes as a function of crop development stage

Crop	BBCH code[(a),(b)]				
	00–09	**10–19**	**20–39**	**40–89**	**90–99**
Beans (vegetable and field)	–	0.60	0.75	0.80	0.35
Cabbage	–	0.60	0.80	0.40–0.00[(c)]	0.00[(c)]
Carrots	–	0.75	0.85	0.50–0.00[(c)]	0.00[(c)]
Cotton	–	0.65	0.75	0.65	0.45
Linseed	–	0.55	0.75	0.60	0.30
Maize	–	0.45	0.65	0.70	0.55
Oil seed rape (summer)	–	0.40	0.50	0.60	0.50
Oil seed rape (winter)	–	0.10	0.40	0.55	0.30
Onions	–	0.60	0.75	0.55–0.00[(c)]	0.00[(c)]
Peas	–	0.40	0.60	0.65	0.35
Potatoes	–	0.30	0.50	0.60	0.35
Soya beans	–	0.55	0.75	0.80	0.35
Strawberries	–	0.50	0.70	0.75	0.50
Sugar beets	–	0.40	0.60	0.60–0.00[(c)]	0.00[(c)]
Sunflower	–	0.60	0.75	0.80	0.55
Tobacco	–	0.55	0.75	0.80	0.85
Tomatoes	–	0.55	0.75	0.70	0.35

Crop	BBCH code[(d)]						
	00–09	**10–19**	**20–29**	**30–39**	**40–69**	**70–89**	**90–99**
Spring cereals	–	0.40	0.50	0.50	0.65	0.65	0.55
Winter cereals	–	0.10	0.40	0.60	0.55	0.60	0.40

BBCH: Biologische Bundesanstalt, Bundesortenamt und Chemische Industrie; na denotes not applicable (no crop canopy present).
(a): The BBCH code is a decimal code ranging from 0 to 99 to characterise the crop development stage (Meier, 2001).
(b): BBCH 00–09: bare to emergence; BBCH 10–19: leaf development; BBCH 20–39: stem elongation; BBCH 40–89: flowering; BBCH 90–99: senescence and ripening.
(c): As these crops are harvested at BBCH 50, the lower value of 0.00 should be used for BBCH code 50–99.
(d): BBCH 00–19: bare to leaf development; BBCH 20–29: tillering; BBCH 30–39: stem elongation; BBCH 40–69: flowering; BBCH 70–99: senescence and ripening.

Table 10: Default foliar wash-off fractions (f_w) of the dose intercepted by the canopy in permanent crops used at Tier-2 considering canopy processes as a function of crop development stage or season

Crop	BBCH code[(a)]			
	00–09[(a)]	**10–69**	**71–75**	**76-89**
Apples	0.55	0.60	0.60	0.55

	BBCH code[(a)]		
	00–09[(a)]	**10–69**	**71–89**
Bush berries	0.50	0.60	0.55
Hops	0.50	0.55	0.60

	BBCH code[(a)]				
	00–09[(a)]	**11–13**	**14–19**	**53–69**	**71–89**
Vines	0.45	0.40	0.50	0.55	0.60

	Season			
	Jan–Mar	Apr–Jun	Jul–Sep	Oct–Dec
Citrus	0.50	0.30	0.15	0.55
Olives	0.50	0.30	0.15	0.50
Permanent grass	0.45	0.55	0.55	0.50
Grass between rows	0.45	0.55	0.55	0.50

(a): Without leaves.

For cultivations of protected crops, it has been recommended to apply the same approaches as for open field crops (see EFSA, 2014b). However, crops grown under cover are generally drip irrigated and protected from rainfall and therefore wash-off from the canopy is not relevant. Therefore, for annual crops grown under cover, we recommend using the crop interception tables published in Appendix C to EFSA (2014a). Please note that there is no wash-off for in-field drip irrigation or under-canopy spray applications either.

2.7. Applicability of the tiered assessment scheme for microbial active substances

Only Tier-1 predefined soil properties should be used for calculating PEC of colony forming units (CFU) of microbial active substances in the bulk soil.[5] Tier-1 calculations should assume no crop interception, a maximum total annual dose and the soil bulk densities that are presented in Table 1 (Section 2.2). The PERSAM tool can be used for this calculation, with the option for microbial active substances being selected. The tool will report just Tier-1 calculations and concentration in total soil when this option is selected. The annual total dose in CFU/ha should be used as input in the tool with it being specified as a single application. Internally the tool applies a default K_{oc} of 2,000 mL/g (high value) consequent to the lack of applicability of the adsorption concept for microorganism propagules. A default DT_{50} for CFU of 1,000 days should usually be used (entered by the user). Alternatively, a decline rate derived from soil investigations assessed as reliable, if such decline was observed, can be used. Organism PECs are reported as CFU/kg.[6] Crop interception might be accounted for in PEC to reduce the CFU calculated to be in the soil. This represents a refinement possibility. This is however only appropriate when experimental data are available for representative microorganism propagules and relevant crops demonstrating their adherence to foliage or the proportion of CFU being measured as initially intercepted being recovered as CFU from the ground (i.e. washed off). In this situation, crop interception values may be taken from Tables 1.4 and 1.5, Appendix C of EFSA (2014a) combined with the experimentally derived foliar wash-off values as appropriate. It would not be appropriate to use the default foliar wash-off factors in Tables 9 and 10 (Section 2.6). When this option is followed, the calculation procedure reduces the dose rate input into PERSAM in CFU/ha according to the proportion experimentally estimated not to reach the soil.

2.8. Applicability of the tiered assessment scheme for soil metabolites

The scenarios described in this Guidance Document can be considered appropriate for both parent compounds and metabolites. The reason is that the scenarios described here were selected using a version of the analytical model that includes leaching. PERSAM for Tier-1 and Tier-2 can handle primary and secondary metabolites. For additional metabolites, the numerical models (Tier-3) should be used if relevant.

[5] Degradation rate is not a credible primary parameter that would drive exposure levels for living microorganism that have the potential to reproduce as well as decline. The concept of adsorption is also not applicable to microorganism propagules. As pore water concentration estimates at Tier-1 and scenario selection at Tier-2 and Tier-3 depend on these factors that are not applicable for microorganism propagules, pore water concentrations at all tiers and bulk soil concentrations at Tier-2 and Tier-3 cannot be relied upon for calculating soil PEC for microbial active substances.

[6] The tool output for the organism PEC (CFU/kg), are internally calculated by the tool from the mg/kg units that it would calculate for a chemical, by using a factor of $1 \times 10^{-6}/3$. The reason of the divisor of 3 in this factor, is to cancel the model adjustment factor (described in Section 2.5) that is not needed when higher tier scenario selection approaches are not applicable, as is the case for microbial active substances.

Additional work may be needed if soil photometabolites are formed that are not detected in the soil metabolism studies:

- Estimate the kinetic formation fraction from the soil photolysis study.
- Perform a soil exposure assessment in which the total amount of metabolite that is eventually formed is assumed to be applied to the soil surface as a parent substance (this amount is calculated as the dose of the parent substance multiplied with the formation fraction and multiplied with the molar mass of the metabolite divided by the molar mass of the parent).

If this approach results in an unacceptable risk, a possible way forward would be to refine the formation fraction of this photometabolite based on field dissipation studies.

2.9. Exposure assessment based on the total amount in soil

If a robust Regulatory Acceptable Concentration (RAC) can be calculated in mg/kg, it should be compared with the PEC in mg/kg in the appropriate soil layer. This requires knowledge of the distribution of the substance and the nature of the test media in the ecotoxicological effect study. However, older soil ecotoxicological studies sometimes expressed exposure in terms of only the applied rate (in kg/ha). If such studies have to be used in the risk assessment, it is proposed to perform the exposure assessment based on the concentration in the top 20 cm of soil (i.e. to recalculate the PEC in total soil given in mg/kg into kg/ha exposure estimate to allow comparison with the ecotoxicological end-point). The value of 20 cm should be used because this is the largest value for the ecotoxicological averaging depth. This is a conservative approach for estimating the total amount in soil (EFSA PPR Panel, 2012) as the total amount increases as the thickness of the evaluation layer increases.

Only the scenarios for the concentration in total soil are relevant for such cases, and the total amount in the topsoil, Z (kg/ha), is calculated from the PEC in total soil (in mg/kg) for an ecotoxicological averaging depth (z_{eco}) of 20 cm and the dry bulk density ρ (in kg/dm^3) with:

$$Z = a\rho\text{PEC} \qquad (2)$$

where $a = 2$ kg dm^3/ha mg (parameter a is needed to convert the concentration in the top 20 cm into the total amount in kg/ha). Therefore, if e.g. $\rho = 1.05$ kg/dm^3 and the PEC is 1 mg/kg then $Z = 2 \times 1.05 \times 1 = 2.1$ kg/ha.

The procedure in this section may not be applied to Tier-1 because an inappropriate value of the bulk density would be applied. The applicant should therefore start at Tier-2 and apply Tier-3A when a risk is identified. The value of ρ should be obtained from the PERSAM output.

2.10. Exposure assessment for no-tillage systems in annual crops

The main difference between no-tillage and conventional or reduced tillage systems is that the latter are ploughed annually over 20 cm depth, which will usually lead to reduction of the concentration in the top centimetres of soil for substances that are not yet to a large extent degraded at the time of ploughing. This makes no difference for the types of concentration based on an ecotoxicological averaging depth (z_{eco}) of 20 cm as these types of concentrations are anyhow averaged over this 20-cm ploughing depth. However, the concentrations for $z_{eco} < 20$ cm (i.e. for z_{eco} of 1, 2.5, 5 or 10 cm) will be higher for no-tillage systems in case there is still a non-negligible fraction of the annual dose left at the time of ploughing. So, the exposure assessment for annual crops under conventional/reduced tillage is expected to underestimate concentrations of persistent substances for annual crops under no tillage for $z_{eco} < 20$ cm.

Despite this, no specific guidance is provided for no-tillage systems in annual crops for the following reasons. First, the GAP tables included in regulatory submissions do not yet include information whether the substance is applied in systems with conventional tillage, reduced tillage, or no tillage. Second, no-tillage farming practices are not abundant in EU. The surface area of no-tillage farming systems for annual crops ranges between 0% and 7% of the arable land in 15 MSs (EFSA PPR Panel, 2010d, Table 2; percentage is below 5% for 13 MSs and 7% for Finland and Greece).

Until guidance for no-tillage systems is developed, the only option is to use the guidance for tilled systems for annual crops using the currently used assessment depth of 5 cm (FOCUS, 1997).

3. Exposure assessment in soil for spray applications

This section provides practical guidance on how to perform exposure assessments in soil for active substances of PPPs and for the metabolites of these active substances (see Figure 4 for an overview of the tiered approach). This section is applicable to spray applications in crops covering the entire field. The guidance also applies to crops grown on ridges and non-uniform applications in annual crops (so row, band, strip, or spot application); however, additional guidance in Section 4 needs to be considered. Section 4 also gives additional guidance for other application types (seed treatments and granules). This section starts with the tiers using the simple analytical model (Tier-1 and Tier-2) and then describes the tiers based on the numerical models (Tier-3A and Tier-3B) and post-registration monitoring (Tier-4).

3.1. Required software tools

To be able to perform the assessments in this section, the following versions of the software tools should be available:

- The PERSAM software tool, which can be downloaded from the website of the European Soil Data Centre: http://esdac.jrc.ec.europa.eu/content/european-food-safety-authority-efsa-data-persam-software-tool. Applicants might want to use the analytical model outside the PERSAM software. Applicants should demonstrate that their own software reproduces the same output (identical output) as PERSAM, e.g. by comparison for the predefined scenarios (see Section 1.4).
- An appropriate version of the numerical models PEARL or PELMO. These models can be downloaded from the FOCUS website.

Please refer to the manuals of the respective software tools for instructions on how to install the software.

3.2. Tier-1: Predefined scenarios using the PERSAM tool

As described earlier, Tier-1 is based on a simple analytical model and on one scenario per regulatory zone North–Centre–South for each of the two types of PECs (i.e. the concentration in total soil and the concentration in the liquid phase). Tier-1 is a fast, simple and conservative procedure. The PERSAM tool provides an option by pressing a button to produce a Tier-1 report for submission to regulatory authorities. There is one set of predefined scenarios, which applies to both annual and permanent crops. The scenarios were selected based on the total area of annual and permanent crops (excluding permanent grassland). The scenarios at Tier-1 are not designed for substances whose properties depend on soil properties, such as pH or clay. For such substances, the applicant should therefore go to Tier-2 or Tier-3A directly.

The Tier-1 scenarios are based on the properties given in Tables 1 and 2. However, the top soil properties of the scenarios for permanent crops are different within the 0–30 cm layer (Table 3). Therefore, the Tier-1 scenarios for the permanent crops have top soil properties that depend on the ecotoxicological averaging depth, z_{eco}: for each z_{eco} value, the average properties over this z_{eco} depth are taken. In addition, the water flux q for the calculation of the leaching term depends on the ecotoxicological relevant averaging depth; see Appendix B for details.

EFSA (2014a) provides guidance for the calculation of the rapidly dissipating fraction at the soil surface (F_{field}) from field dissipation studies. This correction should, however, be applied to only those tiers where the numerical models (PEARL or PELMO) are used. The reason is that the fraction of the dose reaching the soil surface depends on the crop development stage. Such a dependency cannot be introduced into the analytical model.

Tier-1 is implemented in the PERSAM software tool. Practical guidance on how to input the substance properties and how to perform the calculations is given in the PERSAM manual (Decorte et al., 2016a,b; and updates). The PERSAM software can generate an output report in pdf format for use in regulatory submissions to competent authorities. The values given by the PERSAM software tool already include the model adjustment factor and the default scenario adjustment factor (Tables 5 and 8). The factors were added to ensure that Tier-1 delivers more conservative values than higher tiers.

At Tier-1, interception by the canopy is not considered and therefore the input for this analytical model is restricted to:

- the crop type (annual or permanent). In case of annual crops, the user has to specify if an assessment is conducted for a crop that is grown more than one time per year (i.e. carrot, cabbage and vegetable field beans);
- the application scheme, i.e. the number of applications per year, the rate of each application (expressed as mass applied per surface area treated) (kg/ha), the crop development stage (BBCH code) of each application and the time (in days) between the individual applications;
- the application cycle (years);
- the organic matter/water distribution coefficient (K_{om}) or the organic carbon/water distribution coefficient K_{oc} (dm^3/kg). Note that in PERSAM either of these two values can be input;
- the half-life for degradation (*DegT50*) in topsoil at 20°C and a moisture content corresponding to field capacity (days);
- the Arrhenius activation energy (kJ/mol);
- the molar mass of the molecule (g/mol);
- in the case of a transformation product: the molar fraction of formation (–) of the metabolite as formed from its precursor.

For pH- or clay-dependent substances, Tier-1 should not be used and the reader is advised to go directly to Tier-2.

3.2.1. Additional guidance for non-uniform applications in annual crops and permanent crops

In the case of non-uniform applications in annual crops (i.e. applications in crops grown on ridges, and row, band, strip or spot applications), the procedure above can be used to calculate concentrations in the soil averaged over the entire field. However, for such non-uniform applications the concentration in treated and non-treated areas may need to be assessed separately. In those cases, the procedure described in Section 4.2.1 must be followed. An important additional input parameter is the fraction of the field that is treated ($f_{treated}$). Given the large variety of possible crops, a default value for this parameter is not given with the exception of ridge/furrow properties for potatoes (refer to Section 4.2). However, the application must justify the choice of this parameter.

Also, in permanent row crops, both the exposure concentration in and between the crop rows may need to be assessed (Figure 3). In case of application below, the crop canopy guidance for spray applications in annual crops should be followed keeping in mind that the dose rate has to be related to the soil surface area treated. In the case of air blast applications, the dose will generally be targeted to the crop canopy, so the canopy will receive more than the dose averaged over the whole field and the area between the rows will receive less than this dose. How to deal with non-uniform distribution in permanent row crops is described in more detail in Section 4.3.

3.2.2. Guidance for substance-specific parameters

In general, the selection of substance-specific input values should follow recommendations given in FOCUS (2006) and in the generic guidance for Tier-1 FOCUS groundwater assessments (Anonymous, 2014 and subsequent amendments). This Guidance Document has further incorporated the following amendments (EFSA, 2008, 2014a; EFSA PPR Panel, 2012):

- Guidance on deriving the degradation half-life in topsoil at reference conditions is given by EFSA (2014a). This Guidance Document prescribes using the geometric mean from laboratory and/or field experiments following normalisation to reference conditions (20°C, pF 2).
- The default value for the molar activation energy is 65.4 kJ/mol (EFSA, 2008) and should be changed only when based on experimental evidence.
- The geomean K_{om} or K_{oc} of dossier values should be used as the geomean is the best estimator of the median value of a population (EFSA, 2014a).
- In the analytical model, the formation fraction is based on molar fractions and is usually derived from kinetic fitting procedures in line with FOCUS (2006). Formation fractions should be derived following the stepped approach in the section below.

3.2.3. Guidance for the 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 (i.e. Tier-1, Tier-2 and Tier-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 forms two molecules of methyl isothiocyanate, so 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. 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 and that they are retained in the regulatory context. The arithmetic mean should be calculated from all the available reliable formation fractions associated with the selected *DegT50* values and pertinent degradation pathway description. Refer to the EFSA *DegT50* guidance (EFSA, 2014a) for additional guidance on whether field data and laboratory data should be taken together or not. If the number of formation fractions is below the minimum of 3, laboratory and field formation fractions should be combined even if the *DegT50* are not combined (analogous to what is described in EFSA (2014a,b) when there are insufficient *DegT50* values). If the concentration of a soil metabolite remains below the limit of quantification (LOQ) at a number of sampling times in a soil metabolism or field study for a single soil, such that a reliable formation fraction is not available for this soil, it should be excluded from calculating the arithmetic mean (see also footnote[7]).

3.3. Tier-2: Spatially distributed modelling using PERSAM

Tier-2 provides the option of an exposure assessment with the simple analytical model for a particular crop and a particular substance. Tier-2 provides the option to introduce canopy processes for the selected crop as a refinement option to reduce the exposure of the substance to the soil. The PERSAM tool provides an option by pressing a button to produce a Tier-2 report for submission to regulatory authorities. Tier-2 is based on a spatially distributed version of the analytical model described in Tier–1. This implies that the exposure concentration is known for every $1 \times 1\text{-km}^2$ pixel, and therefore, the 95th spatial percentile can be directly obtained from the spatial frequency distribution of the exposure concentration. At Tier-2, the default scenario adjustment factors as listed in Table 5 are not applied; therefore, Tier-2 simulates less conservative values than Tier-1.

Tier-2 is implemented in the PERSAM software tool. Practical guidance on how to input the substance properties and how to perform the calculations is given in (Decorte et al., 2016a,b; and updates). The PERSAM software can generate an output report in pdf format for use in regulatory submissions to competent authorities. Note that the values given by the PERSAM software tool include the model adjustment factor (Table 8). This factor was added to account for differences between PERSAM and the numerical models (EFSA PPR Panel, 2012).

The PERSAM tool only provides the final outcome of the assessment in terms of the 95th percentile of the exposure concentration. Should the user wish to view the concentration distribution in the entire use-area, PERSAM has the option to export an ASCII GRID file. This file can be easily imported into most commonly used geographic information systems (GIS) programmes.

The user has to select a FOCUS crop for which the exposure assessment will be carried out. The crop selected is linked to the CAPRI or permanent crops as listed in Tables 6 and 7.

Tier-2 offers the possibility of incorporating the effect of crop interception in the PEC calculation. In Tier-2, the effects of crop interception and subsequent crop canopy processes are lumped into a single parameter, i.e. the fraction of the dose reaching the soil (f_{soil}, see Section 2.5 for details). This parameter is calculated by PERSAM for each individual application based on the crop interception and BBCH code specified by the user and the default wash-off fraction for that BBCH code given in Table 9 for annual crops and in Table 10 for permanent crops. Tables 9 and 10 are based on simulations with

[7] When a reliable formation fraction is not available for a soil, an upper limit of the formation fraction could in principle be estimated and this upper limit be included in the calculation of the average. However, this is currently not possible because there is no agreed guidance for estimating such an upper limit. Application of an upper limit would improve the calculation procedure, because there is *a priori* no reason to exclude low values. This can be illustrated by comparing the following two example cases: case A consists of three formation fractions of 2, 3, and 4% which gives an average of 3% and case B consists of three formation fractions of < 1%, 3% and 4% which gives an average of 2.7% based on the proposed procedure. Elimination of the < 1% value would have given 3.5% for case B, so a higher value than for case A, which seems difficult to defend.

PEARL and PELMO using a half-life for the decline of the dislodgeable residue of 10 days and a wash-off factor of 0.1 mm^{-1}. Should the applicant wish to refine these parameters, an assessment with the numerical models should be carried out at Tier-3A.

The other model inputs are the same as those in Tier-1 with the exception of substance properties that depend on soil properties such as pH or clay. PERSAM basically provides two options for the relationship between soil properties and substance properties:

- The K_{om} or K_{oc} depends on the pH of the soil. In this case, the sigmoidal function for sorption of weak acids, as described by Van der Linden et al. (2009), may be applied (see Section 3.3.1).
- The K_{om} or *DegT50* depends on soil pH or clay according to other mathematical rules. When this option is used, the applicant should provide statistical evidence that such a relationship exists.

3.3.1. pH-dependent sorption

For weak acids, the following equation may be used to calculate the coefficient for sorption on organic matter (Van der Linden et al., 2009):

$$K_{om} = \frac{K_{om,acid} + K_{om,anion} \frac{M_{anion}}{M_{acid}} 10^{pH-pKa-\Delta pH}}{1 + \frac{M_{anion}}{M_{acid}} 10^{pH-pKa-\Delta pH}} \tag{3}$$

where $K_{om,acid}$ (m^3/kg) is the coefficient for sorption on organic matter under acidic conditions, $K_{om,anion}$ (m^3/kg) is the coefficient for sorption on organic matter under basic conditions, M (kg/mol) is the molar mass, pKa is the negative logarithm of the acid dissociation constant and ΔpH is a constant accounting for surface acidity.

According to the Organisation for Economic Co-operation and Development (OECD) Guideline 106, at least four sorption experiments should be submitted, which have been selected from a wide range of soils (OECD, 2000). More specifically, for ionisable substances, the selected soils should be selected so that it is possible to evaluate the adsorption of the substance in its ionised and unionised forms. Values in normal agricultural soils range between 4 and 8, so it is recommended to select soils covering this pH range. It should then be possible to fit the parameters of the equation as described by Van der Linden et al. (2009).

Section 3.6 in Boesten et al. (2012) provides additional guidance on estimating sorption coefficients for weak acids with pH-dependent sorption. The most essential item in this guidance is that Equation 3 can be fitted to experimental sorption data using any software package capable of fitting non-linear functions to data. However, because of the existence of at least three different pH-measuring methods, the pH values in the sorption experiments must first be brought in line with the type of pH data in the PERSAM data set (i.e. pH_{H2O}). This is performed using the two equations below (Boesten et al., 2012):

$$pH_{H2O} = 0.982 pH_{CaCl2} + 0.648 \tag{4a}$$

$$pH_{H2O} = 0.860 pH_{KCl} + 1.482 \tag{4b}$$

where pH_{H2O} refers to the measurement of pH in water, pH_{CaCl2} is the pH measured in 0.01 M $CaCl_2$ and pH_{KCl} is the pH measured in 1 M KCl. Please note that these equations differ somewhat from the equations given in EC (2014). As the equations in EC (2014) were based on preliminary figures, Equation 4a and 4b should be used instead of the equations in EC (2014). The parameters of the sigmoidal function should be fitted using the corrected pH values. Because this function has four parameters, at least four pH–K_{om} values are required for an adequate fit (see also requirements above). Furthermore, it should be checked that the surface acidity is in a plausible range (i.e. ΔpH should be between 0.5 and 2.5). For further details, refer to Section 3.6 in Boesten et al. (2012).

3.3.2. Clay-dependent sorption

For substances with K_{om} depending on the clay content, a regression equation may be established based on sorption experiments and used at Tier-2 in PERSAM. Notice that in PERSAM clay content is roughly specified via the soil texture classes 'Coarse', 'Medium', 'Medium Fine', 'Fine' and 'Very Fine'. For each of these texture classes, clay contents are specified as follows (for details refer to Appendix B):

- 'Coarse': 5.2%;
- 'Medium' 19.0%;
- 'Medium Fine': 20.3%;
- 'Fine': 44.6%;
- 'Very Fine': 64.5%.

If experimental data do not allow covering the full range of clay content (5.2–64.5%) given in the PERSAM database, minimum and/or maximum K_{om} values should be specified on basis of the range in clay contents in the experiments, so avoiding excessive extrapolation.

3.4. Tier-3A: Crop- and substance-specific scenarios using the numerical models

Tier-3A offers the possibility of simulating exposure concentrations with numerical models for crop- and substance-specific scenarios focusing on only the type of concentration (pore water or total soil) that is required. Therefore, neither a model adjustment factor nor a scenario adjustment factor is needed in Tier-3A.

Scenario development at Tier-3A consists of two steps, i.e. (i) selection of the pixel coordinates of the pixel that corresponds to the 95th percentile for the crop and substance under consideration; and (ii) building the actual scenario. The first step is carried out in the PERSAM tool. The second step is automatically carried out in the shells of PEARL and PELMO. These model shells and documentation will be made available at the website of the respective models (see Section 3.1 for details and conditions). Guidance on performing these two steps is given in Sections 3.4.1 and 3.4.2; a full description of the applied procedure is given in Appendix B. Applicants and rapporteurs are advised to report simulations with at least two numerical models (e.g. PEARL and PELMO) and provide the highest PEC for regulatory submissions (this procedure is in line with EC (2014)).

To guarantee consistency in the tiered approach, substance-specific input values and application schedules that were used in Tier-2 should be used in Tier-3A (see Section 3.2). However, the numerical models require some more substance-specific input values. The selection of these additional substance-specific input values should follow recommendations given in FOCUS (2006) and in the generic guidance for Tier-1 FOCUS groundwater assessments (Anonymous, 2014). Section 3.4.3 gives some amendments to these guidance documents.

3.4.1. Selection of the Tier-3A scenarios

The scenarios are selected by running Tier-2 in the PERSAM tool. The PERSAM tool will return the geographical coordinates (X and Y) and soil and climate properties of the selected pixel but will not run the numerical models. PERSAM writes the location properties to a comma-separated value (csv) file (PERSAM transfer file). This file is read by the PEARL and PELMO shells, which then use this information to build automatically the complete scenario. Please refer to the PERSAM manual for practical guidance on scenario selection at Tier-2. As described in EFSA PPR Panel (2012), the selected pixel is dependent on the selected substance, the selected evaluation depth (1–20 cm) and the selected type of concentration (concentration in total soil or in pore water) and whether it is a parent or metabolite. For this reason, different Tier-3A scenarios are needed for each substance (parent and metabolites), for each evaluation depth and for each type of concentration. However, it is considered justified to base the scenario selection solely on the peak concentration, so it is not necessary to select different scenarios for each TWA window. In the case of permanent crops grown in rows, the scenario selection is based on the crop map for the in-row crop.

3.4.2. Building and running the Tier-3A scenarios

In the next step, the applicant generates and runs the Tier-3A scenarios with the shells of the numerical models (PEARL or PELMO). The following steps must be carried out by the user:

- Specify the transfer file generated by PERSAM to get the geographical coordinates and scenario properties of the Tier-3A scenario. This transfer file also contains the application and tillage schedule, and substance properties that are used by PERSAM (i.e. *DegT50*, K_{om}/K_{oc} and the Arrhenius activation energy).
- Specify the remaining substance properties.
- Reconsider the application schedule and type of application.
- Run the scenarios and generate reports.

All PERSAM transfer files stored in one file directory will be included in one project. This will allow the user to generate a summary report for the regulatory submissions with one push on the button. Please refer to the manual of the models for details.

3.4.3. Model inputs

To run the models, the following inputs are needed:

- the dominant FOCUS zone and FOCUS crop for which the simulations are carried out;
- the mean annual temperature and precipitation of the scenario;
- the topsoil organic-matter content;
- the application cycle (1 year, 2 years or 3 years);
- the application scheme of the PPP;
- properties of the active substance and its transformation products (when applicable).

Notice that the user only needs to input the information that is not in the transfer file provided by PERSAM; please refer to the manuals of the numerical models for details.

Application scheme

In general, the application scheme entered in the numerical models should reflect the application scheme used at Tier-2. However, application timing (according to GAP) may be different in different regulatory zones and MSs. PPPs can be applied to the crop canopy, sprayed onto the soil surface or incorporated into the soil. For each application, the applicant must introduce the application date, the rate of application (kg/ha) and the crop interception if applicable.

As mentioned in EFSA PPR Panel (2012), the exposure-assessment scheme has been developed for spray applications. It is proposed to apply the current exposure-assessment scheme also to granules and small treated seeds that are uniformly distributed over the surface area of the field, incorporated (homogeneously mixed over a certain soil depth) or placed at a certain soil depth (Section 4.4). When the latter two options are used, the applicant should use the options 'incorporation in the soil' or 'placed at a certain soil depth' and provide the appropriate soil depth. The exposure-assessment scheme also covers crops grown on ridges as well as row, band, and spot treatments; refer to Sections 4.1 and 4.3 for additional guidance on application schemes for such treatments.

In permanent crops, both the exposure in the rows and between the rows may need to be assessed (Figure 3). In the case of spray applications, the dose will generally be targeted to the crop canopy, so the canopy will receive more than the dose expressed in kg/ha of the whole field and the area between the rows will receive less than this dose. How to deal with this non-uniform distribution is described in Section 4.2. In general, applicants are advised to always specify the application rate in terms of surface area treated.

Canopy processes

When PPPs are applied to the crop canopy, the numerical models will simulate canopy processes. In these simulations crop interception should always be based on EFSA (2014a). The most important properties affecting canopy processes are the half-life for the decline of the dislodgeable residue on plants and the wash-off factor. These properties are generally not available in the dossier and therefore EFSA PPR Panel (2012) proposed to use as default values in the exposure assessment a wash-off factor of 0.1 mm^{-1} (100 m^{-1}) and a half-life for the dislodgeable foliar residue on plants of 10 days. It is considered acceptable to override these default values by experiments with the substance considered and plants under a range of relevant conditions. Refinements of the wash-off factor should be based on experiments with relevant formulated products and not with the active ingredient (EFSA PPR Panel, 2012, p. 59). General recommendations on how to perform such experiments can be found in Olesen and Jensen (2013, p. 48).

The rapidly dissipating fraction at the soil surface (F_{field})

EFSA (2014a) provides guidance for the calculation of the rapidly dissipating fraction at the soil surface (F_{field}) from field dissipation studies. This correction should apply only to the fraction of the dose that directly reaches the soil surface (see Figure 6) as it is unlikely that fast dissipation processes play an important role for the fraction that is washed off from the canopy. The application rate to the soil surface can be calculated using the following equation:

$$A_{soil} = (1 - f_i)(1 - F_{field})A + f_i f_w A \quad (5)$$

where f_i is the fraction of the dose intercepted by the canopy, F_{field} (–) is the rapidly dissipating fraction and f_w is the fraction of the intercepted dose washed off from the canopy. Detailed guidance on the use of F_{field} in the regulatory process is given in Appendix F. Equation 5 implies that F_{field} is related to a certain application (see Appendix F for details).

Note that such a correction is only defensible when used in combination with an appropriately derived geometric mean $DegT50_{matrix}$ as described in EFSA (2014a). So, the geomean $DegT50_{matrix}$ may be based on a mixture of $DegT50_{matrix}$ values obtained from laboratory studies, tailored $DegT50_{matrix}$ field studies, or legacy field studies. However, only experiments with surface application can be used to derive the rapidly dissipating fraction provided that a clear biphasic decline is observed (see Equation 3 in EFSA (2014a)).

The sorption coefficient under air-dry conditions

As mentioned in EFSA PPR Panel (2012), the all-time-high concentration in pore water in the top centimetre may occur when this top centimetre is very dry. This is, however, not realistic as the sorption of pesticide may increase by several orders of magnitude if the soil becomes very dry. In PEARL and PELMO, a simple approach to describe this effect has therefore been included (see Van and Leistra, 2004). Application of this approach needs one additional parameter, i.e. the sorption coefficient for air-dry soil (in PELMO, the ratio between the sorption coefficient at air-dry conditions and the sorption coefficient at reference conditions has to be specified). Petersen et al. (1995) and Hance (1977) found the sorption coefficient in air-dry soil to be roughly 100 times higher than the sorption coefficient measured under reference conditions. A maximum sorption coefficient that is 100 times the sorption coefficient measured under reference conditions is therefore implemented as a default in PEARL and PELMO. Please note that the sorption coefficient will not be affected when the soil is wetter than wilting point. Introduction of this additional parameter will therefore not affect leaching assessments.

3.4.4. Warming-up period

The Tier-3A scenarios are based on a time series of 20 years of daily meteorological information, such as rainfall and temperature. EC (2014) used a warming-up period of 6 years in the leaching simulations before starting the 20-year evaluation period. As described in EFSA PPR Panel (2012), for persistent substances a longer warming-up period is needed to ensure that the plateau value of the exposure concentration is closely approximated before the evaluation starts. The length of the warming-up period was re-evaluated using PEARL and PELMO. It was concluded that the warming-up period ranges between 6 and 54 years, depending on the K_{om} and *DegT50* of the substance (Table 11). For ease of implementation, it was decided to repeat the same time series of 6 years for this purpose (see Appendix B.2 for background information). The updated versions of PEARL and PELMO will automatically apply the appropriate warming-up period, based on the K_{om} and *DegT50* of the parent and transformation products so the user does not need to input the length of the warming-up period.

Table 11: Warming-up periods (years) needed to reach the plateau concentration as a function of *DegT50* (days) and K_{om} (L/kg). Please note that the half-life refers to the half-life at the average temperature of the scenario and not to the half-life at reference conditions

DegT50	$K_{om} < 100$	$100 \leq K_{om} < 500$	$K_{om} \geq 500$
$DegT50 < 100$	6	6	6
$100 \leq DegT50 < 200$	12	12	12
$200 \leq DegT50 < 500$	12	24	30
$500 \leq DegT50 < 1{,}000$	18	30	30
$DegT50 \geq 1{,}000$	24	30	54

3.5. Tier-3B: Spatially distributed modelling with the numerical models

A further tier may be considered (Tier-3B) that would consist of spatially distributed modelling with numerical models. This tier should, however, only be used when agreed tools and guidance is made available, which is currently not the case. 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) of either the parent substance or any soil metabolite can be derived by statistical analysis of the output of the model runs, so avoiding the need for simplifications in the scenario selection procedure.

Using the procedure described below, it is, in principle, possible to parameterise each 1×1 km^2 grid cell in the whole EU. In view of computation time, it is, however, not desirable to perform calculations with a numerical model for each individual grid cell of the whole EU. It is therefore necessary to reduce the number of grid cells for which calculations are performed by clustering them into groups of similar pedoclimatic properties. This process is called 'schematisation'. Therefore, simulation with spatially distributed models consists of the following three steps:

- creating a spatial schematisation;
- assigning scenarios to each individual cluster;
- calculating the 95th spatial percentile of the concentration distribution.

These three steps are briefly described in the sections below.

3.5.1. Setting up the spatial schematisation

A spatial schematisation may be obtained by overlaying maps with spatially distributed parameters. The maps available in EFSA spatial data set version 1.1 (Hiederer, 2012) should be used for this purpose. Before creating the overlay, grid cells with significant land uses other than annual or permanent crops should be removed. It is advised to include the following maps in the spatial overlay:

- the map with EU regulatory zones;
- the map with FOCUS zones;
- the soil textural map of Europe;
- the map of topsoil organic matter;
- the map of topsoil pH;
- the map of mean annual temperature;
- the map of mean annual precipitation.

Because the last four maps are continuous maps, the spatial overlay would result in a very large number of combinations. For this reason, these maps must be classified so that each category covers an equal area. Some 10 categories for each of these maps will generally be sufficient because this will result in a spatial schematisation consisting of some 10,000 unique combinations. Notice that despite the fact that only 10 classes of temperature, organic matter and precipitation are proposed each scenario will have a unique value of these parameters because they are refined in the parameterisation procedure below. So the number of 10 is only used to reduce the number of unique combinations.

3.5.2. Parameterisation of the unique combinations

Once the schematisation is obtained, a scenario must be assigned to each individual unique combination. As a first step, average values of topsoil organic matter, pH, precipitation and temperature should be derived for each unique combination. This may be carried out by applying the so-called zonal mean function in a GIS package. Once the mean values of topsoil organic matter, temperature, precipitation, and pH are known, the Tier-3A procedure for building the scenario can be applied to each individual unique combination (refer to Appendix B for details). However, in contrast with Tier-3A, it is advised to always use the weather conditions and crop conditions at the scenario location.

3.5.3. Calculation of the 95th spatial percentile of the concentration distribution

The 95th spatial percentile of the PEC within each regulatory zone should be based on a cumulative frequency distribution of the PEC in the area of one of the PERSAM crops. When constructing the cumulative frequency distributions, the crop area in each unique combination must be used as a weighting factor. Maps of the crop area are available in the EFSA spatial data set (see Hiederer (2012) for file names).

3.6. Tier-4: Post-registration monitoring

The PPR Panel proposes to include post-registration monitoring as Tier-4 (EFSA PPR Panel, 2012). As described in Section 2.1, 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 4, 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 PPP is applied.

For Tier-4, this implies that this percentile has to be assessed via one of the following procedures:

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

It is to be expected that hundreds of samples will be needed to assess the 90th percentile with sufficient accuracy based on measurements alone. The alternative would be to use one of the models 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 from the population above the 95th spatial percentile. To demonstrate that this condition is met, the notifier must report for each monitoring site the substance properties, soil properties, climatic conditions, application procedures, and crop management practices. Monitoring sites that do not meet these conditions should be excluded from the analysis. As described in EFSA PPR Panel (2012), 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 based on modelling (so for these substances the approach based on random sampling has to be followed).

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. As the PECs at individual monitoring sites are expected to vary because of variation in K_{om} and *DegT50* (normalised by temperature), 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 PPPs 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, for example, 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 of EFSA, 2012). It is recommended that the applicant contacts the competent authority for agreement on the vulnerable sites for post-registration monitoring.

The proposed methodology in this guidance may also be relevant for identifying locations for dedicated terrestrial field dissipation studies.

Post-registration monitoring is not suitable to assess the annual peak concentration because it is not feasible to sample always immediately after application. Instead, this monitoring can give information on the background concentration. So, it is recommended to sample a few weeks before the first application.

4. Additional guidance for non-spray applications and for non-uniform applications

As described in Section 1.3, it is assumed that for applications of granular products and small treated seeds (to the soil surface or incorporated), the procedure in Section 3 can be used as well. With small modifications, the procedure also covers reasonably well non-uniform applications (crops grown on ridges as well as row, band, strip, and spot treatments). This chapter provides calculation procedures for row, band, strip, and spot treatments in annual crops (Section 4.1), for treatments in crops grown on ridges (Section 4.2), for row treatments in permanent crops (Section 4.3) and for small seeds and granules incorporated in the soil or placed at a certain soil depth (Section 4.4). These calculation procedures should be used in addition to the guidance in Chapter 3.

4.1. Additional guidance for non-uniform applications (row, band, strip and spot applications) in annual crops

When using guidance for non-uniform applications (row, band, strip and spot applications) this use must be specified with sufficient detail in the GAP table to be submitted with the application to the competent authority.

For row, band, strip and spot applications, the part of the field to consider in risk assessment depends on the mobility of species groups for which the risk assessment has to be carried out. Further guidance on the appropriate spatial scale will be given in the guidance on in-soil risk assessment. There are at least three options for the spatial scale: (i) the concentrations in the soil averaged over the whole soil surface; (ii) the concentrations in the soil below the fraction of the soil surface that is treated (so e.g. below the treated rows) and (iii) the concentrations in the soil below the untreated part of the soil surface (e.g. between the treated rows).

The exposure assessment in Chapter 3 will provide appropriate concentrations for option (i) if the dosage used in the exposure assessment is defined as mass of active ingredient applied per surface area of the whole field. If the dosage is defined as the mass of active ingredient per surface area treated, the methodology will also give conservative estimates for options (ii) and (iii). The latter is, however, a very conservative assumption because it implicitly implies that the crop rows or the treated areas are always at the same position. For this reason, a more realistic exposure-assessment procedure has been included in PERSAM and the numerical models. This procedure assumes that the location of the treated rows or the treated areas changes from year to year by calculating the background concentration using an application rate that is defined in kg/ha of the entire field. As these calculations are done internally in the models, the only parameter that the user needs to specify additionally is the fraction of the area treated ($f_{treated}$). The calculation procedure is described in more detail for the analytical model in PERSAM (Appendix A) and in the numerical models (Appendix E).

Note that the fraction of the soil surface treated is not necessarily the same as the fraction of cropped rows (Figure 7) because pesticides may be applied to either the crop rows or the intercrop rows, depending on the type of treatment. Selection of $f_{treated}$ should be justified and supported by a thorough description of the method and rate of application.

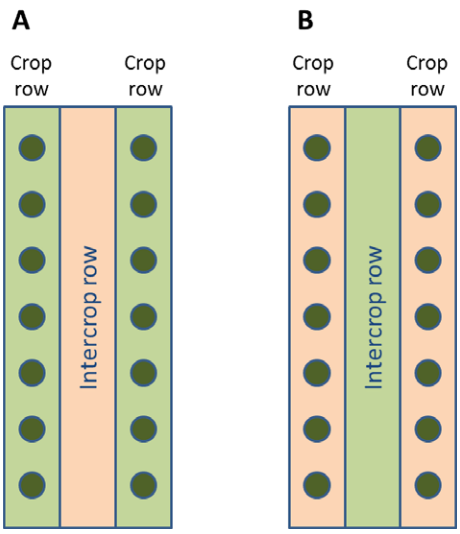

Figure 7: Graph showing the fraction of the soil surface treated (indicated in orange) and the fraction of the soil that is not treated (green). There are two possible situations. (A) The pesticide is applied to the intercrop row (usually herbicide treatments) so $f_{treated}$ equals the relative area of intercrop rows. (B) The pesticide is applied to the crop row (usually fungicide or insecticide treatments) so $f_{treated}$ equals the area of crop rows

This methodology does not only apply to row treatments but is considered appropriate for each kind of non-uniform application to level soil in annual crops covering band, strip as well as spot applications.

4.1.1. Crop interception

Crop interception should not be included in calculations for row, band, strip, and spot applications unless the spray is targeted on just the crop canopy or the crop canopy has closed between the rows.

Full overspray of a field with significant areas not covered by the crop (e.g. before the crop cover is closed) is not addressed by the above stated methodology. In this case, it is recommended that a full dose application to bare soil is used (following Section 3) as a conservative assessment. If the area between the crops is covered by grass, the application should account for either the crop or the grass cover, whichever is the worst case with respect to the soil load (f_{soil}).

4.2. Additional guidance for spray applications in crops grown on ridges

For spray applications onto the whole field after ridge–furrow formation, the recommendation is to use the exposure-assessment methodology developed for spray applications to level surfaces (Section 3). This is justifiable because the initial concentrations in the top layer are expected to be the same for both tillage systems and because the long-term accumulation is expected to be the same.

For spray application onto only the ridge or only the furrow, the guidance in Section 4.1 should be used additionally. For furrow applications, it should be assumed that there is no interception by the crop. The exposure assessment of row applications in Section 4.1 defines $f_{treated}$ as the fraction of the surface area of the field that was treated. So, for ridge applications $f_{treated} = f_{ridge}$ and for furrow applications $f_{treated} = f_{furrow}$ where f_{ridge} (–) is the fraction of the surface area occupied by ridges and f_{furrow} (–) is the fraction of the surface area occupied by furrows.

The 50th percentiles for potatoes of f_{ridge} for the three regulatory zones, determined by Beulke et al. (2015), as given in Table 12 should be used. The same applies to f_{furrow}. Use of the 50th percentiles is considered acceptable because the scenario selection procedure generates spatial 95th percentile cases for potatoes and there are no reasons to assume that the expected value of f_{ridge} or f_{furrow} differs from the 50th percentiles for these spatial 95th percentile cases. For other crops grown on ridges, the recommendation is to use the same f_{ridge} values in the absence of better information.

Use of 2D/3D modelling for refinement of exposure in ridges should only be used if the approach and methodology is agreed with the competent authority.

Table 12: Values of f_{furrow} and f_{ridge} to be used for spray applications onto only the ridge or only the furrow

Regulatory zone	f_{ridge} (–)	f_{furrow} (–)
North	0.55	0.45
Centre	0.72	0.28
South	0.62	0.38

4.2.1. Crop interception

Crop interception should not be included in calculations for ridge–furrow systems unless the spray is targeted on just the crop canopy or the crop canopy has closed between the rows.

4.3. Additional guidance for applications in permanent crops grown in rows

Air blast application in permanent crops usually leads to non-uniform distribution of pesticides depending on the application technique used. Non-uniform pesticide distribution in permanent crops should not be ignored because this may lead to underestimation of pesticide loads to areas directly under the crop canopy as well as neglecting exposure to off-target deposition loads in areas between the rows. Consequently, it may be necessary to perform two separate soil exposure assessments in case of air blast spraying in permanent crops: one for the in-row and one for the between-row situation, the latter typically with bare soil or grass cover (Section 1.3.2). As pesticide application is usually targeted to the crop canopy, soil areas covering the crop rows typically receive higher amounts of pesticides than the application rate averaged over the whole field, whereas areas between the crop rows will typically receive less.

The relationship between the application rate averaged over the whole field and the actually received application rate for the in-row or between-row exposure may be expressed by a simple dose rate assessment factor, f_{dose}:

$$f_{dose} = \frac{A_{actual}}{A_{averaged}} \tag{6}$$

where A_{actual} (kg/ha) is the actually received application rate per surface area and $A_{averaged}$ (kg/ha) is the averaged application rate over the whole field. In the case of a uniform pesticide distribution, $f_{dose,in\text{-}row}$ equals $f_{dose,between\text{-}row}$. However, in practice $f_{dose,in\text{-}row}$ will typically be greater than one and $f_{dose,between\text{-}row}$ less than one. In the extreme case of no deposition in areas between the treated crop rows (e.g. using tunnel spray techniques), $f_{dose,in\text{-}row}$ equals $f_{treated}$ as defined in Section 4.1. Considering that there are no losses to areas outside the whole field, $f_{dose,in\text{-}row}$ and $f_{dose,between\text{-}row}$ are linked to each other depending on the row distance and the crop canopy width:

$$f_{dose,in\text{-}row} = 1 + \frac{(1 - f_{dose,between\text{-}row})(d_{row} - d_{crop})}{d_{crop}} \tag{7}$$

where d_{row} (m) is the distance between the rows and d_{crop} (m) is the width of the crop canopy (Figure 8). If the application rate is expressed in terms of the whole field, in principle the application rate should be multiplied by the corresponding dose rate assessment factors.

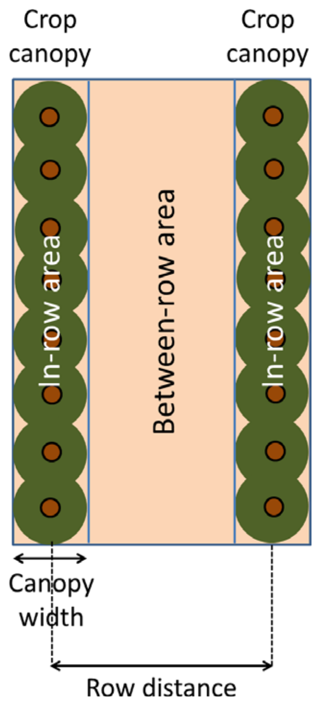

Figure 8: Graph showing the two soil exposure areas, i.e. the in-row and between-row area, in permanent crops depending on the row distance (d_{row}) and the canopy width (d_{crop})

At present, there is no common agreement how to account for non-uniform distribution of spray deposition within the field. Therefore, the working group recommends further data collection to adequately address non-uniform distribution of pesticides in permanent crops. However, until more tailored data become available, the recommendation is to apply a default dose rate assessment factor of 2.9, which can be derived on the basis of a standard row distance of 3.5 m and a crop canopy width of 1.2 m (EPPO, 2012) assuming no drift (so the entire dosage is targeted to the crop canopy). Note that assuming no drift can be considered a worst case for in-row exposure-assessment assessments. The dose rate assessment factor equals $1/f_{treated}$ for such cases. This default dose rate assessment factor is not necessary if the dose rate is already related to the soil surface area treated. If applicants or competent authorities wish to assess the soil exposure between the rows due to drift from airblast application in the row crop, it is recommended to simply assume uniform overspraying of in-row and between-row areas (so $f_{dose,in\text{-}row}$ equals $f_{dose,between\text{-}row}$). Notice that the default dose rate assessment factor of 2.9 should only be refined if justified (e.g. in case of different row dimensions or canopy widths). In general, the applicant is encouraged to define always the application rate related to the surface area treated (i.e. related to the soil surface area directly under the crop canopy).

4.4. Additional guidance for granules and treated small seeds

4.4.1. Applications to crops on level surfaces followed by soil incorporation

The approach in Section 3 can be used for granules and treated small seeds (< 0.5 cm)[8] incorporated into the soil when the agricultural practice aims to result in even horizontal spatial distribution across the field. It does not cover annual crops where treated seed is drilled in widely spaced rows or when granules are placed within or between crop rows, as this will result in locations having higher concentrations within the crop row in the year of drilling or treatment. An example of a crop with small seeds that can have this pattern of drilling in widely spaced rows is *Brassica* vegetables.

The definition of the ecotoxicologically relevant type of concentrations in this guidance is based on the concept that concentrations are averaged over the evaluation depth, z_{eco} (ranging from 1 to 20 cm). The consequence is that the procedure for calculations for homogeneously incorporated granules and treated small seeds in PERSAM is identical to that for spray applications unless the incorporation depth is deeper than z_{eco}. If the incorporation depth is deeper than z_{eco} then in PERSAM z_{eco} is replaced by the incorporation depth. If the incorporation depth is greater than 20 cm the increased concentration resulting from the last application has to be based on averaging over the incorporation depth and not on averaging over the evaluation depth (Appendix A.4.1). Both the numerical models and PERSAM will account for this.

4.4.2. Placing at a certain soil depth

In case of granules and treated small seeds placed at a certain soil depth (z_{inc}), the ecotoxicological mixing depth is considered to start at $z_{inc,}$ because at this depth the maximum concentration occurs. In the numerical models, this is realised by setting the top and the bottom of the evaluation depth to z_{inc} and $z_{inc} + z_{eco}$, respectively. In the analytical model, moving of the ecotoxicological averaging depth is not possible, so only the reference soil depth for the water flux (*fq*) is set to $z_{inc} + z_{eco}$. Notice that in the numerical models z_{inc} always has to start slightly below the top of the evaluation depth to cover adequately the peak concentration occurring after placing at that soil depth. Therefore, z_{inc} should always be increased by 0.5 cm in the numerical models.

4.4.3. Granule applications in crops grown on ridges

Appendix A.4.2 describes a first-tier exposure-assessment procedure for the following application method and subsequent tillage operation: (i) the granules are applied to a level soil surface at a dosage of *A* kg/ha; (ii) they are incorporated to a depth z_{inc}; and (iii) thereafter the top layer with a thickness z_{rf} (ridge furrow) of this level soil system is transformed into a ridge-furrow system. It is assumed that the incorporation depth z_{inc} is larger than z_{rf}. This is commonly the case because this application method is usually used for nematicides in potatoes and protection of the potato roots against the nematodes is expected to be insufficient when z_{inc} is smaller than z_{rf}.

Developing a sophisticated higher-tier approach for these granule applications would be rather complicated in view of the two-dimensional structure of the tillage system. However, as a pragmatic solution, it is proposed that also a Tier-3A scenario is used assuming incorporation to the depth z_{inc} in the numerical models.

5. Documentation to be provided

This section briefly summarises the documentation requirements. The assumption is that the notifier uses one of the standardised tools as described in this Guidance Document (i.e. PERSAM for

[8] Definition of small seeds is taken from draft SANCO guidance on seed treatments (SANCO/10553/2012). For this EFSA guidance it is proposed to handle maize seeds and pelleted seeds as small seeds.

lower tier assessments and PEARL or PELMO for higher-tier assessments). If this is not the case, the notifier should demonstrate that the scenarios used in the tiered approach are adequately parameterised and that the alternative models provide results comparable with existing software tools (see also EFSA PPR Panel (2014) for guidelines on model development and model documentation).

As long as new ecotox effects guidance of PPPs for soil organisms is not available, only results for the concentration in the total soil based on an ecotoxicological averaging depth of 5 cm need to be provided (FOCUS, 1997). In case of soil incorporation (homogeneously distributed over a certain soil depth or placed at a certain soil depth), recommendations in this Guidance Document should be followed. TWA values are to be reported only when used in the risk assessment. Pore water concentrations are currently not used in the soil risk assessment and are currently not to be provided. However, this may change when new ecotox effects guidance of plant production products for soil organisms has been agreed by competent authorities for regulatory use. Pore water concentrations in upper soil layers may need to be reported when used as a surrogate for puddle concentrations for the risk assessment of, e.g. birds and mammals.

The substance properties and the application regime according to the GAP table (i.e. application rate, type of application including placement depth when appropriate, frequency of application and crop interception according BBCH code) determine largely the outcome of a regulatory assessment and should therefore be well documented. Whenever possible, harmonised approaches, as described in this guidance, should be used. Justifications should be provided for using approaches, assumptions, or inputs other than those recommended in this guidance.

As described in Section 2, the selected crop has a large effect on the outcome of the regulatory assessment. A justification for the selected crop should therefore be provided with specific attention to how the crop links to the area of the intended use of the PPP. If the notifier imports his own crop map, its suitability and reliability should be demonstrated.

As described in EFSA PPR Panel (2014), sufficient information should be provided so that the calculations can be reproduced. In practice, this means that the following information must be provided to the regulator:

- The versions of the models that have been used in the regulatory assessment. If non-standard software tools have been used, a description of these models, including a justification of their applicability, should be provided (see first paragraph of this section).
- All relevant input values and results generated by PERSAM (Tier-1 or Tier-2) or the numerical models (Tier-3A).
- For PERSAM, the short report option should be selected for regulatory submissions. If calculations are done outside the model, a document describing all manual calculations done outside the model shells should be provided.

Tier-1 and Tier-2 are simple to perform. However, the applicant may move directly to higher tiers without performing assessments for lower tiers. Only results from one modelling tier, e.g. either Tier-1, Tier-2 or Tiers-3 need to be reported.

If a numerical model is to be used at Tier 3-A, applicants and rapporteurs are advised to report simulations with at least two numerical models (e.g. PEARL and PELMO) and provide results from both models using the highest PEC from either model for the regulatory risk assessments (this procedure is in line with EC (2014)).

Conclusions or recommendations

Recommendations

- For regulatory purposes, applicants must use commonly agreed versions of the software tools and data sets. It is therefore recommended that a procedure for version control and updating the software tools and data sets be developed, including PERSAM, PEARL, PELMO and the EFSA spatial data set.
- The currently used map of organic matter in soil underestimates soil organic matter in arable soils. It is therefore recommended that separate organic matter maps are developed for annual crops, permanent crops, and grassland. The Land Use/Cover Area frame statistical Survey (LUCAS) data set could be a starting point for developing such maps.
- Land use is currently based on the CAPRI data set. This data set refers to the situation in 2010 and has not been updated since then. Furthermore, the data set does not apply to all land

uses covered by this Guidance Document. It is therefore recommended to provide an update of this data set on a regular basis.

- In view of harmonised exposure assessments, the recommendation is to also align the FOCUS groundwater scenario definitions and model implementation with respect to crop canopy processes and to take into account wash-off from the crop canopy for the groundwater exposure assessment as well.

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Glossary and Abbreviations

analytical model	Analytical models are mathematical models that have a closed form solution, i.e. the solution to the equations used to describe changes in a system can be expressed as a mathematical analytic function
application rate	See dose
BBCH code	Biologische Bundesanstalt, Bundesortenamt und Chemische Industrie code: decimal code ranging from 0 to 99 to characterise the crop development stage (Meier, 2001)
CAPRI	Common Agricultural Policy Regionalised Impact modelling system. An economic model developed to support EU policy
CFU	colony forming unit, relates to microbial active substances
CTC	Scenario for the total concentration in the Centre Zone
CTN	Scenario for the total concentration in the North Zone
CTS	Scenario for the total concentration in the South Zone
CLC	Scenario for the concentration in pore water for the Centre Zone
CLN	Scenario for the concentration in pore water for the North Zone
CLS	Scenario for the concentration in pore water for the South Zone

DOSE	The mass of substance applied per unit surface area treated (kg/ha). Substances may be applied uniformly or be applied in rows
ERC	Ecotoxicological Relevant Concentration
f_{dose}	Dose rate adjustment factor for the in-row and between-row exposure assessment to account for non-uniform spray drift in permanent crops
F_{field}	Rapidly dissipating fraction that is not related to degradation in the soil matrix (EFSA PPR Panel, 2010c)
f_{ridge}	Fraction of the surface area of the field that is occupied by the ridge (–)
f_{furrow}	Fraction of the surface area of the field that is occupied by the furrow (–)
FOCUS	Forum for Co-ordination of Pesticide Fate Models and their Use
f_{soil}	Fraction of the dose that reaches the soil
f_{ref}	Refinement factor describing the ratio of the concentrations of the non-uniform and uniform applications
$f_{treated}$	Fraction of the surface area of the field that is treated (–). This fraction may refer to the intercrop row or the crop row, depending on where the pesticide is applied, as well as to treated and non-treated areas in case of strip, band, and spot applications
f_w	Fraction of the intercepted dose washed off from the crop canopy (–)
GAP	Good Agricultural Practice
GIS	geographic information systems
Incorporation	Homogenous distribution of granules or treated small seeds within a certain soil layer; also applies to incorporation via cultivation activity following spray application or broadcasting granules or treated small seeds at the soil surface
JRC	Joint Research Centre
LOQ	limit of quantification
model adjustment factor (f_M)	A factor that accounts for differences between the simple analytical model used at lower tiers and the more realistic numerical models used at higher tiers. The model adjustment factor should ensure that lower tiers are more conservative than higher tiers
numerical model	Numerical models are mathematical models that use a numerical time-stepping procedure to obtain the models behaviour over time
OECD	Organisation for Economic Co-operation and Development
PEARL	Pesticide Emission At Regional and Local Scales. A pesticide fate model intended for higher-tier exposure and leaching assessments
PEC	Predicted Environmental Concentration
PELMO	Pesticide Leaching Model. A pesticide fate model intended for higher-tier exposure and leaching assessments
PERSAM	Persistence in Soil Analytical Model. Software tool for performing lower tier soil exposure assessments
placing at a certain soil depth	Placing of granules or small treated seeds at a certain soil depth without soil mixing; implies moving the evaluation layer in the numerical models below the placing depth (z_{inc})
PPP	Plant Protection Product
PPR	Plant Protection Products and their Residues
RAC	Regulatory Acceptable Concentration
scenario adjustment factor (f_S)	A factor that accounts for the effect of using in lower tiers the total area of annual crops instead of the area of intended use. The scenario adjustment factor should ensure that lower tiers are more conservative than higher tiers
SCoPAFF	Standing Committee of Plant Animal Food and Feed
TWA	time-weighted average

Appendix A – Description of the persistence in soil analytical model

Tier-1 and Tier-2 are based on a simple analytical model (Section 2) that is parameterised for the three zones (North/Centre/South). This model is also used to select the Tier-3A scenarios for the numerical models. Therefore, this analytical model plays a key role in the exposure-assessment procedure. This appendix gives a description of the model (first in terms of a conceptual model and thereafter mathematically). It starts with the model for spray applications in the whole field. Sections A.2 and A.3 describe the model for non-uniform spray applications in row crops and ridge-furrow systems and Section A.4 gives the model for granular applications.

A.1. Spray applications in crops covering the whole field

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

- The substance is applied to the soil surface as a single dose on the same date every year or every 2 or 3 years. This single dose may consist of multiple applications within a year. Between these applications, first-order degradation is assumed.
- At Tier-2, this dose may be corrected to account for crop interception and crop canopy processes based on other models or data.
- The only loss processes from the soil are degradation and leaching. The degradation rate is a function of only soil temperature and leaching is assumed to result from convective flow only.
- Soil properties such as moisture content and temperature are constant in time.
- The soil organic-matter content is averaged over the ecotoxicological mixing layer.
- The model does not consider the time course of concentrations; instead the maximum of the exposure concentration after infinite time is considered.
- The effect of tillage or mechanical cultivation is accounted for by assuming complete mixing over the tillage depth at the moment of tillage. Tillage depth is assumed to be 20 cm for annual crops (EFSA, 2010a) and 5 cm for permanent crops (when applicable).
- Adsorption is described by a linear isotherm using the concept of a sorption coefficient that is proportional to organic-matter content (K_{om}).
- The average exposure concentration over a certain depth is calculated from the sum of the maximum concentration after infinite time and the concentration resulting from a last application.
- A flexible approach is taken for introducing relationships between *DegT50* or K_{om} and soil properties when used for Tier-2.
- Concentrations of metabolites are based on the assumption that each metabolite is applied at the application time of the parent at a dose that is corrected for the kinetic formation fraction and the molar mass of the metabolite.

A.1.1. Parent substances

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

$$C_{T,ini} = \frac{A_{year}}{\rho z_{eco}} \tag{A1}$$

where $C_{T,ini}$ (mg/kg) is the initial concentration in total soil, A_{year} is the annual application rate (kg/ha^{-1} or mg/dm^2), z_{eco} (dm) is the ecotoxicological averaging depth (i.e. 1–20 cm), and ρ is the dry soil bulk density (kg/dm^3). In the second step, the background concentration ($C_{T,plateau}$ mg/kg), just before the next application after an infinite number of annual applications, is calculated:

$$C_{T,plateau} = \frac{z_{eco}}{z_{til}} C_{T,ini} \frac{X}{1-X} \tag{A2}$$

where z_{til} (dm) is the plough depth (fixed at 20 cm or 5 cm for permanent crops when applicable based on EFSA, 2010a) and X is defined as:

$$X = \exp(-t_{cycle}(f_T k_{ref} + k_{leach})) \tag{A3}$$

where t_{cycle} is the time between applications (365, 730 or 1,095 days), f_T is a factor describing the effect of soil temperature on the degradation rate coefficient, 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, and k_{leach} (d^{-1}) is a rate constant accounting for leaching. Although the soil temperature is constant in time, the factor f_T is needed because dossiers are based on degradation rate normalised to 20°C and f_T converts this rate to the rate at the scenario temperature. As follows from the combination of Equations A1 and A2, the background concentration does not depend on the ecotoxicologically relevant averaging depth but depends only on the ploughing depth.

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

$$T > 0^oC \quad f_T = \exp\left(\frac{-E}{R}\left[\frac{1}{T + 273.15} - \frac{1}{T_{ref} + 273.15}\right]\right) \tag{A4a}$$

$$T \leq 0^oC \quad f_T = 0 \tag{A4b}$$

where E is the Arrhenius activation energy (kJ/mol), R is the gas constant (0.008314 kJ/mol K), T (°C) is the soil temperature and T_{ref} (°C) is the temperature at reference conditions (20°C). The coefficient k_{ref} is calculated from the degradation half-life by:

$$k_{ref} = \frac{\ln(2)}{DegT_{50}} \tag{A5}$$

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:

$$C_{T,peak} = C_{T,ini} + C_{T,plateau} \tag{A6}$$

where $C_{T,peak}$ (mg/kg) 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:

$$C_{L,peak} = \frac{C_{T,peak}}{\theta/\rho + f_{om}K_{om}} \tag{A7}$$

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

The model also includes the calculation of *TWA* concentrations. 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:

$$C_{T,TWA} = \frac{C_{T,peak}}{t_{avg} f_T k_{ref}}\left[1 - \exp(-f_T k_{ref} t_{avg})\right] \tag{A8}$$

The TWA concentration in the liquid phase, $C_{L,TWA}$, is calculated from an equation akin to Equation A8 but with the $C_{L,peak}$ instead of the $C_{T,peak}$.

Leaching from the ecotoxicological mixing layer

The rate coefficient k_{leach}, which accounts for leaching from the ecotoxicological averaging layer, is calculated assuming only convective flow and perfect mixing. So, the substance flux J (mg/dm^2 d) at the bottom of the evaluation layer is described by:

$$J = qC_L \tag{A9}$$

where q (dm/d) is the mean annual downward water flow rate at the bottom of the layer. The conservation equation for the evaluation layer can then be written as:

$$S\, z_{\text{eco}} \frac{dC^*}{dt} = S\, z_{\text{eco}} \left(-k_{\text{ref}} f_T C^*\right) - S\, J \tag{A10}$$

where S (dm^2) is the surface area considered and C^* is the mass of substance divided by the volume of soil (mg/dm^3). Assuming linear sorption, we get:

$$C^* = C_L(\theta + \rho\, f_{\text{om}}\, K_{\text{om}}) \tag{A11}$$

Combination of the above equations and rearranging gives:

$$\frac{dC^*}{dt} = -C^*(k_{\text{ref}} f_T + k_{\text{leach}}) \tag{A12}$$

where k_{leach} (d^{-1}) is

$$k_{\text{leach}} = \frac{q}{z_{\text{eco}}(\theta + \rho f_{\text{om}} K_{\text{om}})} \tag{A13}$$

The analytical model is based on X, i.e. the remaining fraction at the moment of the next application, so equal to the C_T at this moment divided by the initial C_T. This is given by Equation A3. Note that k_{leach} is accounted for neither in the calculation of TWA concentrations nor in the case of multiple applications. The reason is that it cannot be assumed that the mean annual leaching rate also applies to short periods of time between, e.g. multiple applications in spring and summer.

Multiple applications in a year

In the original description of the simple analytical model (EFSA PPR Panel, 2012), all applications within a year were summed to a single application. Because this assumption is very conservative, the model has been extended so that degradation between individual applications can be considered. So the annual application rate A_{year} in Equation A1 is calculated as follows:

$$A_{\text{year}} = \sum_{i=1}^{n} \left(f_{\text{soil,i}} A_i \exp\left(-f_T k_{\text{ref}} \left[t_{\text{app,n}} - t_{\text{app,i}}\right]\right)\right) \tag{A14}$$

where A_i (kg/ha) is the application rate of application i, n is the number of applications in a year, $f_{\text{soil,i}}$ is the fraction of the dose reaching the soil for application i (to be taken from Tables 9 and 10; see Equation 1 for definitions) and $t_{\text{app,i}}$ is the Julian day number of application i.

There is the complication that A_{year} as calculated for the total number of applications may be lower than when calculated for a smaller number of applications (e.g. because there is a large time interval between the last two applications or because the last application rate is lower than earlier rates). Therefore, A_{year} has to be calculated n times: the first A_{year} calculation assumes that the first application is the last application, the second A_{year} calculation assumes that the second application is the last application and so on. At the end, the maximum of all A_{year} values has to be taken.

A.1.2. Metabolites

For soil metabolites, the calculation procedures are the same recursive procedure as described above for the active compound with one exception: the annual application rate A_{year} 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). Considering multiple applications, for a soil metabolite formed from the parent, this equivalent rate is given by:

$$A_{\text{year}} = \sum\nolimits_{i=1}^{n} \left(f_{\text{soil,i}} A_i \exp(-f_T k_{\text{ref}} [t_{\text{app,n}} - t_{\text{app,i}}]) \frac{M_{\text{met}}}{M_{\text{parent}}} \sum_{j=1}^{m} (F_{\text{f,p,j}}\, F_{\text{f,s,j}}) \right) \tag{A15}$$

where $F_{\text{f,p,j}}$ and $F_{\text{f,s,j}}$ (–) are formation fractions (i.e. the stoichiometric coefficient of the formation of this metabolite from its precursor, kinetically determined). $F_{\text{f,p,j}}$ is the formation fraction for the primary metabolite j, which is formed directly by the parent, whereas $F_{\text{f,s,j}}$ is the formation fraction for the secondary metabolite, which is formed by primary metabolite j. m is the number of primary metabolites that are transformed into the secondary metabolite. When primary metabolites are calculated the sum of the formation fractions $F_{f,p,j} \times F_{f,s,j}$ over m can be replaced by the single formation fraction $F_{f,p,j}$. Similar to Equations (A9) and (A10) A_i (kg/ha) is the application rate of application i, and $f_{soil,i}$ is the fraction of the dose reaching the soil for application i (to be taken from Tables 9 and 10). Finally, M_{met} (g/mol) is the molar mass of the metabolite considered (primary or secondary) and M_{parent} (g/mol) is the molar mass of the parent substance.

As for parent substances, there is the complication that A_{year} as calculated for the total number of applications may be lower than when calculated for a smaller number of applications. Therefore, A_{year} has to be calculated n times: the first A_{year} calculation assumes that the first application is the last application, the second A_{year} calculation assumes that the second application is the last application and so on. At the end, the maximum of all A_{year} values has to be taken.

A.2. Non-uniform applications in annual crops (row, band, strip and spot applications)

As described in Section 4.2, three types of concentrations may be relevant in the case of non-uniform applications in annual crops, i.e. the concentration averaged over the entire field, the concentration in the treated area (e.g. in the crop row) and the concentration in the non-treated area (e.g. between crop rows). For the concentration averaged over the entire field, the model in Section A.1 can be used when the annual application rate (A_{year}) is expressed in kg/ha of the whole field. If the dosage is defined as the mass of active ingredient per surface area treated, the methodology will also give conservative estimates for options (ii) and (iii). The latter is, however, a very conservative assumption because it implicitly implies that the crop rows or the treated areas are always at the same position. For this reason, a more realistic exposure-assessment procedure has been included in PERSAM. This procedure assumes that the location of the treated rows or the treated areas changes from year to year by calculating the background concentration using an application rate that is defined in kg/ha of the entire field (so the application rate is multiplied by the fraction of the soil that is treated, $f_{treated}$). This refined calculation procedure is described in more detail below.

The simple analytical model considers the situation of an application after a steady-state plateau concentration has been reached. Based on the foregoing assumptions, it seems justifiable to assume that in the non-treated area (e.g. between the crop rows) the maximum concentration is equal to the steady-state plateau concentration in the treated area (e.g. in the crop rows). So the maximum concentration in the non-treated area as well as the plateau concentration in the treated area are calculated with an equation akin to Equation A2:

$$C_{T,\text{non-treated}} = f_{\text{treated}} \frac{z_{\text{eco}}}{z_{\text{til}}} C_{T,\text{ini}} \frac{X}{1 - X} \tag{A16}$$

where $C_{T,\text{non-treated}}$ (mg/kg) is the maximum concentration in the non-treated area as well as the plateau concentration in the treated area and $f_{treated}$ (–) is the fraction of the soil surface that is treated. Notice that the only difference between Equation A2 and Equation A16 is the incorporation of the factor $f_{treated}$.

The maximum concentration in the treated area ($C_{T,treated}$ mg/kg) will be highest after the last application and is the sum of the plateau concentration (which is the same as the concentration in the non-treated area) and the concentration generated by this last application:

$$C_{T,\text{treated}} = C_{T,\text{ini}} + C_{T,\text{non-treated}} \tag{A17}$$

The concentration in pore water is calculated by an equation akin to Equation A7 in which the $C_{T,peak}$ is replaced by $C_{T,treated}$ and $C_{T,\text{non-treated}}$, respectively.

A.3. Applications in ridge–furrow systems

The exposure of soil organisms in ridge–furrow systems may depend strongly on the type of application. Many different application techniques in ridge–furrow tillage systems exist at Member State level (e.g. Boesten et al., 2015) but these are not all relevant for the soil exposure assessment at EU level everywhere in Europe. This section only describes the following applications:

- full overspray after the ridge–furrow formation;
- application in only the ridge or only the furrow.

We define f_{ridge} as the fraction of the surface area of the field occupied by the ridges and f_{furrow} as the fraction of the surface area of the field occupied by the furrows. So

$$f_{ridge} + f_{furrow} = 1 \quad \text{(A18)}$$

Spraying over the full surface area of field after ridge formation

For spray applications onto the whole field after the ridge–furrow formation, the recommendation is to use the model for spray applications to level surfaces; therefore, the model described in Section A.1. This is justifiable because the initial concentrations in the top layer are expected to be the same for both tillage systems and because the long-term accumulation is expected to be the same.

Application in only the ridge or only the furrow

Application to only the ridge or only the furrow can be handled in the same way as the exposure for non-uniform applications in annual crops grown on level surfaces as described in Section A.2. This exposure assessment of non-uniform applications defines $f_{treated}$ as the fraction of the surface area of the field that was treated. So for ridge applications $f_{treated} = f_{ridge}$ and for furrow applications $f_{treated} = f_{furrow}$.

A.4. Applications of granules and small-treated seeds

A.4.1. Applications of granules and small-treated seeds in level soils following incorporation

As described in Section 4.1, the analytical model in Section A.1 may be used for granular and small treated seeds applications with an incorporation depth less than z_{eco}. For greater depths, this needs to be slightly changed. The reason is that the increase of the concentration has to be based on averaging over the incorporation depth instead of averaging over z_{eco} or z_{til}. If the incorporation depth exceeds z_{til} Equation A2 needs to be replaced by Equation A19a:

$$C_{T,plateau} = \frac{A_{year}}{\rho z_{inc}} \frac{X}{1 - X} \quad \text{(A19a)}$$

where z_{inc} (dm) is the incorporation depth.

If the incorporation depth exceeds z_{eco}, Equation A1 needs to be replaced by Equation A19b:

$$C_{T,ini} = \frac{A_{year}}{\rho z_{inc}} \quad \text{(A19b)}$$

A.4.2. Placing of granules and small treated seeds at certain soil depth

In case of placing granules and small-treated seed application to a certain soil level depth (e.g. 10 cm), the mean annual water flux is assessed at a soil of $z_{inc} + z_{eco}$. Therefore, if the incorporation depth is e.g. 10 cm and z_{eco} is 5 cm, the ecotoxicological mixing layer is considered to start at 10 cm and the mean annual water flux is therefore assessed at 15 cm soil depth.

A.4.3. Applications of granules in ridge–furrow system

The procedure in Section A.4.1 is also valid for the combination of the following application method and subsequent tillage operation in ridge–furrow systems: (i) the granules are applied to a level soil surface at a dosage of A_{year} kg/ha; (ii) they are incorporated to a depth z_{inc}; and (iii) thereafter the top layer with a thickness z_{rf} (ridge furrow) of this level soil system is transformed into a ridge-furrow system. It is assumed that the incorporation depth z_{inc} is larger than z_{rf}. This is commonly the case because this application method is usually used for nematicides in potatoes and protection of the potato roots against the nematodes is expected to be insufficient when z_{inc} is smaller than z_{rf}.

A.5. Comparison of PERSAM and PEARL

A.5.1. PERSAM version with leaching

Results of PERSAM and PEARL were compared for some 2,000 different scenarios for permanent crops obtained using the Tier-3B procedure. Simulations were done for five substances, i.e. P1 (*DegT50* = 10 days, K_{om} = 10 days), P4 (*DegT50* = 31 days, K_{om} = 31 days), P8 (*DegT50* = 100 days, K_{om} = 100 days), P13 (*DegT50* = 316 days, K_{om} = 316 days) and P19 (*DegT50* = 1,000 days, K_{om} = 1,000 days). Simulations were done for annual crops assuming tillage to 20 cm and for permanent crops assuming no mixing. Application was in spring (1 kg/ha to the soil surface at May 1). In the annual crop simulations, soil properties were uniform to a depth of 30 cm whereas in the permanent crops soil properties were adjusted according to Table 3.

Results for spring applications (Figures A.1 and A.2) show an excellent correlation between PERSAM results and PEARL results for both annual crops and for permanent crops. The absolute level is, however, different which implies that a model adjustment factor is still necessary to ensure that results based on PERSAM are more conservative than results based on the numerical models (Appendix C).

Simulations have also been done for summer applications (application at 1 July) and for autumn applications (application at 1 October). Results for summer applications in annual crops (Figure A.3) show that results are comparable to that of the spring applications; however, a number of different trend lines can be distinguished for the concentration in pore water in this case. Further investigation revealed that each of these trend lines corresponds to a FOCUS scenario. Apparently, different seasonal patterns of the FOCUS scenarios cause different soil moisture conditions at the time that the maximum concentration is reached. Results for the other application times are comparable and therefore not shown.

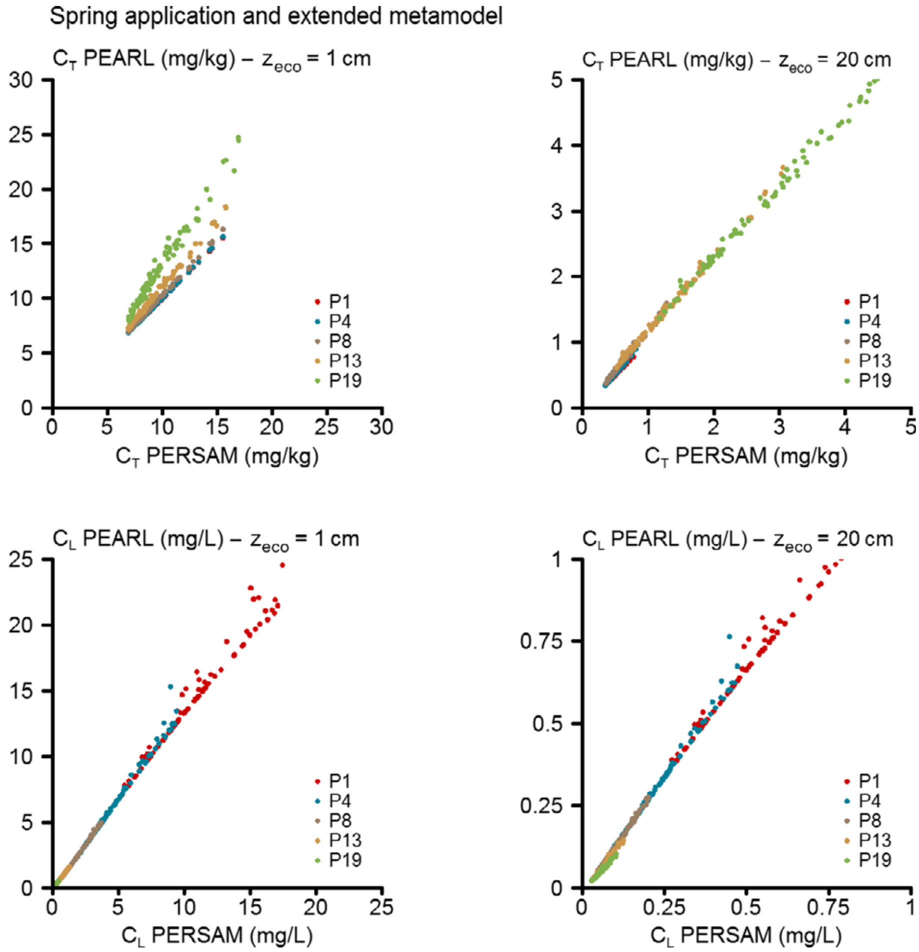

Figure A.1: Comparison of PERSAM and PEARL results for some 2,000 scenarios in annual crops derived using the Tier-3B procedure. Application was in spring (1 May) with a dose of 1 kg/ha (see further text)

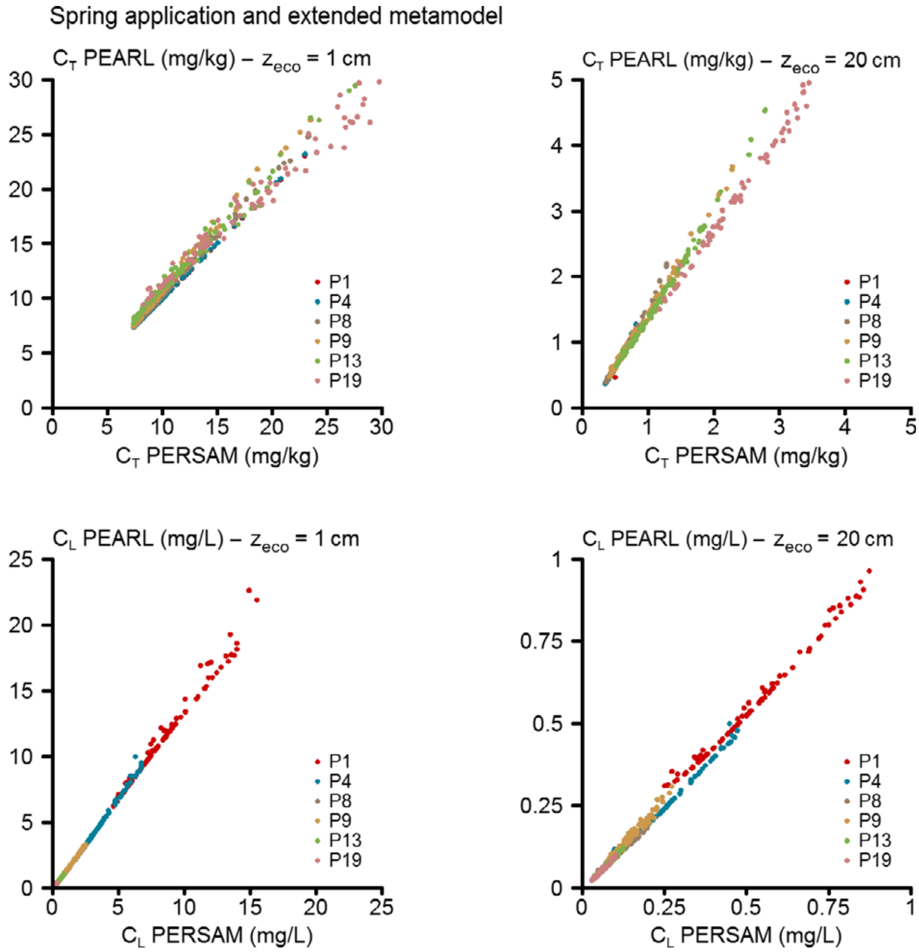

Figure A.2: Comparison of PERSAM and PEARL results for some 2,000 scenarios in permanent crops derived using the Tier-3B procedure. Application was in spring (1 May) with a dose of 1 kg/ha (see further text)

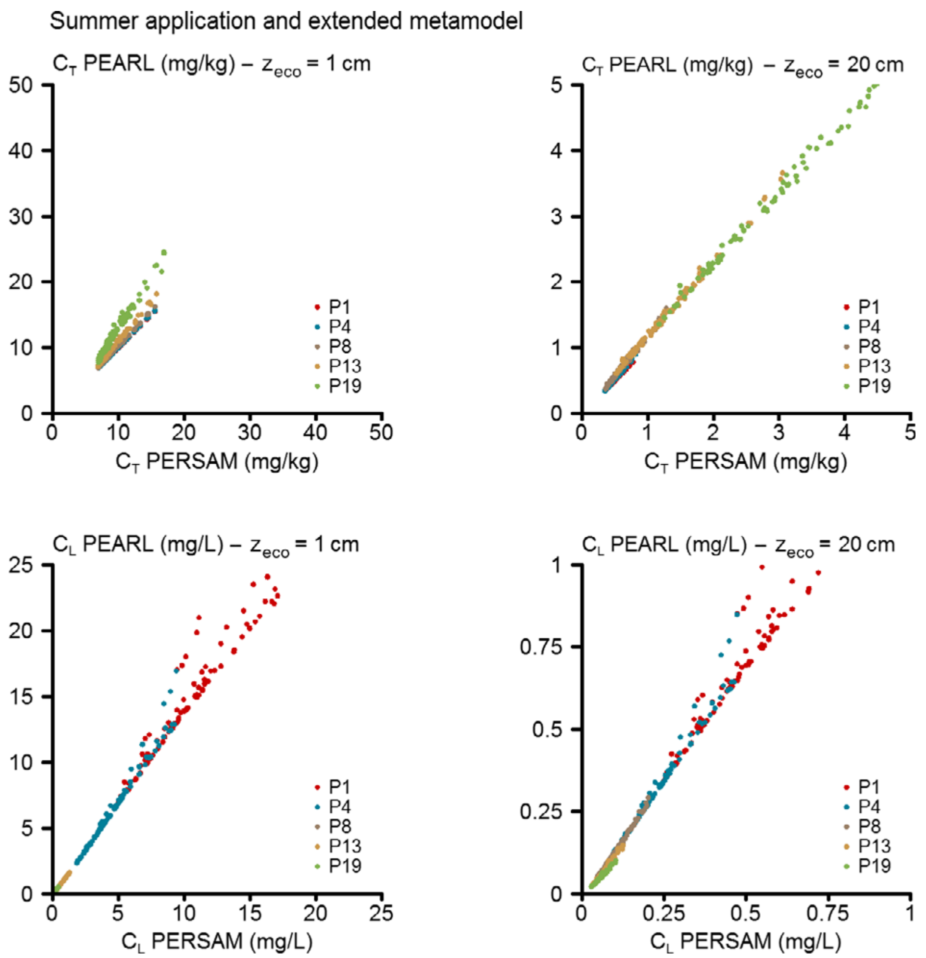

Figure A.3: Comparison of PERSAM and PEARL results for some 2,000 scenarios in annual crops derived using the Tier-3B procedure. Application was in summer (1 July) with a dose of 1 kg/ha (see further text)

A.5.2 PERSAM version without leaching

We performed exactly the same comparison using the PERSAM version described in EFSA (2012), i.e. the version that does not include the leaching term. The agreement between both models is still reasonably good for annual crops (Figure A.4). However, for permanent crops the agreement between the two models is not as good (Figure A.5). Therefore, the addition of the leaching term is essential for creating a suitable model for scenario selection.

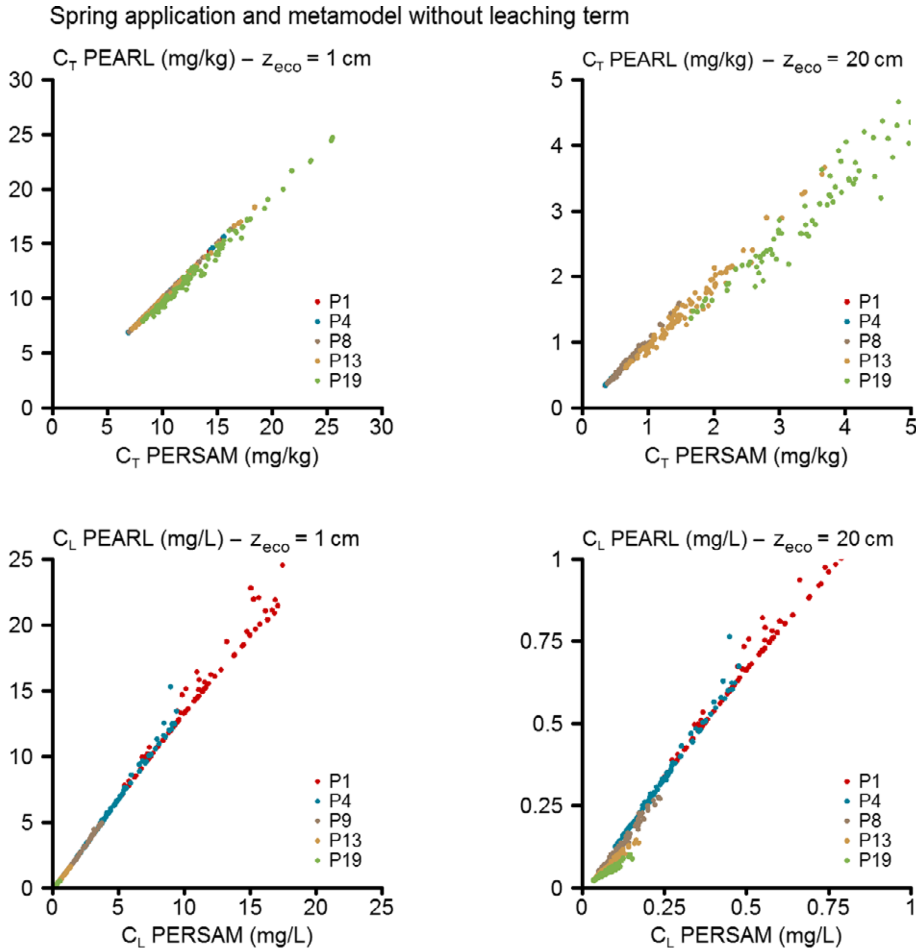

Figure A.4: Comparison of PERSAM and PEARL results for some 2,000 scenarios in annual crops derived using the Tier-3B procedure. Application was in spring (1 May) with a dose of 1 kg/ha (see further text)

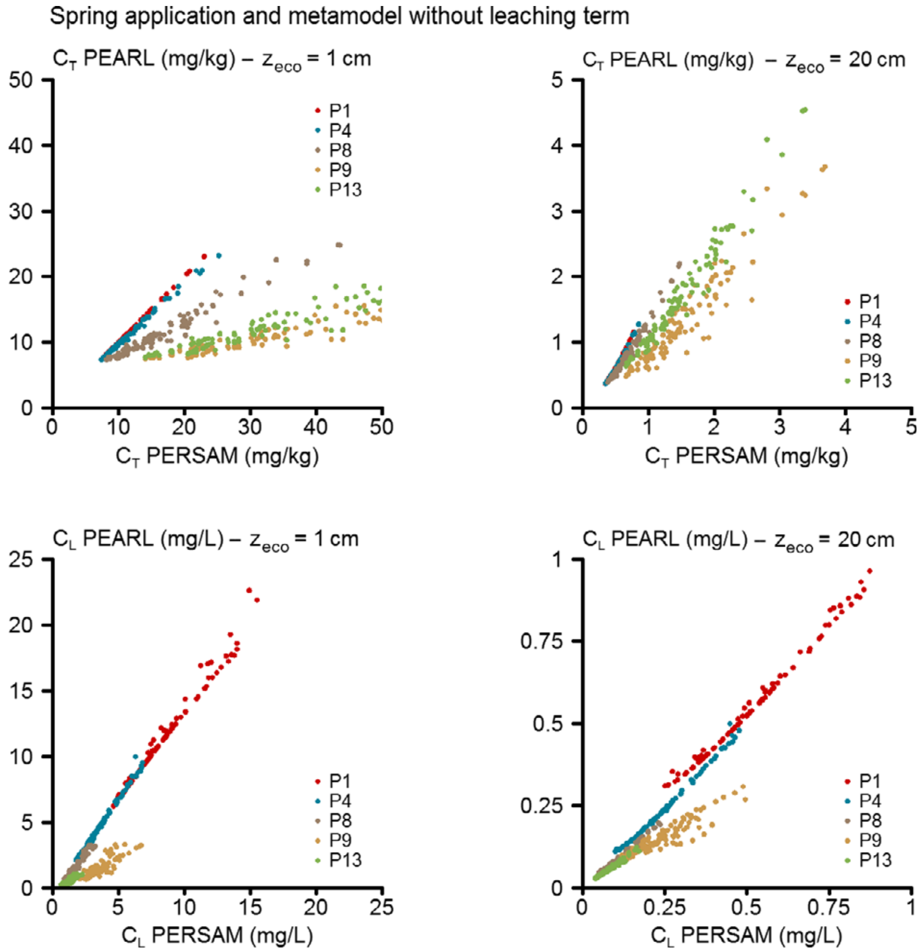

Figure A.5: Comparison of PERSAM and PEARL results for some 2,000 scenarios in permanent crops derived using the Tier-3B procedure. Application was in spring (1 May) with a dose of 1 kg/ha (see further text)

Appendix B – Parameterisation of the exposure scenarios

This appendix gives a description of the parameterisation of the exposure scenarios for annual crops and for permanent crops. A comprehensive description of the procedure can be found in EFSA (2010a), EFSA PPR Panel (2010b, 2012) and Beulke et al. (2015); the data are described in Hiederer (2012). Because the procedures have slightly changed for the sake of harmonisation, a summary of the final procedure is given here.

B.1. Scenarios for the analytical model

This section first describes in general how the site-specific input data for the simple analytical model were derived from the EFSA spatial data set. Then specific considerations are given for Tier-1 and Tier–2.

B.1.1. General considerations

The simple analytical model as implemented in the PERSAM software tool requires the following five site-specific parameters:

- Arrhenius-weighted mean annual temperature (°C);
- mass fraction of organic matter in the top 30 cm (kg/kg);
- top soil bulk density (kg/L);
- top soil water content at field capacity (m^3/m);
- the mean annual water flux at the lower boundary of the ecotoxicological averaging depth (dm/d).

All basic data to derive these input data are available in the EFSA spatial data set (version 1.1), which is available at the address http://esdac.jrc.ec.europa.eu/content/european-food-safety-authority-efsa-data-persam-software-tool. This data set consists of data that are available at a high spatial resolution (1 × 1 km) for all countries of the European Union.

Soil data

Organic matter was obtained by applying a conversion factor of 1.724 to the topsoil organic carbon map (OCTOP) as described by Jones et al. (2005). This map was chosen because it was the only harmonised map of organic carbon in topsoil available when the draft guidance was developed. The availability of the LUCAS data set (Montanarella et al., 2011) makes it possible to compare the OCTOP map with observations of organic matter in European topsoils. This comparison is described in Section B.3 and reveals that organic matter is generally overestimated by the OCTOP map. However, because better alternatives are not yet available, the OCTOP map has not been replaced.

Soil bulk density was calculated from organic matter using a continuous pedotransfer function (Tiktak et al., 2002):

$$\rho = 1800 + 1236 f_{om} - 2910\sqrt{f_{om}} \qquad \text{(B1)}$$

where ρ (kg/m) is the dry bulk density of the soil and f_{om} (kg/kg) is the organic matter content. The use of this pedotransfer function was justified in Appendix D of EFSA (2010a) where it was concluded that more complex pedotransfer functions including also texture did not perform better than this simple pedotransfer function. The volume fraction of water at field capacity was derived from the soil textural class in the Soil Geographical Database of Europe, using the HYPRES pedotransfer rule (Wösten et al., 1999). Notice that only six different classes are available in the HYPRES database, i.e. course, medium, medium fine, fine, very fine and non-mineral. The Arrhenius-weighted long-term average temperature was derived from the WorldClim database (Hijmans et al., 2005) using the procedure in Appendix A.3 of EFSA (2010a). The mean annual precipitation, necessary to calculate the water flux at the lower boundary of the ecotoxicological averaging depth, was also derived from the EFSA spatial data set.

The soil properties in the EFSA spatial data set refer to the top 30 cm. These soil properties can directly be used for scenarios for annual crops. However, in permanent crops, organic matter cannot be assumed to be uniformly distributed within this top 30 cm soil layer. For this reason, Beulke et al. (2015) introduced correction factors for calculating the depth distribution of organic matter in the top

30 cm (Table 3). Notice that the correction factors corresponding to the ecotoxicological averaging depth have to be applied and that the correction factors are different for situations with and situations without mechanical cultivation (Table 3).

Weather data and the water flux at the bottom of the ecotoxicological averaging depth

The mean annual water flux at the bottom of the ecotoxicological averaging depth is obtained by multiplying the sum of precipitation and irrigation with a ratio f_q, which is defined by:

$$f_q = \frac{q_{avg}}{(P + I)_{avg}} \qquad (B2)$$

where q_{avg} (dm/d) is the mean annual flux at the bottom of the ecotoxicological averaging depth and $(P+I)_{avg}$ (dm/d) is the sum of the mean annual precipitation P and irrigation I. The mean annual water flux at the bottom of the ecotoxicological averaging depth (q_{avg}) was calculated with PEARL and PELMO for all FOCUS crops in Tables 6 and 7. For each FOCUS crop, the dominant FOCUS zone per regulatory zone (Table B.7) was selected for modelling. (The dominant FOCUS zone is defined as the zone with the largest crop area within a regulatory zone.) Table B.1 gives the properties of the FOCUS zones.

Table B.1: FOCUS groundwater climatic zones (Hiederer, 2012) and climate properties of the FOCUS scenarios (FOCUS, 2000)

FOCUS zone	Total mean annual precipitation (mm)	Mean annual temperature (°C)	Mean annual precipitation of FOCUS scenario (mm)	Mean annual temperature of FOCUS scenario (°C)
Châteaudun	< 600	5 to < 12.5	648	11.3
Hamburg	600 to < 800	5 to < 12.5	786	9.0
Jokioinen	All[(a)]	< 5	650	4.1
Kremsmünster	800 to < 1,000	5 to < 12.5	899	8.6
Okehampton	≥ 1,000	5 to < 12.5	1038	10.2
Piacenza	800 to < 1,000	≥ 12.5	857	13.2
Porto	≥ 1,000	≥ 12.5	1150	14.8
Sevilla	< 600	≥ 12.5	493	17.9
Thiva	600 to < 800	≥ 12.5	500	16.2

(a): No distinction in precipitation for temperatures < 5°C (see Hiederer, 2012).

This procedure requires the availability of maps of $(P + I)$ for every pixel and every crop. The following procedure was used to obtain these maps:

- for non-irrigated crop–scenario combinations, precipitation at the respective location was selected from the EFSA spatial data set;
- for irrigated crop–scenario combination, the sum of precipitation and simulated irrigation of the respective FOCUS zone meteo file was selected irrespective of the location; so when a crop is irrigated, it is assumed that the sum of precipitation and irrigation is constant in the entire FOCUS zone; this is justified because low rainfall amounts will be compensated for by high irrigation amounts and vice versa (see also Figure 4 in Tiktak et al., 2004).

The mean annual irrigation amounts for all FOCUS–crop combinations are given in Section B.3. The mean of PEARL and PELMO was used for further calculations. Section B.3 also gives an overview of f_q values for each FOCUS–crop combination. Differences in f_q values between the scenarios are relatively small. The reason is that these ratios are primarily affected by the vertical distribution of roots, which generally shows only limited variability between the FOCUS scenarios. Because of the small differences between the scenarios it was decided to use the mean of all f_q values for use in PERSAM; these values are listed in Table B.2.

Table B.2: Ratio (f_q) of the mean annual water flux at different soil depths and the mean annual precipitation plus irrigation

1 cm	2.5 cm	5 cm	20 cm
0.80	0.75	0.70	0.50

B.1.2. Tier-1 parameterisation

The Tier-1 scenarios apply to the 95th percentile concentration in the entire area of annual and permanent crops (excluding grassland). Parameterisation of Tier-1 scenarios comes down to selecting one of the pixels from the EFSA spatial data set described above. The scenarios were selected using the statistical procedure as described in EFSA PPR Panel (2012), EFSA (2012) and Tiktak et al. (2013). Because leaching was not included in earlier versions of PERSAM, and annual and permanent crops were not combined, the scenario selection was redone.

The scenario selection was redone with the analytical model described in Appendix A. The filters listed in Table B.3 were applied to the EFSA spatial data set (version 1.1) with the aim to avoid unrealistic pixels. The procedure described in EFSA PPR Panel (2012) and summarised in Tiktak et al. (2013) was used for scenario selection. Therefore, for 19 substances, for two evaluation depths (1 cm and 20 cm) and for both crop types (annual and permanent crops) simulations were done with the analytical model and with the parameter settings listed in Table B.4. Next, all locations between the 94 and 96th percentiles were selected for each of the 76 runs. The candidate Tier-1 scenarios were those scenarios that were within the 94 and 96th percentile range in all model runs. The final Tier-1 scenario was the scenario that was closest to the median properties of all Tier-1 candidates (following the procedure as described in Section B.2.1). Properties of the predefined scenarios are given in Tables 1–2.

Table B.3: Filters applied to the EFSA spatial data set

Properties in EFSA data set	Annual and permanent crops
EFSA generalised land use	Annual (class 1) or permanent crops (class 3) excluding grassland (class 2)
Topsoil organic matter	> 0 and < 0.334 (g/g)[(a)]
Topsoil textural class	Only mineral soils (classes 1, 2, 3, 4, and 5)
Topsoil pH	> 0
Topsoil water content at field capacity	> 0 cm^3/cm^3
Total mean annual precipitation	> 0 mm

(a): The upper limit of organic matter for the respective land-use type in the LUCAS data set (see Section B.3).

Table B.4: Parameter settings for selection of the Tier-1 scenarios

Parameters of the analytical model	Annual crops		Permanent crops	
Annual application rate (A_{year})	1 kg/ha		1 kg/ha	
Application cycle (t_{cycle})	365 days		365 days	
Averaging window t_{avg}	0 days		0 days	
Activation energy (E_{act})	65.4 kJ/mol		65.4 kJ/mol	
DegT50 and K_{om}	As defined in Appendix III of EFSA (2012)		As defined in Appendix III of EFSA (2012)	
Total annual irrigation	0 mm		0 mm	
Evaluation depth (z_{eco})	1 cm	20 cm	1 cm	20 cm
Tillage depth (z_{til})	20 cm	20 cm	1 cm	20 cm
Leaching ratio (f_q)	0.80	0.50	0.80	0.50
Depth correction factor $f_{om,corr}$[(a)]	1.00	1.00	1.95	1.19

(a): Obtained from Table 3.

B.1.3. Tier-2 parameterisation

At Tier-2, the analytical model uses the same spatial data as at Tier-1; however, all data including organic-matter content, precipitation, temperature and the dominant FOCUS zone refer to the scenario location. If this location is considered to be irrigated (triggered by the dominant FOCUS zone in Table B.7), the sum of precipitation and irrigation is kept constant all over the regulatory zone. This means that the correction factor for precipitation should be set to 1 in these cases.

When the substance is applied to the canopy, the fraction of the dose reaching the soil is calculated on basis of EFSA crop interception values and default wash-off fractions from the canopy as given in Tables 9 and 10. Notice that these tables are based on average wash-off values over a period of 20 years because this generates exposure concentrations that are close to those simulated with the numerical models (Appendix D). Finally, the worst case of the three regulatory zones was used to derive the default wash-off fraction.

Because Tier-2 is based on the area of intended use and not on the total crop area, this tier also requires the crop areas as derived from the CAPRI2000 data set for annual crops and the assessment done by Beulke et al. (2015) for permanent crops – see Hiederer (2012) and Beulke et al. (2015) for details and file names. Notice that the data set for permanent crops was reassessed by the working group to bring it in line with the 1 $\times$ 1-km^2 resolution used in the EFSA spatial data set (refer to Annex I). A closer inspection of this data set revealed that significant areas of permanent crops are located in pixels with 'EFSA generalised land-use' class 9 (in these pixels 'non-agricultural' areas cover the majority of the pixel area). To include these crop areas at Tier-2, the EFSA general land-use mask for selecting pixels with permanent crops includes class 9 as well (in addition to the general filters applied to the EFSA spatial data set, refer to Table B.3). Notice that slight inconsistencies with respect to different crop areas at Tier-1 and Tier-2 in case of permanent crops are fully covered by the scenario adjustment factor. For permanent grassland, which is not accounted for in the selection of Tier-1 scenarios at all, only pixels covering EFSA general land-use class 2 ('grass') are included at Tier-2. In any case, at Tier-2 the minimum area for the crop of interest has to be 1 ha/km^2 (= 1%) per pixel.

When used for substances whose $DegT_{50}$ or K_{om} is pH- or clay-dependent, the pH or the clay content of the topsoil is needed as well. The pH-value in the EFSA spatial data set is the pH-H_2O so the applicant may need to apply the procedure in Section 3.3.1 to convert the pH value as measured in the sorption or degradation experiment. Note that the clay content in the EFSA spatial data set can be only roughly estimated for a scenario location because only five classes are available (also refer to Section 3.3.2).

The scenario parameterisation for permanent crops is different for in-row and between-row exposure assessments (Section 1.3.2): Between-row areas are typically non-irrigated but often mechanically cultivated (for citrus, vines, olives and hops). In addition, areas between the rows may be without cover (bare soil) or are covered by grass depending on the permanent crop type (Table B.5). Note that the models already account for the correct scenario parameterisation depending on the exposure assessment selected by the user.

Table B.5: Differences in scenario parameterisation with respect to in-row and between-row soil exposure assessment in permanent crops grown in rows (based on common cultivation practices as given in Beulke et al., 2015). These differences apply to both the analytical model and the numerical models

Permanent crop	Exposure assessment	Irrigation	FOCUS crop	Mechanical cultivation[(b)]
Pome and stone fruit	In-row	Yes/No[(a)]	Apples	No
	Between-row	No	Grass	No
Bush berries	In-row	Yes/No[(a)]	Bush berries	No
	Between-row	No	Grass	No
Citrus	In-row	Yes/No[(a)]	Citrus	No
	Between-row	No	No cover (bare soil)	Yes
Olives	In-row	Yes/No[(a)]	Olives[(c)]	Yes
	Between-row	No	No cover (bare soil)	Yes
Vines	In-row	Yes/No[(a)]	Vines	No
	Between-row	No	No cover (bare soil)	Yes

Permanent crop	Exposure assessment	Irrigation	FOCUS crop	Mechanical cultivation[(b)]
Hops	In-row	Yes/No[(a)]	Hops[(c)]	No
	Between-row	No	No cover (bare soil)	Yes

(a): Drip irrigation depending on the FOCUS zone (see Table B.8).
(b): Mechanical cultivation is characterised by a specific top soil organic-matter profile and perfect mixing over the top 5 cm two times a year.
(c): Not a FOCUS GW crop (for parameterisation approach refer to Beulke et al., 2015).

B.2. Scenarios for the numerical models

In Tier-3A, the scenario is first selected in the PERSAM software (Tier-2). PERSAM then generates a file (the so-called PERSAM transfer file) containing the geographical coordinates and the location properties. This file is used by PEARL or PELMO to generate automatically the input files for the Tier-3A scenarios. Further use of the models is almost the same as the FOCUS Groundwater versions.

B.2.1. Scenario selection

The Tier-3A scenarios are selected using the following procedure, which is already implemented in the PERSAM tool (Section 3.5.1):

- For each pixel of the maps obtained in Tier-2, a vulnerability score is calculated. (The vulnerability score is 0% for the pixel with the lowest concentration and 100% for the pixel with the highest concentration; see EFSA (2012) for details.)
- Select all pixels with a vulnerability score between 94% and 96%.
- Calculate for this subset of pixels the median value of temperature, precipitation plus irrigation, organic matter of the top 30 cm of the soil and – when applicable – the pH of the topsoil.
- Select the pixels with properties closest to the median value of these properties. This comes down to optimising the following objective function:

$$O = \sum_{i=1}^{n} \left| \frac{p_i - p_{50}}{p_{50}} \right| \qquad \text{(B3)}$$

where O is the objective function to be minimised, p is the property (temperature, $P+I$, organic matter or pH), p_{50} is the median of these properties, i is an index and n is the number of properties.

This procedure avoids the selection of scenarios with extreme properties. Notice that the effect of leaching is included in the selection of the scenario, because this process is included in the Tier-2 calculation. Wash-off is not included in the selection of the scenarios. As tables in Appendix D are based on average values of 20 years, it cannot fully be ensured that the models used at Tier-3A will not deliver higher wash-off values. However, the effect of these differences is accounted for in the model adjustment factors.

Different scenarios must be selected for the concentration in total soil and the concentration in pore water and for the parent compound and for each metabolite. In principle, a separate scenario needs to be developed for each ecological averaging depth. However, if only one depth is needed in the effects assessment, only one scenario needs to be developed and other results do not need to be reported. It is finally considered acceptable to base the scenario selection only on the peak concentration (so no individual scenarios for different TWA values).

B.2.2. Scenario parameterisation

This scenario selection procedure will deliver the geographical coordinates of the scenario and the following location-specific information as given in the EFSA spatial data set:

- arithmetic mean annual temperature (°C);
- mean annual precipitation (dm/d);
- organic-matter content of the top 30 cm of the soil (kg/kg);
- pH of the topsoil (–);
- soil textural class (course, medium, medium fine, fine and very fine).

Scenarios for PEARL and PELMO are built by combining the above five properties with crop and weather data from the dominant FOCUS Groundwater scenarios (EC, 2014) within each regulatory zone. In permanent crops grown in rows, scenario selection is always based on the map of the row crop.

Soil profiles

In addition to the properties of the topsoil (0–30 cm), PEARL and PELMO need properties of the subsoil (30–200 cm). These can be obtained using average soil profiles, which were based on all arable soil profiles available in the Soil Profile Analytical Database of Europe (v1). Averages were calculated for the 0–30 cm soil layer, the 30–60 cm soil layer, the 60–100 cm soil layer and the 100–200 cm soil layer (cf. FOCUS, 2000) and are shown in Table B.6. The use of average soil profiles is considered acceptable, because the evaluation depth for the exposure assessment is 1–20 cm (see EFSA, 2010aa for additional considerations).

The scenario selection procedure returns the soil textural class at the scenario location. Based on this, the soil textural distribution (clay, silt and sand) can be assigned using the values in Table B.6. Organic matter of the subsoil is calculated with the equation:

$$f_{\mathrm{om}} = f_{\mathrm{z,om}} f_{\mathrm{om,0}} \tag{B4}$$

where f_{om} (kg/kg) is the mass fraction of organic matter, $f_{\mathrm{z,om}}$ (–) is the organic-matter content relative to the topsoil organic-matter content and $f_{\mathrm{om,0}}$ (kg/kg) is the organic-matter content of the topsoil, which has been derived in the scenario selection procedure. Notice that $f_{z,\mathrm{om}}$ depends on the soil textural class, see Table B.6. In the case of permanent crops, additional scaling factors apply to the 0–30 cm soil layer as well – see Section 'Differentiation of soil properties of the topsoil' below.

Soil bulk density is derived from the scaled organic-matter content using Equation B1. Soil hydraulic functions as required by PEARL can be obtained from the soil textural class using the HYPRES pedotransfer rules (Wösten et al., 1999) and are also listed in Table B.6. The consequence of using these so-called class pedotransfer rules is that the soil hydraulic properties are considered to be independent of organic-matter content and density of the soil. The water content at field capacity and the water content at wilting point required by PELMO are estimated with the analytical function proposed by Van Genuchten (1980):

$$\theta(h) = \theta_{\mathrm{r}} + \frac{\theta_{\mathrm{s}} - \theta_{\mathrm{r}}}{\left(1 + |\alpha h|^{n}\right)^{-m}} \tag{B5}$$

where θ (m^3/m^3) is the volume fraction of water, h (cm) is the soil water pressure head, θ_{s} (m^3/m^3) is the volume fraction of water at saturation, θ_{r} (m^3/m^3) is the residual water content in the extremely dry range, α (cm^{-1}) and n (–) are empirical parameters, and m (–) can be taken equal to:

$$m = 1 - \frac{1}{n} \tag{B6}$$

Table B.6: Mean soil profiles for the soil textural classes at the soil map of Europe. The soil profiles (totalling 534) were calculated using all arable soil profiles in the Soil Profile Analytical Database for Europe (SPADE)

Depth[(a)]	Sand	Silt	Clay	$f_{z,om}$[(a)]	f_z	θ_s	θ_r	α	n	K_s	λ
Coarse											
0–30	83.2	11.6	5.2	1.0	1.0	0.4	0.03	0.0383	1.377	0.6	1.25
30–60	84.4	10.6	5.0	0.5	0.5	0.37	0.03	0.0430	1.521	0.7	1.25
60–100	85.6	10.0	4.4	0.3	0.3	0.37	0.03	0.0430	1.521	0.7	1.25
> 100	85.8	9.5	4.7	0.1	0.0	0.37	0.03	0.0430	1.521	0.7	1.25
Medium											
0–30	39.5	41.5	19.0	1.0	1.0	0.44	0.01	0.0310	1.180	0.121	–2.42
30–60	38.8	41.1	20.1	0.5	0.5	0.40	0.01	0.0250	1.169	0.108	–0.74
60–100	40.3	38.9	20.8	0.3	0.3	0.40	0.01	0.0250	1.169	0.108	–0.74
> 100	41.0	38.3	20.7	0.1	0.0	0.40	0.01	0.0250	1.169	0.108	–0.74

Depth[(a)]	Sand	Silt	Clay	$f_{z,om}$[(a)]	f_z	θ_s	θ_r	α	n	K_s	λ
Medium fine											
0–30	8.7	71.0	20.3	1.0	1.0	0.43	0.01	0.0080	1.254	0.023	-0.59
30–60	8.6	68.8	22.6	0.5	0.5	0.41	0.01	0.0080	1.218	0.040	0.50
60–100	7.7	68.4	23.9	0.3	0.3	0.41	0.01	0.0080	1.218	0.040	0.50
> 100	7.5	69.9	22.6	0.1	0.0	0.41	0.01	0.0080	1.218	0.040	0.50
Fine											
0–30	16.2	39.2	44.6	1.0	1.0	0.52	0.01	0.0370	1.101	0.248	–1.98
30–60	16.5	37.9	45.6	0.5	0.5	0.48	0.01	0.0200	1.086	0.085	–3.71
60–100	16.1	38.4	45.5	0.3	0.3	0.48	0.01	0.0200	1.086	0.085	–3.71
> 100	15.9	38.6	45.5	0.1	0.0	0.48	0.01	0.0200	1.086	0.085	–3.71
Very fine											
0–30	4.8	30.7	64.5	1.0	1.0	0.61	0.01	0.0270	1.103	0.150	2.50
30–60	7.2	25.6	67.2	0.5	0.5	0.54	0.01	0.0170	1.073	0.082	0.00
60–100	9.0	23.5	67.5	0.3	0.3	0.54	0.01	0.0170	1.073	0.082	0.00
> 100	10.6	20.0	69.4	0.1	0.0	0.54	0.01	0.0170	1.073	0.082	0.00
Organic											
0–30	61.0	8.8	29.0	1.0	1.0	0.77	0.01	0.0130	1.204	0.080	0.40
30–60	70.0	10.0	20.0	1.1	0.5	0.77	0.01	0.0130	1.204	0.080	0.40
60–100	61.4	10.0	20.0	1.1	0.3	0.77	0.01	0.0130	1.204	0.080	0.40
> 100	69.1	10.0	20.0	1.1	0.0	0.77	0.01	0.0130	1.204	0.080	0.40

(a): Depth (cm) is the depth, sand (%) is the sand content, silt (%) is the silt content, clay (%) is the clay content, $f_{z,om}$ (–) is the organic-matter content relative to the topsoil organic-matter content, f_z (–) is the depth dependence of degradation in soil, θ_s (m^3/m^3) is the volume fraction of water at saturation, θ_r (m^3/m^3) is the residual water content in the extremely dry range, α (cm^{-1}) and n (–) are empirical parameters of the van Genuchten equation, K_s (m/d) is the saturated hydraulic conductivity and λ (–) is a shape parameter.

The depth of the soil profile is assumed to be 2 m. The lower boundary condition of the hydrological model is not expected to have a large effect on the predicted concentration in top soil. For pragmatic reasons, a free-drainage boundary condition was therefore assumed for all scenarios.

For the top 1 cm, the thickness of the numerical compartments in PEARL is set to 2 mm, because the evaluation depth of the exposure assessment can be as small as 1 cm. In PELMO the thickness of the top compartments is 1 mm with 9 mm below. In both models, the layer thickness is 1 cm for the 1–30 cm soil layer, 2.5 cm for the 30–100 cm soil layer and 5 cm for the 100–200 cm soil layer.

The dispersion length is set to a value of 2.5 cm for the layer 0–60 cm and 5 cm for the layer 60–200 cm. The value for the topsoil differs from the value used in FOCUS (2010), because the evaluation depth is 1–20 cm, whereas the evaluation depth for the FOCUS scenarios is 100 cm. For short travel distances, a lower value of the dispersion coefficient is needed (Vanderborght and Vereecken, 2007) All other soil parameters, including the depth dependence of transformation, are set to the default values published by FOCUS (2010).

The scenario parameterisation for permanent crops is different for in-row and between-row exposure assessments (Section 1.3.2): Between-row areas are typically non-irrigated but often mechanically cultivated. In addition, areas between the rows may be without cover (bare soil) or are covered by grass depending on the permanent crop type (Table B.5). Note that the models already account for the correct scenario parameterisation depending on the crop and exposure assessment selected by the user.

Weather data

Weather data are always based on the FOCUS groundwater weather series of the dominant FOCUS scenario within each regulatory zone (see Table B.7 for the list of dominant FOCUS zones). The advantage of this procedure is that there is no need for data in addition to the data that are available in the EFSA spatial database and in the FOCUS groundwater scenarios. This deviation from the original procedure described in EFSA (2010a) is considered justifiable because long-term accumulation of a substance is primarily affected by the long-term average temperature and to a lesser extent by daily weather conditions. To guarantee consistency in the tiered approach, temperatures and precipitation in the FOCUS weather series are scaled to the temperature and precipitation at the scenario location:

$$T_{\text{day,scenario}} = T_{\text{day,FOCUS}} + T_{\text{avg,scenario}} - T_{\text{avg,FOCUS}} \tag{B7a}$$

$$P_{\text{day,scenario}} = \frac{P_{\text{avg,scenario}}}{P_{\text{avg,FOCUS}}} P_{\text{day,FOCUS}} \tag{B7b}$$

where $T_{\text{day,scenario}}$ is the daily mean temperature at the soil exposure scenario location, $T_{\text{avg,scenario}}$ is the mean annual temperature at the soil exposure scenario location, $T_{\text{avg,FOCUS}}$ is the mean annual temperature of the FOCUS groundwater scenarios (Table B.1), $P_{\text{day,scenario}}$ (dm/d) is the daily mean precipitation at the scenario location, $P_{\text{avg,scenario}}$ is the mean annual precipitation at the scenario location, $P_{\text{avg,FOCUS}}$ is the mean annual precipitation of the FOCUS scenario and $P_{\text{day,FOCUS}}$ is the mean annual precipitation of the FOCUS scenario (Table B.1). Scaling of precipitation is not applied if the location is considered to be irrigated (depending on the dominant FOCUS scenario). Notice that scaling of temperatures is based on the 'normal' mean annual temperature and not on the Arrhenius-weighted temperature.

All other weather data – including evapotranspiration – are kept to their original values.

Both PEARL and PELMO have the option to scale temperatures and precipitation automatically using the equation above. The advantage is that the original FOCUS weather files can be kept and that only one parameters needs to be input to the model. The scaling parameters (ΔT (°C) and f_P (–)) that need to be input are given by the equations:

$$\Delta T = T_{\text{avg,scenario}} - T_{\text{avg,FOCUS}} \tag{B8a}$$

$$f_{\text{p}} = \frac{P_{\text{avg,scenario}}}{P_{\text{avg,FOCUS}}} \quad (\text{non-irrigated}) \text{ and } f_p = 1 \quad (\text{irrigated}) \tag{B8b}$$

Crop data

At Tier-3A crop and weather data are taken from the dominant FOCUS scenario[9] in the regulatory zone (Table B.7; see Table B.1 for definitions of FOCUS zones). The crop area is based on the list of CAPRI crops (Hiederer, 2012) and permanent crops (Beulke et al., 2015) (see Tables 6 and 7 for the link between CAPRI and permanent crops and FOCUS crops).

Table B.7: Dominant FOCUS scenario per regulatory zone and crop to be used for modelling with PEARL and PELMO. If a FOCUS crop is not available for the respective combination, a second-best alternative is selected. In the header, DS is the dominant scenario, AR means the relative area of this dominant scenario (as a percentage of the total area of the respective crop in the respective zone) and FO is the FOCUS crop to be used in PEARL and PELMO. Shaded cells indicate combinations in which the dominant scenario does not have a FOCUS crop

Crop		North			Centre			South		
FOCUS	**CAPRI/permanent crop**	**DS**	**AR**	**FO**	**DS**	**AR**	**FO**	**DS**	**AR**	**FO**
Apples	Pome and stone	HA	88	HA	HA	62	HA	SE	46	SE
Beans (field and vegetables)	Pulses	HA	56	HA	CH	50	HA	HA	47	TH
Bush berries	Bush berries	HA	85	HA	CH	65	CH	SE	43	SE
Cabbage	Other vegetables	HA	70	HA	CH	47	CH	SE	33	SE
Carrots	Other vegetables	HA	70	HA	CH	47	CH	SE	33	TH
Citrus	Citrus	–	–	–	–	–	–	SE	82	SE

9 Note amendments were made to the senescence dates of the crop onions at the scenarios Thiva (21/6) and Porto (21/5) compared with that published in Generic guidance for Tier-1 FOCUS groundwater assessments (Anonymous, 2014), as before the amendment the date of senescence was before that of maximum LAI.

Crop		North			Centre			South		
FOCUS	**CAPRI/permanent crop**	**DS**	**AR**	**FO**	**DS**	**AR**	**FO**	**DS**	**AR**	**FO**
Cotton	Texture crops	–	–	–	HA	46	TH	TH	53	TH
Grass	Grass	HA	75	HA	HA	38	HA	HA	55	HA
Hops	Hops	–	–	–	HA	56	HA	HA	68	HA
Linseed	Texture crops	HA	60	OK	HA	46	OK	SE	53	OK
Maize	Maize	HA	52	HA	CH	54	CH	HA	32	HA
No crop (fallow)	Fallow	HA	58	HA	HA	47	HA	SE	31	SE
Oil seed rape (summer)	Rapes	HA	57	OK	HA	50	OK	HA	76	OK
Oil seed rape (winter)	Rapes	HA	57	HA	HA	50	HA	HA	76	HA
Olives	Olives	–	–	–	–	–	–	SE	53	SE
Onions	Other vegetables	HA	75	HA	HA	74	HA	SE	21	TH
Peas	Pulses	HA	56	HA	CH	50	CH	HA	47	HA
Potatoes	Potatoes	HA	68	HA	HA	51	HA	HA	45	HA
Soybean	Soya beans	–	–	–	CH	64	PI	TH	35	PI
Spring cereals	Cereals	HA	56	HA	CH	48	CH	HA	34	HA
Strawberries	Other vegetables	HA	70	HA	CH	47	HA	SE	33	SE
Sugar beets	Sugar beet	HA	63	HA	HA	50	HA	HA	51	HA
Sunflower	Sunflower	–	–	–	CH	83	PI	HA	24	PI
Tobacco	Tobacco	–	–	–	CH	61	PI	SE	37	TH
Tomatoes	Other vegetables	HA	70	CH	CH	47	CH	SE	33	SE
Vines	Vines	–	–	–	CH	57	CH	SE	33	SE
Winter cereals	Cereals	HA	56	HA	CH	48	CH	HA	34	HA

CH: Châteaudun; HA: Hamburg; JO: Jokioinen; KR: Kremsmünster; OK: Okehampton; PI: Piacenza; PO: Porto; SE: Seville; TH: Thiva. See Table B.1 for further details

In some cases, the dominant FOCUS scenario cannot be linked to a FOCUS crop. This is particularly the case for those FOCUS crops that are only parameterised for a few FOCUS scenarios, e.g. linseed and soya beans. In those specific cases, the most appropriate crop was selected for parameterising crop development (i.e. preferably a crop in the same regulatory zone). Note that weather data are in those cases still taken from the dominant FOCUS zone.

Irrigation data

Irrigation is applied at all tiers in line with the respective dominant FOCUS zone (Table B.7). The FOCUS zones where irrigation is considered to take place are Châteaudun, Piacenza, Sevilla, Porto, and Thiva (see Table B.8). If a 'second-best' alternative for a FOCUS crop is not parameterised for irrigation (e.g. linseed) irrigation is not applied at all. In case of annual crops sprinkler irrigation (weekly irrigation) is applied, whereas for permanent crops (in-row exposure assessment) weekly drip (surface) irrigation is assumed. Note that for between-row exposure assessments for permanent crops no irrigation is assumed at all. Irrigation for annual crops is assumed from crop emergence to start senescence. For evergreen permanent crops (citrus and olives), the irrigation period is the entire year. For other permanent crops, the irrigation periods are defined from start of leaf development to the start of senescence.

Table B.8: Irrigation settings for all crop–scenario combinations

	Regulatory zone		
Crop	**North**	**Centre**	**South**
Apples	No	No	Sur
Bare soil (between rows)	No	No	No
Beans (field)	No	Spr	No
Bush berries	No	Spr	Spr
Cabbage	No	Spr	Spr
Carrots	No	Spr	Spr
Citrus	–	–	Sur
Cotton	–	No	Spr
Grass	No	No	No
Grass between rows	No	No	No
Hops	–	No	No
Linseed	No	No	Spr
Maize	No	Spr	No
No crop (fallow)	No	No	No
Oil seed rape (summer)	No	No	No
Oil seed rape (winter)	No	No	No
Olives	–	–	Sur
Onions	No	No	Spr
Peas (animals)	No	No	No
Potatoes	No	No	No
Soybean	–	Spr	Spr
Spring cereals	No	No	No
Strawberries	No	Spr	Spr
Sugar beets	No	No	No
Sunflowers	–	Spr	No
Tobacco	–	Spr	Spr
Tomatoes	No	Spr	Spr
Vines	–	Sur	Sur
Winter cereals	No	No	No

'Sur' indicates surface (drip) irrigation.
'Spr' indicates sprinkler irrigation.

Soil management

Soil cultivation (tillage) is applied in case of annual crops assuming perfect mixing of the top 20 cm of the soil layer 1 month before emergence. In case of permanent crops, situations with mechanical cultivation are already reflected by the top soil organic-matter profile. In addition, situations with mechanical cultivation are considered to account for tillage (perfect mixing) to a soil depth of 5 cm two times a year (1 May and 15 June). In contrast with annual crops, mechanical cultivation for permanent crops is specific to the crop and exposure assessment (Table B.9).

Table B.9: Soil-management setting for annual and permanent crops

Crop type	Crop	Tillage (ploughing to 20 cm)	Mechanical cultivation[(a)]	
			In-row exposure	Between-row exposure
Annual crops	All	Yes	No	
Permanent crops	Apples	No	No	No
	Bush berries	No	No	No
	Vines	No	No	Yes
	Citrus	No	No	Yes
	Olives	No	Yes	Yes
	Hops	No	No	Yes
Permanent grass	Grass	No	No	

(a): Mechanical cultivation is accompanied by tillage (perfect soil mixing) to a soil depth of 5 cm.

The warming-up period

As described in Section 3.4.2, the warming-up period consists of a multiple of 6 years and each 6-year period consists of the same meteorological time series. It is important that this 6-year time series has an approximately 'average' air temperature. If the temperature of this 6-year series is too low, then the all-time maximum of the concentrations is likely to happen in the first of the 20-year evaluation period, which is undesirable.

Therefore, for each of the FOCUS groundwater scenarios, the 6-year averages of the Arrhenius air temperatures of the meteorological time series were calculated (see Table B.10). This gives 15 possible options for 6-year periods for each scenario (starting in 1907–1921). Next, the average Arrhenius air temperature of all 15 options was calculated (e.g. 10.57°C for Hamburg as shown in Table B.10). Subsequently, the desired 6-year period was selected using the criteria: (i) that its Arrhenius temperature is lower than this average; and (ii) that its Arrhenius temperature is closest to this average. For example, for Hamburg this is the period 1913–1918 because its Arrhenius temperature of 10.49°C is lower than the 10.57°C average and is closer to 10.57°C than all the other periods with an average Arrhenius temperature below 10.57°C.

This gives the following 6-year time series for the warming-up periods:

- FOCUS GW Châteaudun: 1911–1916;
- FOCUS GW Hamburg: 1913–1918;
- FOCUS GW Jokioinen: 1916–1921;
- FOCUS GW Kremsmünster: 1915–1920;
- FOCUS GW Okehampton: 1912–1917;
- FOCUS GW Piacenza: 1910–1915;
- FOCUS GW Porto: 1919–1924;
- FOCUS GW Sevilla: 1917–1922;
- FOCUS GW Thiva: 1918–1923.

Table B.10: Annual average air temperatures and annual average Arrhenius air temperatures of the FOCUS GW scenarios

Year	Scenario Châteaudun			Scenario Hamburg		
	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)
1907	11.04	12.86		9.90	11.84	
1908	11.69	13.97		9.18	11.19	
1909	11.20	12.41		9.32	10.69	
1910	10.64	11.97		8.32	9.88	
1911	10.77	12.43		7.53	9.36	
1912	10.57	12.12	12.63	7.99	9.62	10.43
1913	11.46	13.06	12.66	8.29	10.06	10.13
1914	11.98	13.65	12.61	9.03	11.01	10.10
1915	11.59	13.62	12.81	9.38	11.22	10.19
1916	11.03	12.59	**12.91**	8.47	9.93	10.20
1917	10.29	12.36	12.90	8.23	10.22	10.34
1918	10.58	12.52	12.97	8.75	10.49	**10.49**
1919	10.54	12.59	12.89	8.15	9.80	10.44
1920	11.76	13.08	12.79	9.63	11.09	10.46
1921	12.35	14.13	12.88	9.79	11.30	10.47
1922	12.45	14.15	13.14	10.33	11.64	10.75
1923	11.14	13.12	13.26	9.30	11.00	10.88
1924	11.29	12.91	13.33	9.97	11.87	11.12
1925	10.81	12.24	13.27	8.62	10.15	11.17
1926	12.66	14.24	13.47	9.78	11.80	11.29
Average			**12.97**			**10.57**

Year	Scenario Jokioinen			Scenario Kremsmünster		
	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)
1907	5.49	7.31		8.88	11.01	
1908	2.68	5.06		8.70	10.94	
1909	3.38	5.67		8.88	10.52	
1910	2.60	6.02		7.94	9.74	
1911	3.49	6.25		8.45	10.52	
1912	3.53	6.62	6.15	7.75	9.80	10.42
1913	3.53	5.99	5.93	8.07	10.19	10.28
1914	4.70	6.89	6.24	8.39	10.73	10.25
1915	4.59	7.36	6.52	8.70	11.11	10.35
1916	4.55	6.96	6.68	7.74	9.55	10.31
1917	2.22	6.29	6.68	7.65	10.32	10.28
1918	3.22	6.44	6.65	8.14	10.55	10.41
1919	2.21	5.10	6.50	8.03	10.50	10.46
1920	3.89	6.97	6.52	9.09	11.00	**10.51**
1921	5.75	7.57	**6.55**	9.30	11.03	10.49
1922	5.80	7.31	6.61	8.97	10.86	10.71

Year	Scenario Jokioinen			Scenario Kremsmünster		
	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)
1923	5.80	7.46	6.81	8.65	10.90	10.81
1924	5.77	7.43	6.97	9.28	11.75	11.01
1925	3.49	6.25	7.17	8.93	11.00	11.09
1926	4.70	6.89	7.15	10.43	12.72	11.38
Average			**6.61**			**10.58**

Year	Scenario Okehampton			Scenario Piacenza		
	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)
1907	10.20	11.74		13.15	15.60	
1908	10.53	12.43		12.64	15.01	
1909	10.12	11.17		12.72	14.86	
1910	9.56	10.74		12.26	14.63	
1911	9.38	10.90		12.84	15.51	
1912	9.74	11.11	11.35	13.65	15.85	15.24
1913	10.05	11.37	11.29	13.09	15.67	15.26
1914	10.58	12.20	11.25	13.26	16.10	15.44
1915	10.66	12.24	11.43	14.23	16.76	**15.75**
1916	10.11	11.41	11.54	12.10	14.59	15.74
1917	9.23	10.97	**11.55**	12.41	15.56	15.75
1918	9.61	11.01	11.53	12.91	15.79	15.74
1919	9.46	11.07	11.48	14.44	16.98	15.96
1920	10.69	11.72	11.40	13.25	15.70	15.90
1921	11.11	12.49	11.45	13.04	15.53	15.69
1922	11.19	12.42	11.61	13.48	16.05	15.94
1923	9.99	11.47	11.70	13.73	16.64	16.12
1924	11.00	12.55	11.95	13.77	16.28	16.20
1925	10.31	11.66	12.05	13.61	16.33	16.09
1926	11.41	12.89	12.25	14.04	16.55	16.23
Average			**11.59**			**15.80**

Year	Scenario Porto			Scenario Sevilla		
	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)
1907	14.31	15.26		16.94	18.66	
1908	14.44	15.53		16.94	18.91	
1909	14.37	15.14		17.12	18.33	
1910	14.56	15.44		17.35	19.06	
1911	14.56	15.63		17.58	19.34	
1912	14.56	15.52	15.42	17.63	19.63	18.99
1913	15.23	16.40	15.61	18.26	20.00	19.21

Year	Scenario Porto			Scenario Sevilla		
	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)
1914	14.82	15.72	15.64	17.62	19.23	19.26
1915	14.95	15.93	15.77	17.92	19.54	19.47
1916	14.58	15.60	15.80	17.31	18.88	19.44
1917	15.04	16.55	15.95	17.94	19.65	19.49
1918	14.69	16.04	16.04	17.73	19.00	19.38
1919	14.77	15.83	15.95	18.43	19.52	19.30
1920	15.31	16.20	16.03	18.18	19.10	19.28
1921	15.81	16.76	16.16	18.63	19.71	19.31
1922	14.94	15.99	16.23	18.32	19.39	**19.39**
1923	14.34	15.49	16.05	17.78	19.05	19.29
1924	14.47	14.94	**15.87**	18.64	20.47	19.54
1925	15.17	16.17	15.93	18.42	20.25	19.66
1926	14.85	15.52	15.81	19.68	21.56	20.07
Average			**15.88**			**19.41**

Year	Scenario Thiva		
	Annual average temperature (°C)	Annual average Arrhenius temperature (°C)	Average of Arrhenius temperature of the previous 6 years (°C)
1907	16.61	18.56	
1908	15.72	17.22	
1909	16.51	18.10	
1910	15.73	17.23	
1911	16.29	17.76	
1912	15.78	17.48	17.73
1913	16.30	17.99	17.63
1914	16.12	17.98	17.76
1915	16.00	17.63	17.68
1916	16.08	17.53	17.73
1917	16.63	18.17	17.80
1918	16.18	17.84	17.86
1919	16.30	18.25	17.90
1920	16.59	18.55	17.99
1921	15.61	17.18	17.92
1922	16.27	17.92	17.99
1923	15.31	17.12	**17.81**
1924	16.26	17.91	17.82
1925	16.64	18.33	17.83
1926	17.29	18.86	17.89
Average			**17.82**

B.3. Comparison of the OCTOP map with observations in LUCAS

The LUCAS (Land Use/Cover Area frame statistical survey) topsoil survey (Montanarella et al., 2011) offers the opportunity to compare the OCTOP (top soil organic carbon) data set included in the EFSA spatial data set v.1.1 with measurements of organic matter in European topsoils. Note that in the EFSA spatial data set the organic carbon content is already scaled to organic-matter content applying a factor of 1.724 (Hiederer, 2012). To avoid any confusion the data set is therefore called OMTOP in this context. The LUCAS data set was created in 2009 in response to the scarcity of harmonised up-to-date OC data. The data set contains some 20,000 soil samples taken in 23 MSs. The topsoil samples were sent to a centre laboratory for physicochemical analyses, which included total soil carbon (refer to Tóth et al., 2013 for details).

Because it is known that land use has a large effect on OC content, we used three subsamples from the LUCAS data set, i.e. arable crops, permanent crops, and permanent grassland. The subsets were created using land cover information available at the LUCAS website (please refer to http://ec.europa.eu/eurostat/web/lucas/data/primary-data/2009). The following classification was used (see the file 'LUCAS 2009 classification' at the site above):

- annual crops: categories B10–B55;
- permanent crops: categories B71–B84;
- permanent grassland: category E20.

To compare LUCAS with OMTOP, organic carbon in the LUCAS data set was multiplied by 1.72. Then, cumulative frequency distributions were drawn, which are shown in Figure B.1. From this figure, it is obvious that organic-matter contents are generally overestimated by OMTOP. The only exception is permanent grassland, whose frequency distributions compare reasonably well to those of the OMTOP map. This can be explained as follows. The OMTOP map is based on pedotransfer rules with variables like soil type, latitude, temperature and land use as explaining variables (Jones et al., 2005). Despite the fact that land use is the most important influential factor for organic matter in topsoils (e.g. De Brogniez et al., 2014; Van den Berg et al., 2017), only one value of organic matter is predicted for each 1×1 km^2 pixel. So for each pixel, organic matter is an average value for the mixture of land use found within each pixel. This will lead to an overestimation of organic matter in cropland soils if the pixel also contains, e.g. grassland soils or forests. The alternative would be to predict separate maps for cropland and grassland (e.g. Van den Berg et al., 2017).

It should be noted that the frequency distribution of organic matter in the LUCAS data set is based on 20,000 point observations, which are not area weighted. For this reason, the representativeness of the LUCAS data set for the EU as a whole is not known. A better comparison would possible when the point observations would be interpolated onto the 1×1 km^2 grid of the EFSA spatial data set. An example of such a map is the map created by De Brogniez et al. (2014). This map, however, does not make a distinction between cropland and other land uses, so it suffers from the same shortcoming as the OMTOP map. It is therefore recommended to develop a new map of organic matter in European topsoils, which makes a distinction between cropland soils and grassland soils (see e.g. Van den Berg et al., 2017).

Because a true alternative to the OMTOP map is currently not available, it was decided to continue using this map until a better alternative is available. However, it was decided to remove all pixels with organic-matter contents higher than the largest value for the respective land use in the LUCAS data set (see Table 9.1 in Tóth et al., 2013). So, for annual crops all pixels were removed with organic-matter contents above 0.334 g/g and for permanent crops (including grassland) all pixels with organic-matter contents above 0.343 g/g were removed (see Table B.3).

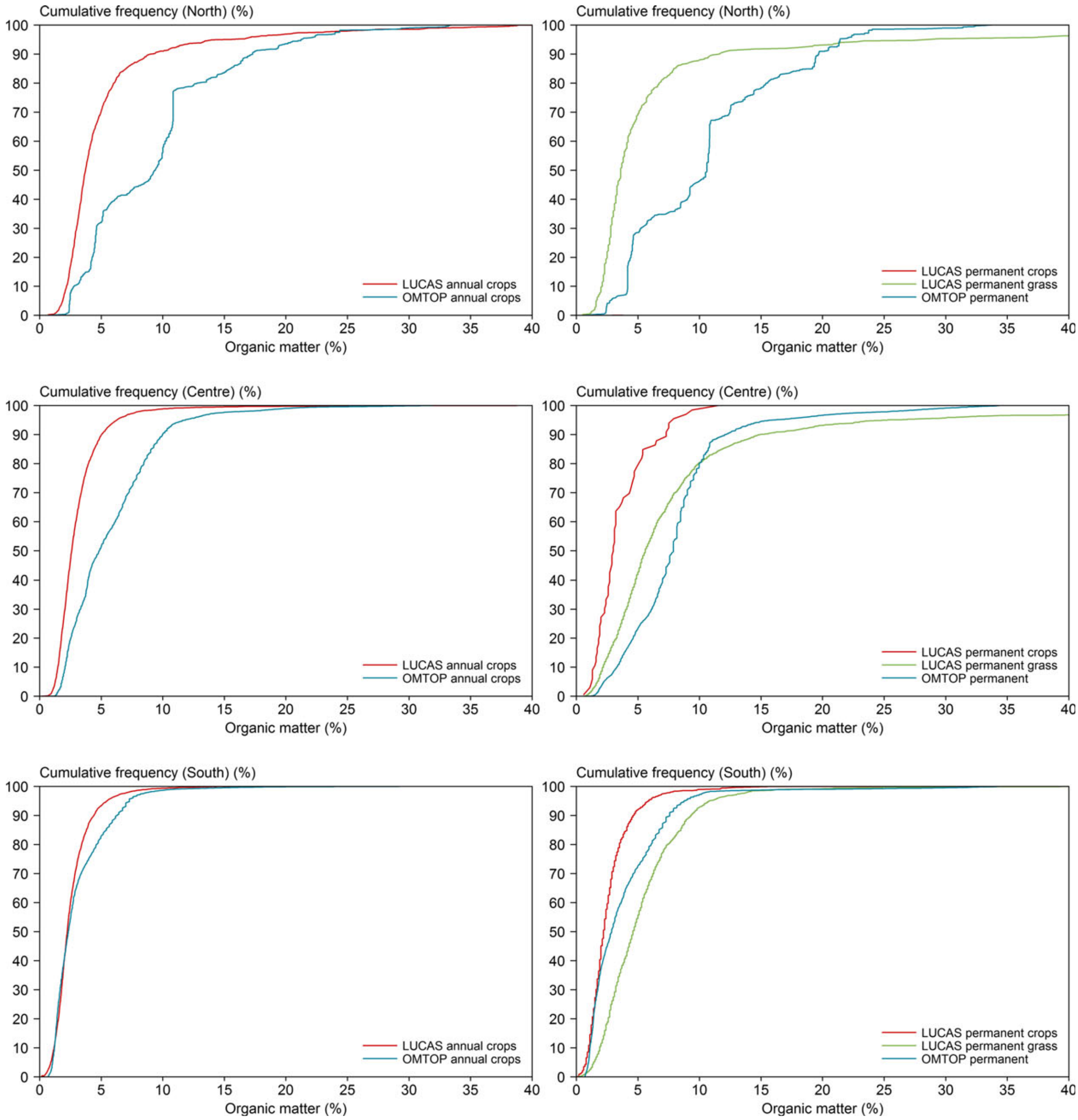

Figure B.1: Frequency distributions of organic matter in the LUCAS data set compared with that of the OMTOP map for the three regulatory zones North, Centre and South. Left-hand side: annual crops. Right-hand side: permanent crops and grassland. Notice that 'permanent' in OMTOP is a combination of grassland and permanent crops

B.4. Supporting information for the calculation of the f_q ratios applied in the analytical model

This section gives supporting information for the calculation of the f_q ratios. Table B.11 provides the annual irrigation applied in all FOCUS–crop combinations. Tables B.12–B.15 provide the f_q-ratio for soil depths of 1, 2.5, 5 and 20 cm. In those cases where the evaluation depth is in between the depths reported in Tables B.12–B.15, it is advised to interpolate linearly.

Table B.11: Irrigation applied for all regulatory zone-crop combinations. The dominant FOCUS zone as listed in Table B.7 was used for modelling

Crop	PEARL			PELMO			Mean		
	Regulatory zone			Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South	North	Centre	South
Apples	0	0	1003	0	0	916	0	0	960
Bare soil (between the rows)	0	0	0	0	0	0	0	0	0
Beans (field and vegetables)	0	260	0	0	263	0	0	262	0
Bush berries	0	266	771	0	237	648	0	252	710
Cabbage	0	185	496	0	209	661	0	197	579
Carrots	0	175	524	0	170	639	0	173	582
Citrus	–	–	737	–	–	729	–	–	733
Cotton	–	0	238	–	0	315	–	0	277
Grass	0	0	0	0	0	0	0	0	0
Grass (between the rows)	0	0	0	0	0	0	0	0	0
Hops	–	0	0	–	0	0	–	0	0
Linseed	0	0	612	0	0	745	0	0	679
Maize	0	267	0	0	265	0	0	266	0
No crop (= fallow)	0	0	0	0	0	0	0	0	0
Oil seed rape (summer)	0	0	0	0	0	0	0	0	0
Oil seed rape (winter)	0	0	0	0	0	0	0	0	0
Olives	–	–	721	–	–	729	–	–	725
Onions	0	0	90	0	0	273	0	0	182
Peas (animals)	0	0	0	0	0	0	0	0	0
Potatoes	0	0	0	0	0	0	0	0	0
Soybean	–	247	491	–	265	574	–	256	533
Spring cereals	0	0	0	0	0	0	0	0	0
Strawberries	0	277	505	0	263	746	0	270	626
Sugar beets	0	0	0	0	0	0	0	0	0
Sunflower	–	384	0	–	327	0	–	356	0
Tobacco	–	360	657	–	288	823	–	324	740
Tomatoes	0	181	155	0	178	185	0	180	170
Vines	–	241	790	–	237	756	–	239	773
Winter cereals	0	0	0	0	0	0	0	0	0

Table B.12: Ratio (f_q) of the mean annual water flux at 1 cm depth and the mean annual precipitation plus irrigation for all regulatory zone–crop combinations. The dominant FOCUS zone as listed in Table B.7 was used for modelling

Crop	PEARL			PELMO		
	Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South
Apples	0.72	0.72	0.79	0.96	0.96	0.96
Beans (field and vegetables)	0.65	0.63	0.65	0.94	0.95	0.94
Bush berries	0.72	0.68	0.72	0.96	0.96	0.95
Cabbage	0.64	0.61	0.57	0.94	0.95	0.94
Carrots	0.64	0.61	0.64	0.94	0.95	0.94

Crop	PEARL			PELMO		
	Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South
Citrus	–	–	0.88	–	–	0.98
Cotton	–	0.65	0.59	–	0.94	0.93
Grass	0.72	0.72	0.72	0.96	0.96	0.96
Hops	–	0.62	0.62	–	0.96	0.96
Linseed	0.67	0.67	0.61	0.94	0.94	0.94
Maize	0.66	0.64	0.66	0.94	0.95	0.94
No crop (= fallow)	0.54	0.54	0.46	0.92	0.92	0.93
Oil seed rape (summer)	0.65	0.65	0.65	0.94	0.94	0.94
Oil seed rape (winter)	0.65	0.65	0.65	0.95	0.95	0.95
Olives	–	–	0.71	–	–	0.98
Onions	0.63	0.63	0.55	0.94	0.94	0.92
Peas (animals)	0.65	0.58	0.65	0.94	0.93	0.94
Potatoes	0.63	0.63	0.63	0.94	0.94	0.94
Soybean	–	0.69	0.68	–	0.95	0.94
Spring cereals	0.67	0.59	0.67	0.94	0.93	0.94
Strawberries	0.66	0.63	0.62	0.95	0.96	0.94
Sugar beets	0.67	0.67	0.67	0.94	0.94	0.94
Sunflower	–	0.70	0.69	–	0.96	0.95
Tobacco	–	0.67	0.64	–	0.95	0.94
Tomatoes	0.68	0.64	0.58	0.94	0.94	0.92
Vines	–	0.72	0.74	–	0.97	0.96
Winter cereals	0.64	0.58	0.64	0.95	0.94	0.95
Mean of all crops	0.66	0.64	0.65	0.94	0.95	0.95
Overall mean (rounded)	0.80					

Table B.13: Ratio (f_q) of the mean annual water flux at 2.5 cm depth and the mean annual precipitation plus irrigation for all regulatory zone–crop combinations. The dominant FOCUS zone as listed in Table B.7 was used for modelling

Crop	PEARL			PELMO		
	Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South
Apples	0.72	0.72	0.79	0.91	0.91	0.91
Beans (field and vegetables)	0.65	0.63	0.65	0.86	0.88	0.86
Bush berries	0.72	0.68	0.71	0.91	0.91	0.88
Cabbage	0.64	0.60	0.56	0.87	0.88	0.85
Carrots	0.64	0.61	0.63	0.87	0.88	0.87
Citrus	–	–	0.88	–	–	0.95
Cotton	–	0.65	0.58	–	0.86	0.85
Grass	0.71	0.71	0.71	0.91	0.91	0.91
Hops	–	0.62	0.62	–	0.90	0.90
Linseed	0.66	0.66	0.60	0.87	0.87	0.86
Maize	0.66	0.63	0.66	0.87	0.88	0.87
No crop (= fallow)	0.54	0.54	0.46	0.82	0.82	0.83
Oil seed rape (summer)	0.65	0.65	0.65	0.87	0.87	0.87
Oil seed rape (winter)	0.65	0.65	0.65	0.89	0.89	0.89

Crop	PEARL			PELMO		
	Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South
Olives	–	–	0.71	–	–	0.95
Onions	0.63	0.63	0.54	0.86	0.86	0.83
Peas (animals)	0.65	0.57	0.65	0.86	0.84	0.86
Potatoes	0.62	0.62	0.62	0.86	0.86	0.86
Soybean	–	0.68	0.67	–	0.88	0.86
Spring cereals	0.67	0.58	0.67	0.87	0.84	0.87
Strawberries	0.65	0.63	0.59	0.89	0.90	0.86
Sugar beets	0.66	0.66	0.66	0.87	0.87	0.87
Sunflower	–	0.70	0.69	–	0.90	0.88
Tobacco	–	0.67	0.63	–	0.89	0.85
Tomatoes	0.67	0.64	0.57	0.86	0.87	0.83
Vines	–	0.74	0.86	–	0.93	0.91
Winter cereals	0.64	0.58	0.64	0.89	0.86	0.89
Mean of all crops	0.66	0.64	0.65	0.87	0.88	0.87
Overall mean (rounded)	0.75					

Table B.14: Ratio (f_q) of the mean annual water flux at 5 cm depth and the mean annual precipitation plus irrigation for all regulatory zone–crop combinations. The dominant FOCUS zone as listed in Table B.7 was used for modelling

Crop	PEARL			PELMO		
	Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South
Apples	0.71	0.71	0.78	0.83	0.83	0.83
Beans (field and vegetables)	0.64	0.62	0.64	0.76	0.79	0.76
Bush berries	0.71	0.67	0.70	0.83	0.83	0.79
Cabbage	0.63	0.59	0.54	0.77	0.78	0.72
Carrots	0.63	0.60	0.61	0.78	0.78	0.76
Citrus	–	–	0.87	–	–	0.90
Cotton	–	0.64	0.57		0.75	0.74
Grass	0.70	0.70	0.70	0.84	0.84	0.84
Hops	–	0.61	0.61	–	0.81	0.81
Linseed	0.64	0.64	0.59	0.78	0.78	0.74
Maize	0.65	0.62	0.65	0.77	0.78	0.77
No crop (= fallow)	0.54	0.54	0.46	0.70	0.70	0.71
Oil seed rape (summer)	0.64	0.64	0.64	0.77	0.77	0.77
Oil seed rape (winter)	0.64	0.64	0.64	0.81	0.81	0.81
Olives	–	–	0.70	–	–	0.90
Onions	0.62	0.62	0.53	0.76	0.76	0.70
Peas (animals)	0.64	0.56	0.64	0.76	0.71	0.76
Potatoes	0.61	0.61	0.61	0.75	0.75	0.75
Soybean	–	0.66	0.65	–	0.77	0.75
Spring cereals	0.66	0.56	0.66	0.77	0.71	0.77
Strawberries	0.64	0.62	0.55	0.80	0.82	0.73
Sugar beets	0.65	0.65	0.65	0.77	0.77	0.77
Sunflower	–	0.69	0.68	–	0.82	0.79

Crop	PEARL			PELMO		
	Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South
Tobacco	–	0.66	0.61	–	0.81	0.73
Tomatoes	0.66	0.63	0.56	0.75	0.76	0.70
Vines	–	0.72	0.73	–	0.87	0.83
Winter cereals	0.63	0.57	0.63	0.81	0.75	0.81
Mean of all crops	0.65	0.63	0.64	0.78	0.78	0.78
Overall mean (rounded)	0.70					

Table B.15: Ratio (f_q) of the mean annual water flux at 20 cm depth and the mean annual precipitation plus irrigation for all regulatory zone–crop combinations (PEARL). The dominant FOCUS zone as listed in Table B.7 was used for modelling

Crop	PEARL			PELMO		
	Regulatory zone			Regulatory zone		
	North	Centre	South	North	Centre	South
Apples	0.64	0.64	0.68	0.57	0.57	0.53
Beans (field and vegetables)	0.55	0.54	0.55	0.51	0.47	0.51
Bush berries	0.63	0.59	0.58	0.59	0.52	0.42
Cabbage	0.55	0.50	0.36	0.52	0.44	0.29
Carrots	0.56	0.53	0.45	0.53	0.46	0.37
Citrus	–	–	0.79	–	–	0.65
Cotton	–	0.55	0.45		0.51	0.34
Grass	0.58	0.58	0.58	0.58	0.58	0.58
Hops	–	0.60	0.60	–	0.57	0.57
Linseed	0.53	0.53	0.44	0.53	0.53	0.34
Maize	0.57	0.53	0.57	0.52	0.43	0.52
No crop (= fallow)	0.54	0.54	0.46	0.49	0.49	0.36
Oil seed rape (summer)	0.54	0.54	0.54	0.51	0.51	0.51
Oil seed rape (winter)	0.59	0.59	0.59	0.56	0.56	0.56
Olives	–	–	0.66	–	–	0.65
Onions	0.55	0.55	0.41	0.52	0.52	0.32
Peas (animals)	0.55	0.44	0.55	0.50	0.37	0.50
Potatoes	0.53	0.53	0.53	0.51	0.51	0.51
Soybean	–	0.53	0.47	–	0.43	0.33
Spring cereals	0.58	0.45	0.58	0.52	0.37	0.52
Strawberries	0.57	0.55	0.19	0.54	0.51	0.22
Sugar beets	0.55	0.55	0.55	0.52	0.52	0.52
Sunflower	–	0.62	0.60	–	0.53	0.54
Tobacco	–	0.61	0.43	–	0.51	0.32
Tomatoes	0.57	0.54	0.45	0.51	0.43	0.35
Vines	–	0.66	0.66	–	0.63	0.53
Winter cereals	0.57	0.48	0.57	0.55	0.41	0.55
Mean of crops	0.57	0.55	0.53	0.53	0.50	0.46
Overall mean (rounded)	0.50					

B.5. Re-assessment of the permanent crop distribution database

The spatial distribution of permanent crops in the EU was assessed by Beulke et al. (2015). The crop data collation was based on CORINE Land Cover data as well as orchard and farm structure surveys at the NUTS 2 level (EUROSTAT). Finally, 2013 unique combinations ('plots') were identified by GIS spatial overlay of permanent crop cover, FOCUS climatic zone, regulatory zone and soil mapping unit/dominant typological unit. As these plots cover considerably large areas, merging with the EFSA spatial data set (1 km^2 raster) was not considered appropriate by the working group. Therefore, it was decided to re-assess the permanent crop database based on the information available in Beulke et al. (2015).

In a first step, the CORINE Land Cover 2012 (shape file, version 18.5, 2/2016) was overlaid with the EFSA spatial data set (Inspire, 1 km^2 raster) to obtain ready-to-use crop distribution maps for vines (CORINE Land Cover code 221), olives (code 223) and pasture (permanent grassland, code 231). All other permanent crops in Beulke et al. (2015) (i.e. pome fruits, stone fruits, bush berries, hops and citrus) are considered to be lumped in CORINE Land Cover code 222 ('fruit trees and berry plantations'). So in a next step, the EFSA spatial data were overlaid with the permanent crop plot data set (shape file, Beulke et al., 2015) to determine the dominant (largest) plot for each raster cell which is covered by CORINE Land Cover code 222 and by one of the 2013 permanent crop plot. Raster cells not covering one of the plots were discharged from the final data set. Crop areas for pome fruits, stone fruits, bush berries, hops and citrus are defined for each of the 2013 plots (Beulke et al., 2015). Based on this information, plot specific fractions of area covered by each of these five crops were calculated. Finally these fractions were applied to the total area covered by CORINE Land Cover code 222 in each individual raster cell (based on the dominant plot found at that location). Notice that in the final data set pome and stone fruits were lumped together into one crop, used as a crop distribution estimate for FOCUS apples and similar crops.

Appendix C – Scenario and model adjustment factors

C.1. Derivation of scenario adjustment factors

In EFSA PPR Panel (2012), the assessment of the predefined scenarios for annual crops (95th spatial percentile of the concentration in total soil and soil pore water for the total area of annual crops in the EU), as well as the scenario adjustment factors (then called crop extrapolation factors), were based on the first release of a set of spatial data published in 2011, later referred to as the EFSA Spatial Data Version 1.0 (Hiederer, 2012). In 2012, the new release of the EFSA Spatial Data Version 1.1 was made available and published on the European Soil Portal of the EC JRC (http://eusoils.jrc.ec.europa.eu/library/data/efsa/).

Following the introduction of revised Tier-1 scenarios (refer to Appendix B), the working group reassessed the scenario adjustment factors, which are based on the 95th percentile crop ratio as follows:

$$\zeta = \frac{P_{95,x}}{P_{\mathrm{Tier1}}} \qquad \text{(C1)}$$

where $P_{95,x}$ is the spatial 95th percentile of the concentration for the area of crop x and P_{Tier1} is the PEC calculated at Tier-1 (calculated with the simple analytical model without any adjustment factors). Calculations were made with the simple analytical model including leaching for all CAPRI crops or crop groups that are in Tables 6 and 7. This was carried out for the standard substances 1–19 (refer to EFSA PPR Panel (2012) for substance properties) for all regulatory zones and for an evaluation depth z_{eco} of 1 and 20 cm considering the peak concentration only. Results are given in Tables C.1–C.4.

Table C.1: Minimum and maximum scenario adjustment factors for concentration in the total soil ($C_{T,peak}$) in annual crops based on the standards substances 1–19

CAPRI crop or crop group	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Cereals[(a)]	0.95	0.96	0.98	0.98	1.00	1.00	0.95	0.98	0.97	0.98	1.00	1.00
Fallow	1.01	1.01	1.00	1.01	0.98	0.98	1.01	1.02	0.99	1.01	0.93	0.98
Maize	0.72	0.75	0.88	0.91	0.99	0.99	0.63	0.75	0.73	0.91	0.95	0.99
Other fresh vegetables	0.97	0.98	0.93	0.95	0.93	0.95	0.97	0.98	0.82	0.95	0.74	0.95
Potatoes	0.93	0.93	1.01	1.01	1.03	1.04	0.93	0.96	0.99	1.01	1.03	1.06
Pulses	0.87	0.87	0.93	0.94	1.00	1.00	0.87	0.90	0.90	0.94	1.00	1.02
Rapes	0.93	0.93	0.93	0.94	1.02	1.03	0.93	0.95	0.93	0.97	1.02	1.05
Soya	NC	NC	0.84	0.87	0.83	0.86	NC	NC	0.64	0.87	0.53	0.86
Sugar beet	0.84	0.84	0.92	0.93	1.01	1.01	0.79	0.84	0.89	0.93	1.01	1.05
Sunflower	NC	NC	0.82	0.86	0.96	0.96	NC	NC	0.56	0.86	0.87	0.96
Texture crops	1.25	1.28	0.93	0.94	0.90	0.91	1.25	1.31	0.93	0.98	0.70	0.91
Tobacco	NC	NC	0.91	0.94	0.94	0.97	NC	NC	0.73	0.94	0.71	0.97

Max: maximum; Min: minimum; NC: no crop.
(a): Based on the combined crop area of barley, common wheat, durum wheat, oats and rye.

Table C.2: Minimum and maximum scenario adjustment factors for the concentration in the liquid phase ($C_{L,peak}$) in annual crops based on the standards substances 1–19

CAPRI crop or crop group	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Cereals[a]	1.02	1.04	0.95	1.00	0.92	1.00	1.00	1.04	0.96	1.02	0.92	1.04
Fallow	1.02	1.04	0.95	1.03	1.00	1.06	1.00	1.04	0.95	1.03	1.00	1.07
Maize	1.00	1.02	1.03	1.17	0.85	0.95	0.99	1.02	0.80	1.17	0.85	1.00
Other fresh vegetables	1.00	1.00	1.02	1.05	1.08	1.15	0.97	1.01	0.84	1.05	0.75	1.15
Potatoes	1.00	1.00	0.95	1.02	0.92	1.06	0.97	1.08	0.96	1.02	0.92	1.06
Pulses	0.96	1.00	0.95	0.98	0.98	1.00	0.95	1.00	0.95	1.02	0.98	1.08
Rapes	1.02	1.04	0.92	0.96	0.79	0.90	1.02	1.05	0.91	1.01	0.79	0.97
Soya	NC	NC	1.03	1.24	0.85	0.98	NC	NC	0.82	1.24	0.71	0.98
Sugar beet	1.02	1.04	1.00	1.05	0.85	0.97	0.99	1.04	1.00	1.05	0.85	0.98
Sunflower	NC	NC	1.03	1.24	0.95	1.00	NC	NC	0.76	1.24	0.95	1.02
Texture crops	0.62	0.77	0.95	0.97	1.01	1.10	0.62	0.84	0.95	1.01	1.01	1.10
Tobacco	NC	NC	1.02	1.05	0.91	1.10	NC	NC	0.74	1.05	0.63	1.10

Max: maximum; Min: minimum; NC: no crop.
(a): Based on the combined crop area of barley, common wheat, durum wheat, oats and rye.

Table C.3: Minimum and maximum scenario adjustment factors for concentration in the total soil ($C_{T,peak}$) in permanent crops based on the standards substances 1–19

Permanent crop	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Apples – between row	0.78	0.80	0.86	0.90	0.88	0.95	0.83	0.86	0.87	0.93	0.87	0.96
Apples – in row	0.78	0.80	0.86	0.90	0.58	0.95	0.83	0.86	0.87	0.93	0.64	0.96
Berries – between row	0.86	0.88	1.01	1.06	0.79	0.89	0.89	0.92	0.97	1.02	0.79	0.92
Berries – in row	0.86	0.88	0.80	1.02	0.56	0.89	0.89	0.92	0.87	1.02	0.62	0.92
Citrus – between row	NC	NC	NC	NC	0.58	0.74	NC	NC	NC	NC	0.57	0.83
Citrus – in row	NC	NC	NC	NC	0.43	0.79	NC	NC	NC	NC	0.43	0.84
Hops – between row	NC	NC	0.68	0.77	0.94	0.98	NC	NC	0.83	0.89	1.05	1.11
Hops – in row	NC	NC	0.84	0.87	1.09	1.15	NC	NC	0.86	0.91	1.06	1.14
Olives – between row	NC	NC	NC	NC	0.54	0.76	NC	NC	NC	NC	0.58	0.85
Olives – in row	NC	NC	NC	NC	0.40	0.76	NC	NC	NC	NC	0.46	0.85
Permanent grass	0.97	0.97	1.10	1.17	1.16	1.24	0.98	0.99	1.07	1.14	1.13	1.35
Vines – between row	NC	NC	0.60	0.74	0.67	0.82	NC	NC	0.73	0.86	0.74	0.91
Vines – in row	NC	NC	0.59	0.83	0.55	0.89	NC	NC	0.67	0.88	0.60	0.92

Max: maximum; Min: minimum; NC: no crop.

Table C.4: Minimum and maximum scenario adjustment factors for concentration in the liquid phase ($C_{L,peak}$) in permanent crops based on the standards substances 1–19

Permanent crop	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Apples – between row	0.97	1.04	1.00	1.05	1.04	1.13	1.01	1.11	0.97	1.04	1.03	1.09
Apples – in row	0.97	1.04	1.00	1.05	0.89	1.10	1.01	1.11	0.97	1.04	0.61	1.08
Berries – between row	0.98	1.04	0.85	0.96	0.98	1.12	1.02	1.12	0.84	0.99	0.93	1.17
Berries – in row	0.98	1.04	0.75	0.91	0.83	1.12	1.02	1.12	0.76	0.92	0.66	1.17
Citrus – between row	NC	NC	NC	NC	1.20	1.53	NC	NC	NC	NC	1.10	1.21
Citrus – in row	NC	NC	NC	NC	0.90	1.10	NC	NC	NC	NC	0.68	1.08
Hops – between row	NC	NC	1.04	1.13	0.80	0.87	NC	NC	0.92	1.00	0.67	0.91
Hops – in row	NC	NC	0.91	0.94	0.65	0.77	NC	NC	0.89	0.98	0.64	0.88
Olives – between row	NC	NC	NC	NC	1.26	1.56	NC	NC	NC	NC	1.08	1.29
Olives – in row	NC	NC	NC	NC	1.26	1.56	NC	NC	NC	NC	0.75	1.29
Permanent grass	0.91	0.96	0.67	0.78	0.73	0.86	0.92	0.98	0.64	0.80	0.70	0.93
Vines – between row	NC	NC	1.16	1.47	1.17	1.45	NC	NC	1.04	1.20	1.09	1.17
Vines – in row	NC	NC	0.93	1.17	0.90	1.09	NC	NC	0.80	1.14	0.67	1.08

Max: maximum; Min: minimum; NC: no crop.

In line with the approach taken in EFSA PPR Panel (2012), the working group proposes to use the maximum of the values in Tables C.1–C.4 to be used as scenario adjustment factor in Tier-1 for all regulatory zones (Table C.5).

Table C.5: Ranges (and final values) of the new scenario adjustment factors for annual and permanent crops for the three regulatory zones and for both the concentration in total soil ($C_{T,peak}$) and the concentration in the liquid phase ($C_{L,peak}$)

	Scenario adjustment factor[(a)]			
	$C_{T,peak}$		$C_{L,peak}$	
	Min	Max	Min	Max
North	0.63	1.31	0.62	1.12
Centre	0.56	1.17	0.64	1.47
South	0.40	1.35	0.61	1.56
Final[(b)]	–	**1.40**	–	**1.60**

(a): Based on the standard substances 1–19.
(b): Rounded up to ensure consistency in the tiered approach.

C.2. Derivation of model adjustment factors

The model adjustment factors (f_M), as derived in EFSA PPR Panel (2012), were based on simulations with PEARL for 19 substances. In these simulations, only *DegT50* and K_{om} were changed. However, at Tier-3A, users have to apply other substance properties, such as the Freundlich adsorption coefficient (*1/n*), the transpiration stream concentration factor (*TSCF*) or the vapour pressure. Changing these parameters may affect the model adjustment factors because it cannot *a priori* be guaranteed that the predicted concentrations are lowered by changing these parameters. In addition, a leaching term (k_{leach}) was added to the analytical model which was not considered for in EFSA PPR Panel (2012) as well.

To investigate the effect on the model adjustment factors of both the additional substance properties in the numerical models, and the leaching term, a comparative assessment applying PERSAM and PEARL was carried out. To ensure maximum concentrations in the numerical model for both the total soil and the pore water, the *TSCF* and the vapour pressure were set to zero. As the impact of *1/n* on the concentration is not unambiguous, two runs were performed with *1/n* set to either 0.7 or 1.0. This range is based on Boesten et al. (2012).

To cover a wide range of possible crop/tillage/location settings, calculations were performed for winter cereals, tomatoes, apples (in-row), apples (between-row, grass modelled) and vines (between-row, bare soil modelled). The application rate was set to 1 kg/ha applied 1 day before emergence (annual crops) or on 1 May (permanent crops) each year. In a second set of calculations, multiple applications (five times 1 kg/ha with an interval of 14 days) starting 1 day before emergence (annual crops) or on 1 May (permanent crops) were applied. Application was done to the soil surface.

Results are given for the peak as well as for the 56-day TWA concentration applying an ecotoxicological averaging depth of 1, 5 and 20 cm (C.1–C.4).

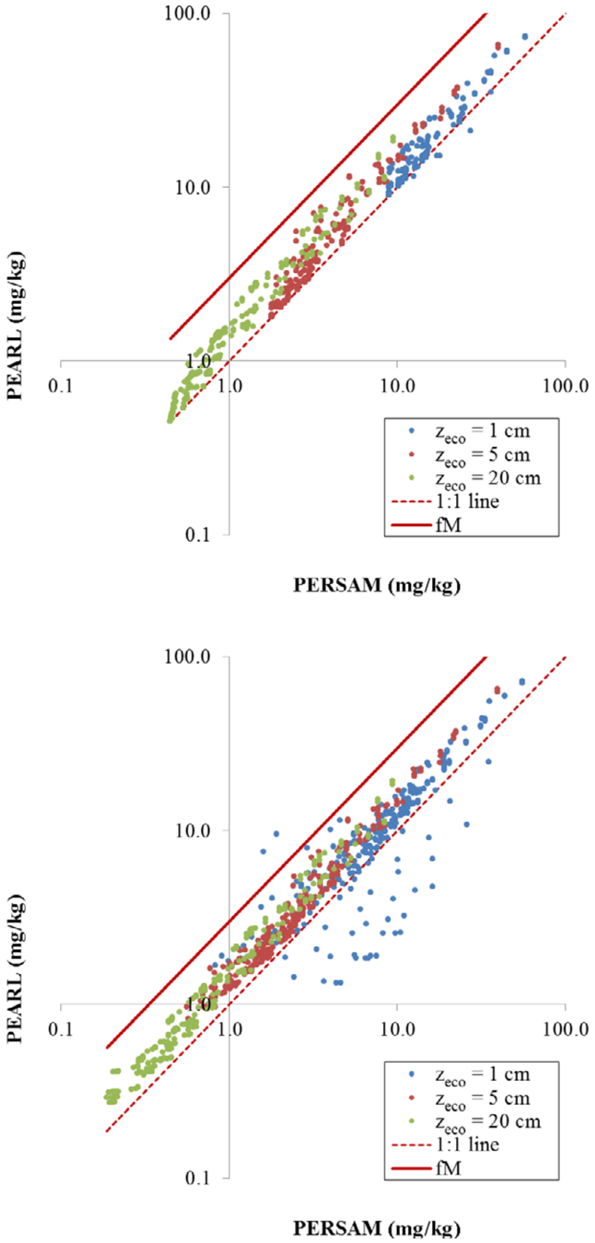

Figure C.1: Concentration in the total soil for PERSAM vs PEARL following a single application of 1 kg/ha covering a wide range of possible crop/tillage/location settings (refer to text). Top: peak concentration, bottom: 56-day TWA concentration, left: *1/n* = 0.7, right: *1/n* = 1.0. Model adjustment factor (f_M) set to 3

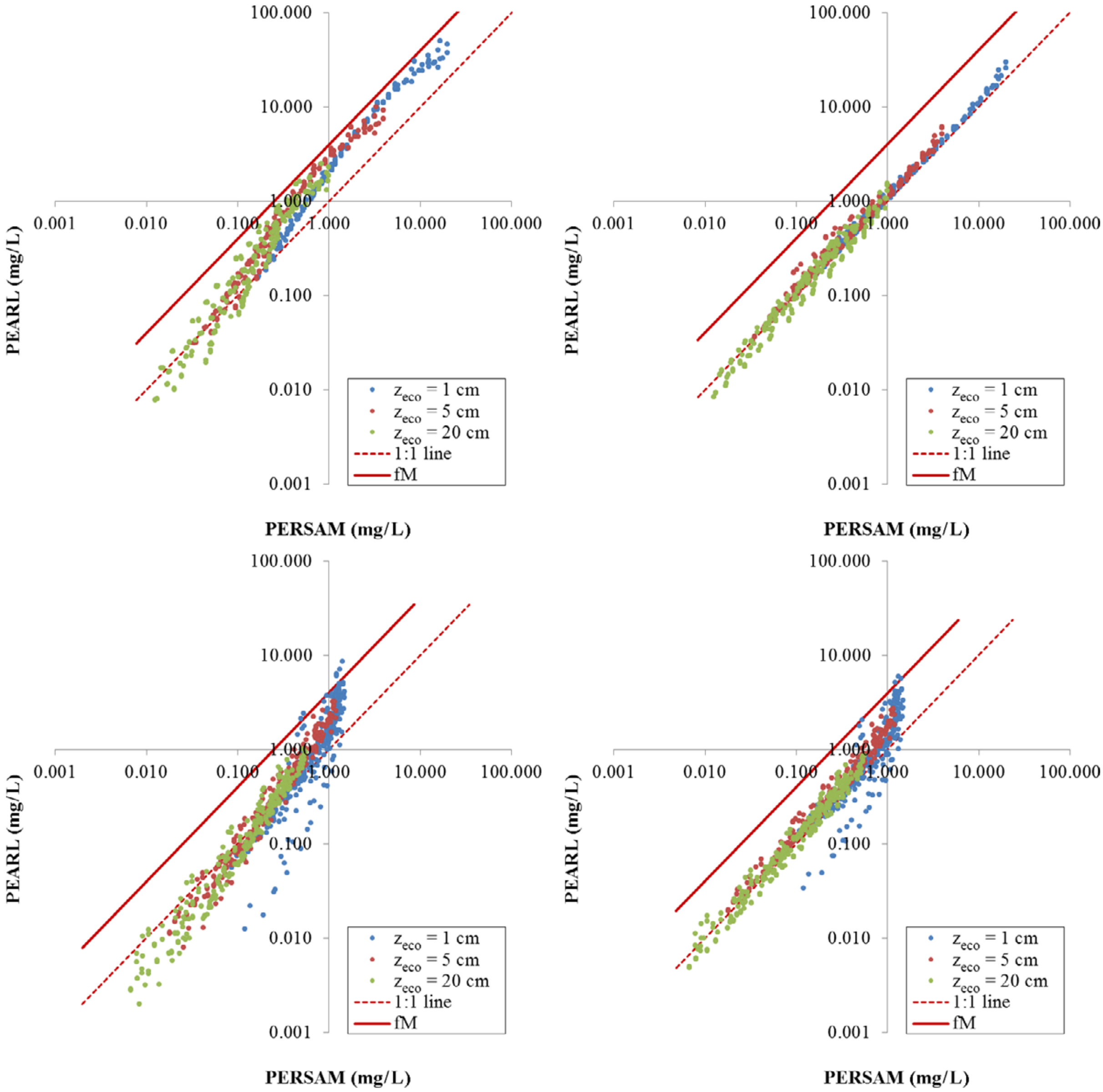

Figure C.2: Concentration in the soil pore water for PERSAM vs PEARL following a single application of 1 kg/ha covering a wide range of possible crop/tillage/location settings (refer to text). Top: peak concentration, bottom: 56-day TWA concentration, left: *1/n* = 0.7, right: *1/n* = 1.0. Model adjustment factor (f_M) set to 4

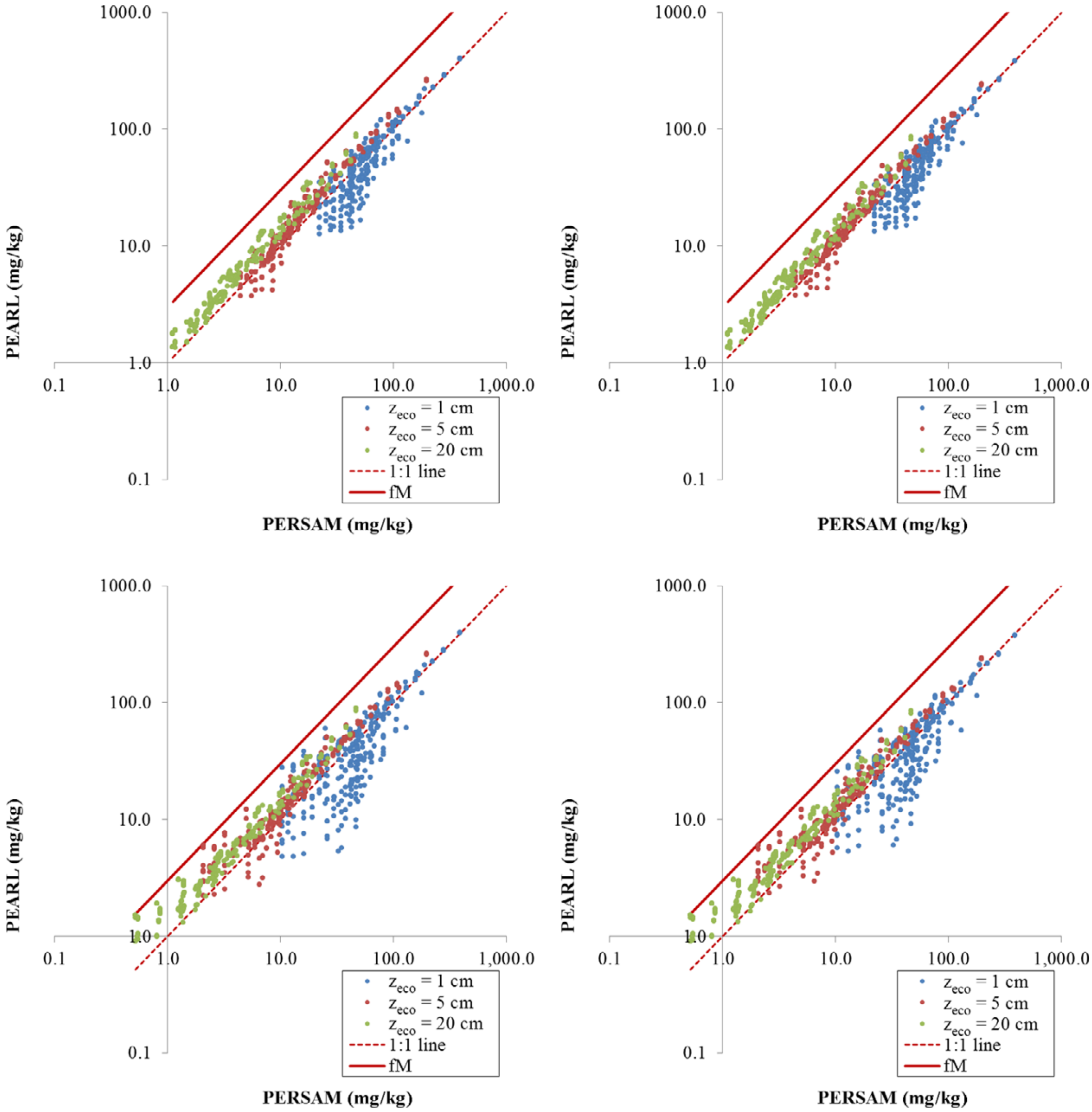

Figure C.3: Concentration in the total soil for PERSAM vs PEARL following a multiple application of 1 kg/ha (5 times, 14-day interval) covering a wide range of possible crop/tillage/location settings (refer to text). Top: peak concentration, bottom: 56-day TWA concentration, left: $1/n$ = 0.7, right: $1/n$ = 1.0. Model adjustment factor (f_M) set to 3

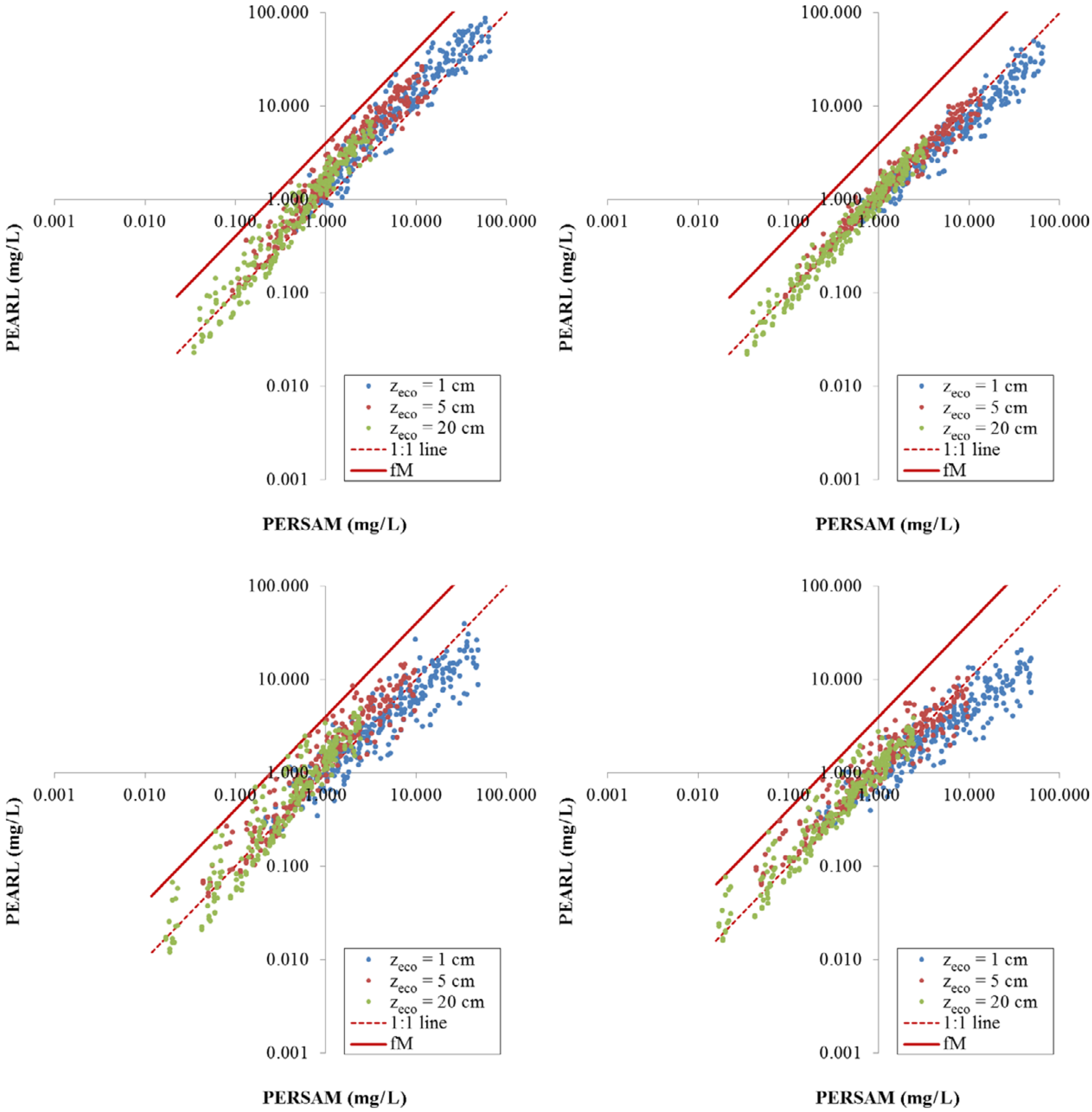

Figure C.4: Concentration in the soil pore water for PERSAM versus PEARL following a multiple application of 1 kg/ha (five times, 14-day intervals) covering a wide range of possible crop/tillage/location settings (refer to text). Top: peak concentration, bottom: 56-day TWA concentration, left: *1/n* = 0.7, right: *1/n* = 1.0. Model adjustment factor (f_M) set to 4

As can be concluded from this modelling exercise, differences between PERSAM and PEARL may be considerable for the top 1-cm soil layer. Differences are smaller for the top 5 and 20 cm. Differences are also higher for the 56-day TWA than for the peak concentration and for *1/n* values of 0.7 compared with *1/n* values of 1.0.

Based on these findings, it is proposed to apply a default model adjustment factor (f_M) of 3 for the concentration in the total soil and a default model adjustment factor of 4 for the concentration in the pore water.

As can be seen in Figures C.1–C.4, there are some rare situations (2 for total soil and 11 for pore water concentration out of 3,192 calculations each) still exceeding these default model adjustment factors. A closer inspection of the data revealed that this happened in the following situations:

- 56-day TWA concentration in total soil, standard substances 1 and 2, apples (between-row exposure), Southern zone, z_{eco} = 1 cm;

- 56-day TWA concentration in the pore water, standard substances 1 and 2, apples (between-row exposure), Southern zone, z_{eco} = 1, 5, and 20 cm;
- 56-day TWA concentration in the pore water, standard substances 1 and 2, apples (in-row exposure), Southern zone, z_{eco} = 1;
- 56-day TWA concentration in the pore water, standard substances 1, 2 and 6, winter cereals, Centre and Southern zone, z_{eco} = 1 and 20 cm.

No exceedance of the suggested default model adjustment factors was observed in the case of the peak concentration. In view of these rare exceedances at rather extreme conditions, the default model adjustment factors as proposed above are considered justifiable.

Notice that this comparison did not take into account multiple applications in winter and early spring as these applications are not considered that often to occur. As PERSAM applies, the annual average temperature for degradation all over the year the model will overestimate degradation in periods with daily temperatures below the annual average temperature. For multiple applications in December, January and February, it is therefore recommended to directly move to Tier-3A using Tier-2 for selection of the location only.

Appendix D – The fraction of the dose reaching the soil for Tier-2 assessments

D.1. Introduction

Since the introduction of the FOCUS groundwater scenarios in 2001, it has been common practice in the leaching assessment at the EU level to use the FOCUS interception tables to correct the dosage that reaches the soil surface. It was assumed that all intercepted substances will dissipate on the plant surface and will so never reach the soil. EFSA PPR Panel (2012) considered this approach not defensible and proposed to use, as defaults in the exposure assessment, a wash-off factor of 0.1/mm and a half-life of 10 days for the decline of dislodgeable foliar residue on plants. Crop canopy processes and foliar wash-off can be simulated by PEARL and PELMO. However, for Tier-2, this would require running one of the numerical models before running PERSAM. For this reason, tables of default wash-off fractions from the crop canopy were created. This was carried out by calculating this fraction for all relevant crop–location combinations with PEARL and PELMO with the intention to use the average result in the form of a table similar to the EFSA crop interception tables. The calculation procedure was as follows:

- Runs were made with one application per year, so the simulation time was 26 years of which the last 20 years were evaluated.
- At the application time, a dose of 1 kg/ha was applied to the plant surface.
- For each year, the annual wash-off (kg/ha) was calculated using a wash-off factor of 0.1 mm^{-1} and a half-life of 10 days for the decline of dislodgeable foliar residue on plants, and this annual wash-off was transformed into an annual fraction washed off (division by 1 kg/ha).

Calculations were made with PEARL and PELMO with applications on the 5th, 15th and 25th day of each month. Calculations were made only for periods when a crop was present.

The results in the wash-off tables are based on absolute application dates. The EFSA crop interception tables are based on crop development stages using so-called BBCH codes (Meier, 2001). How these two tables are linked is described in Section D.4.

D.2. How to deal with differences in wash-off between the 20 years?

The above-mentioned runs provided 20 fractions washed off, each corresponding to a different year over 20 years. It is a point of debate whether the correction of the FOCUS interception tables should be based on the maximum of these 20 fractions or on the average fraction. To explore the consequences of these two options, scenario calculations were made with PEARL for the scenario annual crops for concentration in total soil in zone north. (ACTN)[10] sugar beets, substance P3 (*DegT50* = 200 days, K_{om} = 1,000 L/kg), annual application of 1 kg/ha on 25 August (a simulation period of 26 years) and ecotoxicological averaging depths of 1 and 20 cm. The interception (according to the FOCUS interception table) was 90%. The PEARL wash-off calculations for this scenario, as described above, showed that the average annual wash-off fraction was 0.639 and that the maximum annual wash-off was 0.974.

Subsequently, three types of PEARL calculations were made and results compared:

- Annual application of 0.1 kg/ha to the soil, 0.9 kg/ha on the crop and simulation of wash-off by PEARL using the wash-off factor of 0.1/mm and a half-life of 10 day for the decline on plants; this calculation is referred to as 'simulated wash-off'.
- Annual application of 0.675 kg/ha to the soil surface, corresponding with the annual average wash-off fraction; this calculation is referred to as 'average wash-off'.
- Annual application of 0.977 kg/ha to the soil surface, corresponding with the maximum annual wash-off fraction; this calculation is referred to as 'maximum wash-off'.

The calculation of these soil loads of 0.675 and 0.977 kg/ha was based on the equation:

$$A_{soil} = ((1 - f_i) + f_i f_w)A \qquad \text{(D1)}$$

where A_{soil} is the soil load (kg/ha), A is the dosage (kg/ha), f_i is the fraction of the dose that is intercepted by the crop (–) and f_w is the fraction (–) washed off.

[10] ACTN is a historical scenario (EFSA, 2015b).

The time course for the concentration in total soil averaged over the top 20 cm in Figure D.1 shows that use of the average wash-off fraction leads to a time course that is close to the PEARL run in which the plant processes were simulated. Use of the maximum wash-off fraction resulted in a considerable overestimation of the plateau value, which is the result of assuming that the maximum wash-off occurs every year.

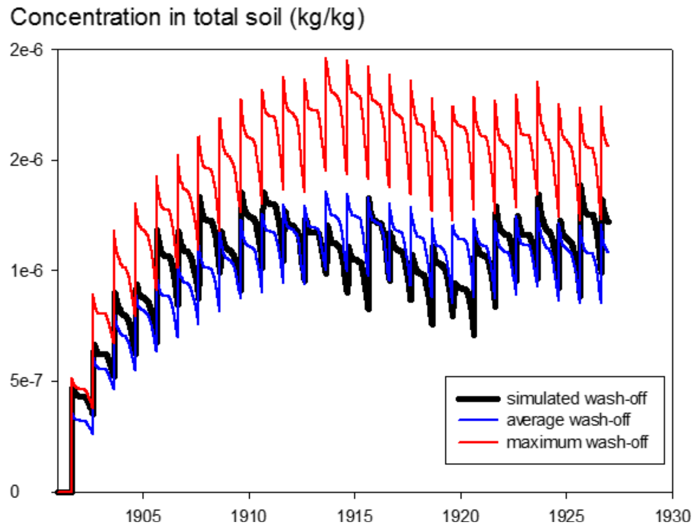

Figure D.1: Concentration in total soil (average over top 20 cm) as a function of time as calculated with PEARL for the scenario ACTN and sugar beets, substance P3 (*DegT50* = 200 days, K_{om} = 1,000 L/kg), annual application of 1 kg/ha on 25 August for the three types of PEARL calculations as indicated in the graph

The results for the concentration in total soil in the top 1 cm (Figure D.2) are different from those of the top 20 cm. In this case, the annual fluctuations dominate the time course of the concentration and the background plateau level does not play a role. Because the end-point of the simulation is the maximum value over the whole simulation period, use of the maximum wash-off leads to a good correspondence with run with the simulated wash-off and use of the average wash-off leads to an underestimation. The pattern, as shown in Figure D.2, is probably representative for this scenario when ecotoxicological averaging depths deeper than 1 cm are considered for substances that do not accumulate.

The results of the PEARL run with the simulated plant processes (Figure D.2) show that the annual peak concentrations vary by a factor near to 3. Comparison of the different runs in Figure D.2 indicates that this variation is mainly caused by the differences in the wash-off from year to year. In the scenario selection procedure for the exposure assessment of soil organisms by EFSA PPR Panel (2012) it was assumed appropriate to use a 100th percentile of the concentration in time based on the assumption that there would be only small differences between peak concentrations between different years (EFSA PPR Panel, 2012, p. 31). The line for the simulated wash-off in Figure D.2 shows that this is not the case for this scenario for the concentration in total soil in the North Zone when combinations of substances and ecotoxicological averaging depths are considered that do not lead to accumulation. So, for uses that lead to a high fraction intercepted by the crop, the exposure assessment goal of an overall 90th percentile, in principle, should have led to a scenario selection procedure that included the wash-off process. However, such a procedure is, as yet, impossible given the limited knowledge on the processes that determine the wash-off (see EFSA PPR Panel, 2012). Moreover, it would also have made the exposure assessment overly complicated because then different approaches would be needed for uses with low and high crop interception.

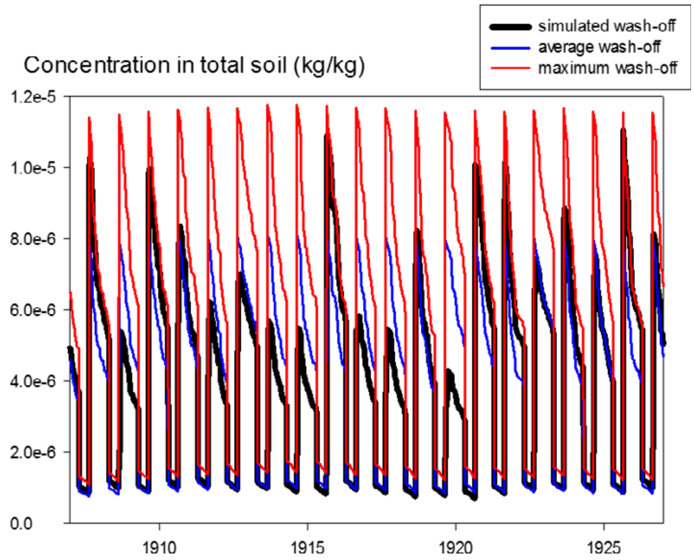

Figure D.2: Concentration in total soil (average over top 1 cm) as a function of time as calculated with PEARL for the scenario ACTN and sugar beets, substance P3 (*DegT50* = 200 days, K_{om} = 1,000 L/kg), annual application of 1 kg/ha on 25 August for the three types of PEARL calculations as indicated in the graph

In view of the foregoing, and because the wash-off factor of 0.1/mm is considered a conservative default value (EFSA PPR Panel, 2012), it is proposed to base the approach on the annual average wash-off fraction; so the maximum annual wash-off will not be considered.

D.3. Fraction of the dose reaching the soil calculated with PEARL and PELMO

Reinken et al. (2013) identified significant differences between PEARL and PELMO with respect to the parameterisation of wash-off calculations. The working group analysed these differences and concluded that these were primarily caused by differences in the calculation of the fraction of the surface area of the soil covered by the crop, i.e. SC. It is assumed that the fraction of the dose intercepted by the crop equals SC. The description of crop development was therefore harmonised.[11] In both PEARL and PELMO, it is now assumed that the LAI increases linearly between emergence date and the date at which the maximum LAI occurs. Furthermore, it was decided to base the soil cover needed in the wash-off calculations on Beer's law:

$$SC = 1 - e^{-\kappa LAI} \tag{D2}$$

in which κ is the extinction coefficient for diffuse solar radiation (set to 0.39 based on Kroes et al., 2008). Following harmonisation, differences between PEARL and PELMO are small, generally, indicating that the harmonisation process has been successful.

D.4. Development of the table for the fraction washed off

The regulatory exposure assessment should consider the worst-case fraction of the dose that reaches the soil (f_{soil}) for each crop. This fraction considers crop interception at the time of application as well as wash-off in the following days (where the latter is affected, of course, by dissipation processes at the plant canopy). Default wash-off fractions for use in Tier-2 were calculated with PEARL and PELMO following the recommendations in EFSA PPR Panel (2012) (i.e. using a default wash-off factor of 0.1/mm and a half-life of 10 days for the decline of pesticide residues on plants).

The wash-off factors from the crop canopy were based on calculations with PEARL and PELMO over 26 years, of which the last 20 years were used considering annual applications for every scenario–crop

[11] Note amendments were made to the senescence dates of the crop onions at the scenarios Thiva (21/6) and Porto (21/5) compared with that published in generic guidance for Tier-1 FOCUS groundwater assessments (Anonymous, 2014), as before amendment, the date of senescence was before that of maximum LAI.

combination. For each of these scenarios, 36 simulations were performed with different application dates (always on the 5th, 15th or 25th day of every month). For sake of simplicity, it was assumed that crop interception was 100%. As PELMO considers harvesting of crops and application of pesticide to crops with different sequences, simulations were not carried out for those situations where application would be on the date of harvest.

The wash-off fraction was calculated based on the average wash-off in PEARL and PELMO for the last 20 years of the simulations (see Section D.2 for a justification for taking the average wash-off fraction).

To combine these wash-off fractions with reasonable crop interception values, all application dates had to be linked to BBCH crop stages (Meier, 2001). Gericke et al. (2010) found a linear relationship between date and the BBCH code for annual crops. This implies that it is justifiable to use linear interpolation starting at the date of emergence (BBCH 09) and ending at the date of harvest (i.e. BBCH 99 in the case of annual crops or BBCH 50 in the case of crops harvested at BBCH 50, such as onions, sugar beet, or cabbage). However, to improve the link for winter crops with dormancy shortly after emergence, BBCH stage 19 was attached to the spring point, which gives two separate linear phases (i.e. BBCH 09–19 and 20–99 or 20–50, respectively). For consistency reasons, a linear relationship between the date and the BBCH code was applied for permanent crops as well, starting from first leaf development (BBCH 09) to start of senescence (BBCH 89).

In case of evergreen permanent crops (citrus and olives) as well as permanent grass (established turf), crop interception is considered the same all year round (EFSA, 2014a). To account for seasonal variability in wash-off fractions due to seasonal changes in rainfall patterns four wash-off periods (January–March, April–June, July–September and October–December) were defined for these evergreen crops.

For spray applications onto crops without leaves (during autumn and winter), a special procedure had to be developed because the LAI is zero or very low, so the SC from Equation D2 would become zero and PEARL and PELMO would simulate no wash-off of water and substance. This was solved in PEARL by specifying a minimum SC that corresponded to the crop interception percentages for apples, bush berries and vines without leaves as specified in Appendix C of EFSA (2014a), so 0.5 for apples and 0.4 for bush berries and vines. For hops, the same value as for vines was used (0.4). In PELMO, a similar procedure was followed but based on specifying a minimum LAI that was calculated back from Equation D2 based on these minimum SC values.

Average wash-off fractions from the canopy (f_w) for predefined BBCH periods considering canopy dissipation processes as a function of crop development stage are given in Tables D.1 and D.2. In PERSAM, the dose that reaches the soil (f_{soil}) following an application to the crop canopy is finally calculated according to Equation A1. Notice that the user only has to specify the crop interception according to EFSA (2014a) and the BBCH code for each individual application. PERSAM internally looks for the correct default wash-off value to apply.

Table D.1: Average foliar wash-off fraction (f_w) considering canopy crop processes as a function of crop development stage for annual crops. Calculations were done for the dominant FOCUS zone and final (default) figures are the maximum of the three regulatory zones rounded to the next higher 0.05

Crop	Regulatory zone	Dominant FOCUS zone	Scenario for crop parameters	BBCH code[(a),(b)]				
				00–09	**10–19**	**20–39**	**40–89**	**90–99**
Beans (vegetable and field)	North	HA	HA (fields)	na	0.35	0.46	0.62	0.31
	Centre	CH	HA (fields)	na	0.44	0.71	0.76	0.23
	South	HA	TH (veg.), 1st	na	0.44	0.53	0.55	0.10
		HA	TH (veg.), 2nd	na	0.57	0.61	0.61	0.30
	Max. (rounded)			**na**	**0.60**	**0.75**	**0.80**	**0.35**
Cabbage[(c)]	North	HA	HA, 1st	na	0.42	0.56	0.36	na
		HA	HA, 2nd	na	0.50	0.59	0.39	na
	Centre	CH	CH, 1st	na	0.55	0.68	0.31	na
		CH	CH, 2nd	na	0.55	0.69	0.38	na
	South	SE	SE, 1st	na	0.41	0.69	0.18	na
		SE	SE, 2nd	na	0.59	0.79	0.31	na
	Max. (rounded)			**na**	**0.60**	**0.80**	**0.40**	**na**
Carrots[(c)]	North	HA	HA, 1st	na	0.51	0.52	0.36	na
		HA	HA, 2nd	na	0.53	0.60	0.49	na
	Centre	CH	CH, 1st	na	0.52	0.61	0.48	na
		CH	CH, 2nd	na	0.59	0.62	0.36	na
	South	SE	TH, 1st	na	0.66	0.68	0.25	na
		SE	TH, 2nd	na	0.72	0.81	0.11	na
	Max. (rounded)			**na**	**0.75**	**0.85**	**0.50**	**na**
Cotton	Centre	HA	TH	na	0.46	0.60	0.63	0.45
	South	TH	TH	na	0.61	0.72	0.39	0.05
	Max. (rounded)			**na**	**0.65**	**0.75**	**0.65**	**0.45**
Linseed	North	HA	OK	na	0.31	0.46	0.60	0.27
	Centre	HA	OK	na	0.31	0.46	0.60	0.27
	South	SE	OK	na	0.51	0.72	0.59	0.08
	Max. (rounded)			**na**	**0.55**	**0.75**	**0.60**	**0.30**
Maize	North	HA	HA	na	0.36	0.54	0.62	0.52
	Centre	CH	CH	na	0.41	0.62	0.70	0.48
	South	HA	HA	na	0.36	0.54	0.62	0.52
	Max. (rounded)			**na**	**0.45**	**0.65**	**0.70**	**0.55**
Onions[(c)]	North	HA	HA	na	0.41	0.60	0.53	na
	Centre	HA	HA	na	0.41	0.60	0.53	na
	South	SE	TH	na	0.57	0.75	0.43	na
	Max. (rounded)			**na**	**0.60**	**0.75**	**0.55**	**na**
Peas	North	HA	HA	na	0.35	0.46	0.62	0.31
	Centre	CH	CH	na	0.36	0.56	0.54	0.20
	South	HA	HA	na	0.35	0.46	0.62	0.31
	Max. (rounded)			**na**	**0.40**	**0.60**	**0.65**	**0.35**
Potatoes	North	HA	HA	na	0.30	0.50	0.59	0.33
	Centre	HA	HA	na	0.30	0.50	0.59	0.33
	South	HA	HA	na	0.30	0.50	0.59	0.33
	Max. (rounded)			**na**	**0.30**	**0.50**	**0.60**	**0.35**

Crop	Regulatory zone	Dominant FOCUS zone	Scenario for crop parameters	BBCH code[(a),(b)]				
				00–09	10–19	20–39	40–89	90–99
Oil seed rape (summer)	North	HA	OK	na	0.37	0.49	0.60	0.47
	Centre	HA	OK	na	0.37	0.49	0.60	0.47
	South	HA	OK	na	0.37	0.49	0.60	0.47
	Max. (rounded)			**na**	**0.40**	**0.50**	**0.60**	**0.50**
Oil seed rape (winter)	North	HA	HA	na	0.09	0.40	0.52	0.28
	Centre	HA	HA	na	0.09	0.40	0.52	0.28
	South	HA	HA	na	0.09	0.40	0.52	0.28
	>**Max. (rounded)**			**na**	**0.10**	**0.40**	**0.55**	**0.30**
Sugar beets[(c)]	North	HA	HA	na	0.40	0.60	0.57	na
	Centre	HA	HA	na	0.40	0.60	0.57	na
	South	HA	HA	na	0.40	0.60	0.57	na
	Max. (rounded)			**na**	**0.40**	**0.60**	**0.60**	**na**
Soybeans	North	HA	PI	na	0.43	0.62	0.64	0.27
	Centre	CH	PI	na	0.53	0.72	0.76	0.32
	South	TH	PI	na	0.52	0.72	0.74	0.13
	Max. (rounded)			**na**	**0.55**	**0.75**	**0.80**	**0.35**
Strawberries	North	HA	HA	na	0.46	0.49	0.57	0.46
	Centre	CH	HA	na	0.50	0.66	0.70	0.33
	South	SE	SE	na	0.47	0.56	0.73	0.07
	Max. (rounded)			**na**	**0.50**	**0.70**	**0.75**	**0.50**
Sunflowers	North	JO	PI	na	0.36	0.50	0.63	0.50
	Centre	CH	PI	na	0.58	0.72	0.78	0.37
	South	HA	PI	na	0.40	0.55	0.62	0.51
	Max. (rounded)			**na**	**0.60**	**0.75**	**0.80**	**0.55**
Tobacco	Centre	CH	PI	na	0.51	0.70	0.77	0.30
	South	SE	TH	na	0.44	0.73	0.80	0.82
	Max. (rounded)			**na**	**0.55**	**0.75**	**0.80**	**0.85**
Tomatoes	North	HA	CH	na	0.42	0.59	0.64	0.33
	Centre	CH	CH	na	0.55	0.70	0.67	0.25
	South	SE	SE	na		0.71	0.46	0.04
	Max. (rounded)			**na**	**0.55**	**0.75**	**0.70**	**0.35**

Crop				BBCH code[(d)]						
				00–09	10–19	20–29	30–39	40–69	70–89	90–99
Spring cereals	North	HA	HA	na	0.36	0.50	0.50	0.61	0.62	0.51
	Centre	CH	CH	na	0.40	0.47	0.45	0.60	0.55	0.28
	South	HA	HA	na	0.36	0.50	0.50	0.61	0.62	0.51
	Max. (rounded)			**na**	**0.40**	**0.50**	**0.50**	**0.65**	**0.65**	**0.55**
Winter cereals	North	HA	HA	na	0.09	0.33	0.44	0.55	0.56	0.38
	Centre	CH	CH	na	0.08	0.38	0.58	0.55	0.53	0.23
	South	HA	HA	na	0.09	0.33	0.44	0.55	0.56	0.38
	Max. (rounded)			**na**	**0.10**	**0.40**	**0.60**	**0.55**	**0.60**	**0.40**

na denotes not applicable (no crop canopy present).
(a): The BBCH code is a decimal code ranging from 0 to 99 to characterise the crop development stage (Meier, 2001).
(b): BBCH 00–09: bare to emergence; BBCH 10–19: leaf development; BBCH 20–39: stem elongation; BBCH 40–89: flowering; BBCH 90–99: senescence and ripening.
(c): These crops are harvested at BBCH 50 and therefore the value 0 should be used for crop stage 50–99.
(d): BBCH 00–19: bare to leaf development; BBCH 20–29: tillering; BBCH 30–39: stem elongation; BBCH 40–69: flowering; BBCH 70–99: senescence and ripening.

Table D.2: Average foliar wash-off fraction (f_w) considering canopy crop processes as a function of crop development stage or season. Calculations are done for the dominant FOCUS zone and final (default) figures are the maximum of the three regulatory zones rounded to the next higher 0.05

Crop	Regulatory zone	Dominant FOCUS zone	Crop parameter	BBCH code			
				00–09[(a)]	10–69	71–75	76–89
Apples	North	HA	HA	0.52	0.59	0.59	0.52
	Centre	HA	HA	0.52	0.59	0.59	0.52
	South	SE	SE	0.42	0.21	0.20	0.37
	Max. (rounded)			**0.55**	**0.60**	**0.60**	**0.55**

Crop	Regulatory zone	Dominant FOCUS zone	Crop parameter	BBCH code		
				00–09[(a)]	10–69	71–89
Bush berries	North	HA	HA	0.48	0.58	0.54
	Centre	CH	CH	0.45	0.53	0.51
	South	SE	SE	0.39	0.21	0.31
	Max. (rounded)			**0.50**	**0.60**	**0.55**
Hops	Centre	HA	HA	0.48	0.52	0.56
	South	HA	HA	0.48	0.52	0.56
	Max. (rounded)			**0.50**	**0.55**	**0.60**

Crop	Regulatory zone	Dominant FOCUS zone	Crop parameter	BBCH code				
				00–09[(a)]	11–13	14–19	53–69	71–89
Vines	Centre	CH	CH	0.45	0.37	0.46	0.55	0.60
	South	SE	SE	0.38	0.35	0.35	0.17	0.46
	Max. (rounded)			**0.45**	**0.40**	**0.50**	**0.55**	**0.60**

Crop	Regulatory zone	Dominant FOCUS zone	Crop parameter	Season			
				Jan–Mar	Apr–Jun	Jul–Sep	Oct–Dec
Citrus	South	SE	SE	0.48	0.29	0.15	0.51
	Max. (rounded)			**0.50**	**0.30**	**0.15**	**0.55**
Olives	South	SE	SE	0.45	0.27	0.14	0.48
	Max. (rounded)			**0.50**	**0.30**	**0.15**	**0.50**
Permanent grass	North	HA	HA	0.43	0.54	0.54	0.46
	Centre	HA	HA	0.43	0.54	0.54	0.46
	South	HA	HA	0.43	0.54	0.54	0.46
	Max. (rounded)			**0.45**	**0.55**	**0.55**	**0.50**
Grass between rows	North	HA	HA	0.43	0.54	0.54	0.46
	Centre	CH	CH	0.40	0.53	0.50	0.43
	South	SE	SE	0.40	0.25	0.13	0.40
	Max. (rounded)			**0.45**	**0.55**	**0.55**	**0.50**

(a): Without leaves.

Appendix E – Non-uniform application (row, band, strip and spot applications) in annual crops in the numerical models

If non-uniform treatments are applied, this should be indicated in the GAP table including the fraction of the area treated ($f_{treated}$).

As described in Appendix A.2, two types of concentrations may be needed in the case of non-uniform treatments in annual crops, i.e. (i) the concentration in the non-treated area (e.g. between the treated rows); and (ii) the concentration in the treated area (e.g. in the treated rows). This appendix describes how the refined exposure-assessment procedure for annual crops is being incorporated into the numerical models.

It is assumed that the maximum concentration in the non-treated area equals the plateau concentration in the treated area (see Equation A16). In the numerical models, this plateau concentration will be reached directly before the application causing the maximum concentration in time. This concentration needs to be calculated by the model. The concentration in the treated area needs to be calculated according to an equation akin to Equation A17. So for the plateau concentration, the models should use the corrected dose A_{year} $f_{treated}$, and for the application causing the highest concentration, the models should use the normal dose A_{year}. The problem with this calculation is that the year that the maximum concentration occurs is not known *a priori*.

The solution to this problem is to do a normal calculation with the numerical models (using the dose expressed per hectare of treated soil, so A_{year}) and to multiply the so obtained PECs with a refinement factor derived from calculations with PERSAM. This refinement factor is defined by the ratio of the concentrations of the non-uniform and uniform concentrations:

$$f_{ref} = \frac{C_{T,treated}}{C_{T,treated,uniform\_application}} = \frac{\frac{z_{eco}}{z_{til}}\frac{X}{1-X}f_{treated} + 1}{\frac{z_{eco}}{z_{til}}\frac{X}{1-X} + 1} \quad \text{(E1)}$$

where $C_{T,treated}$ (mg/kg) is the maximum concentration in the treated area, $C_{T,treated,uniform\_application}$ (mg/kg) is the maximum concentration in the treated area assuming uniform application, $f_{treated}$ (–) is the fraction of the soil treated and $C_{T,ini}$ (mg/kg) is the initial concentration in total soil directly after application as calculated with Equation A1.

A more sophisticated alternative to the refinement above would be to run the numerical models two times:

- In the first run, the model is run using the dose averaged over the whole field ($f_{treated}$ A_{year}) and the year that the maximum concentration occurs is extracted from the output (the models already give this output).
- In the second run, the model uses the normal dose (i.e. A_{year} expressed in kg per hectare treated soil) for all applications in the year that the maximum concentration is reached. The peak concentration needed in the exposure assessment is then the maximum concentration for this year.

The procedures in this Appendix can be combined with the solution for the rapidly dissipating fraction of Appendix F, provided that first the calculation procedure for this rapidly dissipating fraction is carried out and thereafter the procedure described here.

The approach described above for the concentration in the treated area is considered a conservative approach for spot applications in annual crops because it might be assumed that spot applications take place on less than 10% of the surface area of the treated field. Therefore, the probability is low that a certain spot will be treated in the subsequent 2 years.

Appendix F – Use of the rapidly dissipating fraction derived from field dissipation studies

EFSA (2014a) provided guidance for the calculation of the rapidly dissipating fraction at the soil surface (F_{field}) from field dissipation studies. Here, guidance is provided as to how available F_{field} values can be used to estimate the F_{field} for the soil exposure scenario.

This F_{field} approach is a simplified approach. In principle, it would be preferable if the numerical models could be used to simulate the rapid dissipation at the soil surface. However, as described by EFSA PPR Panel (2010c, p. 14–15), the current knowledge of the photodegradation and volatilisation processes in the top millimetres of soil is yet insufficient to use the numerical models for this purpose.

The estimation of F_{field} for the required scenario can be subdivided into two steps:

- Is the fast decline observed in field dissipation studies also expected to occur in the required exposure scenario?
- If yes, which value of F_{field} is to be used?

With respect to the first step, the answer is 'no' ($F_{field} = 0$) unless the notifier provides plausible arguments to support the position that a fast initial decline is expected to occur in the required exposure scenario. Let us consider two examples: case YES where this is indeed expected and case NO where this is not expected. In case YES, the field dissipation study was a spray application in Germany onto bare soil and it showed a fast initial decline of 70% of the dose as a result of photodegradation. The required exposure scenario for this case was spraying onto bare soil in southern Europe in the spring. In case NO, we have the same field study but now the required exposure scenario is spraying onto a crop with 80% deposition on the crop and 20% on the soil with most of the soil usually in the shadow of the plants. The YES/NO answer may be different for different applications in the same crop during the year (e.g. YES for applications in early growth stages and NO in late growth stages). The guidance for providing this yes/no answer is limited in view of the limited experience and available data on fast dissipation processes.

For the second step, it is proposed to use the worst-case value of four accepted values. For example, four field dissipation studies show F_{field} values of 30%, 40%, 60% and 80% for studies in France, the UK, Germany and Spain under normal agricultural use conditions. If fewer or more than four such values are available, the use of an estimate of the 12.5th percentile is proposed. This is approximately the same as the worst-case value of four values (ignoring the difference between a quantile of a sample population and the true population).

Unlike the *DegT50*, for which the uncertainty is accounted for by selecting a scenario that represents a higher spatial percentile (EFSA PPR Panel, 2010b), the uncertainty and spatial and temporal variability of the surface loss processes (F_{field}) are not considered in the scenario selection. Therefore, it is considered appropriate to use a 12.5th percentile of F_{field}. The basis for using the worst-case value of four values is that, in EU regulatory practice, field dissipation studies with four soils are usually required.

Once the 12.5th percentile F_{field} is available, the next step is to use this value in the exposure assessment. We recommend including the fast surface decline only in tiers that use the numerical models.

The correction based on F_{field} should apply to only the fraction of the dose that directly reaches the soil surface (see Figure 7) since it is unlikely that fast dissipation processes play an important role for the fraction that is washed off from the canopy. Significant wash-off will only occur if the crop has covered the soil to a large extent and fast dissipation processes at the soil surface are likely to be less significant when the soil is covered to a large extent.

The guidance below is based on the following assumptions: (i) F_{field} is an input parameter of the simulation model; (ii) F_{field} has to be specified for each application of the substance and (iii) F_{field} is used in the model as follows:

$$A_{ism} = f_{soil}\,(1 - F_{field})\,A \tag{F1}$$

where A_{ism} is that part of the dose (kg/ha) that is assumed to reach the soil surface on the day of application (the part that penetrates immediately into the soil matrix) and *F*field (–) is the rapidly dissipating fraction.

The procedure is to switch off both photochemical transformation (in case this is simulated) and volatilisation (by setting the saturated vapour pressure to zero) in the numerical models because these loss processes are included in F_{field}. This procedure assumes that the runoff of substances is negligibly small (less than 1% of the dose). When this condition is not met, the model input value of F_{field} has to be corrected to result in the sum of F_{field} and runoff equalling the target F_{field}.

The proposed calculation procedure is as follows:

- run the model using this 12.5th percentile F_{field};
- select from this run the year at which the all-time-high concentration occurs;
- in case of the concentration in total soil, this concentration is called $c_{\text{T,uncorrected}}$ because it also includes rapid dissipation of the dosage that generates the all-time high (which is inappropriate as described above);
- the corrected concentration can then be calculated as:

$$c_{\text{T,corrected}} = c_{\text{T,uncorrected}} + \frac{f_{\text{soil,last}}\, F_{\text{field,last}}\, A_{\text{last}}}{\rho\, z_{\text{eco}}} \qquad \text{(F2)}$$

where the subscript '*last*' refers to the last application in the year (assuming that this leads to the all-time high concentration which will usually be the case). This equation adds again the amount that was subtracted in the model simulations to account for rapid dissipation of part of this last application.

In the case of the concentration in pore water, the following steps should be implemented: (i) the maximum pore water concentration should be looked up; (ii) the correction in Equation G2 should be applied to the total concentration; and (iii) the pore water concentration should be calculated using the normal algorithms in the models.

This procedure can be combined with the solution for the in-row applications (Appendix E), provided that first the correction for the rapidly dissipating fraction is carried out and thereafter the procedure for the in-row applications.

A more sophisticated procedure would be to run the numerical models twice (conform the procedure for non-uniform applications in Appendix E). This implies carrying out the following steps:

- run the model for the required simulation period using this 12.5th percentile F_{field};
- select from this run the year at which the all-time-high concentration occurs;
- take the model input file of this run and perform the calculation of the next model run (see next item) outside the shells of the models using this model input file as a starting point;
- run the model a second time but now with a zero F_{field} for the year in which the all-time-high concentration occurs. If there is only one application per year, set F_{field} to zero for this application, when there are more applications per year, set F_{field} to zero only for the application in the all-time-high year that leads to the all-time-high concentration (usually the last application in the year). This implies that for repeated applications it is assumed there is enough time available for the rapid dissipation before the next dosage is applied.

Setting F_{field} to zero in the all-time-high year is necessary because otherwise the all-time-high concentration would be systematically underestimated because the rapid dissipation takes some time.

Appendix G – Examples on how the EFSA Guidance Document can be used

This appendix gives examples on how the EFSA Guidance Document can be used. Calculations were done with the model versions that were available at the time of publication of this Guidance Document and may change when updated model version are released. The model versions at the time of publication were PERSAM version 1.0.2, PEARL kernel version 3.2.8 (16 June 2017) and PELMO version 4.10 (February 2017). Calculations were done using the substance properties in Table G.1 unless stated otherwise in the respective example.

Note that, for illustrative purposes, results for all tiers are given in these examples. However, as stated in Section 5, the soil exposure assessment may start at each individual tier without reporting results from lower tiers.

Table G.1: Summary of substance properties of pesticides and metabolites used in the example

Substance property	Unit	Pesticide							Metabolite	
		A	B	C	D	E	F	G	M1	M2
Molar mass	(g/mol)	300	300	300	300	300	300	300	200	100
Water solubility (20°C)	(mg/L)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	90	90
Vapour pressure (20°C)	(Pa)	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-4}	10^{-8}	10^{-8}	10^{-8}
DegT50(a) (geomean)	(days)	250	250	250	250	250	250	25	100	250
Molar activation energy	(kJ/mol^{-1})	65.4	65.4	65.4	65.4	65.4	65.4	65.4	65.4	65.4
Exponent for the effect of liquid	(–)	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
K_{om} (geomean)	(L/kg)	1,000	1,000	(b)	(c)	(d)	1,000	1,000	10	100
K_{om} in dry soil(e)	(L/kg)	10^5	10^5	–	–	–	10^5	10^5	1,000	10^4
$1/n$	(–)	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9
DegT50 on crop surface	(d)	10	2(f)	10	10	10	10	10	10	10
Wash-off factor(g)	(mm^{-1})	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Plant uptake factor	(–)	0	0	0	0	0	0	0	0	0
Molar formation fraction (arithmetic mean)	(–)	–	–	–	–	–	–	–	0.7(h)	1.0(i)

(a): At 20°C and moisture content corresponding to field capacity, pF2.
(b): pH-dependent using a sigmoidal soil pH–K_{om} relationship.
(c): pH-dependent using a linear soil pH–K_{om} relationship.
(d): Clay dependent using a linear soil clay–K_{om} relationship.
(e): K_{om} in dry soil set to $K_{om} \times 100$ (PEARL); factor for increase of sorption when soil is air dried set to 100 (PELMO).
(f): Based on experimental evidence.
(g): 0.1/mm = 1/cm (PELMO) = 100/m (PEARL).
(h): From pesticide G.
(i): From metabolite M1.

G.1. Example 1 (annual crops, application to the soil surface)

In Example 1, we consider a rather persistent substance (pesticide A) with an average (geomean) *DegT50* of 250 days (at 20°C and moisture content corresponding to field capacity, pF2) and an average (geomean) K_{om} of 1,000 L/kg (Table G.1). Pesticide A is intended to be applied once each year via spraying in maize 1 day before emergence (to the soil surface) with an application rate of 1 kg/ha. Let us further assume that we are interested in results for the concentration in total soil as well as in soil pore water for an ecotoxicological averaging depth (z_{eco}) of 5 cm and for averaging times (t_{avg}) of 0 and 21 days.

Input values at Tier-1 (PERSAM) are the *DegT50* (250 days), the K_{om} (1,000 L/kg), the rate of applications (one time 1 kg/ha) and the application cycle (each year in this case) without further specifying the crop, except that an assessment for annual crops (planted once a year) is intended. At Tier-2 no further input is needed as application is on the soil surface, so there are no canopy processes to be taken into account. The final results at Tier-1 and Tier-2, already corrected for with the default model and scenario adjustment factors, are directly obtained from the model output tables (and respective reports).

At Tier-3A, PERSAM is used to select crop-specific and substance-specific scenarios to be calculated with the numerical models (in this example this is only one scenario with z_{eco} = 5 cm for pesticide A for each regulatory zone). For each of these scenarios, a PERSAM transfer file is generated. Notice that the scenario to be selected in PERSAM for numerical modelling at Tier-3A has to be always based on the ecotoxicological averaging depth (z_{eco}) of interest (5 cm in this example). In contrast, it is considered acceptable to obtain results for individual averaging times (t_{avg}) from the specific scenario, which is based on a t_{avg} = 0 days only. In PEARL and PELMO, only the storage folder of PERSAMs transfer files have to be specified. The models automatically generate the scenario-specific input files for all Tier-3A scenarios in this folder. Substance properties and the application scheme are the same as those at Tier–1 and Tier-2. However, the numerical models require some more substance properties to adequately account for substance behaviour in soil. So, let us assume a water solubility of 0.1 mg/L (at 20°C), a vapour pressure of 10^{-8} Pa (at 20°C), a Freundlich exponent (1/*n*) of 0.9 and a crop uptake factor of 0 for pesticide A (Table G.1). The K_{om} under air-dry conditions is assumed to be 100 times the K_{om} under reference conditions (i.e. 10^5 L/kg). In this example, application in the numerical models is set to 'application to the soil surface' to the FOCUS-crop maize 1 day before emergence. Note that at Tier-3A no adjustment factors are needed. Therefore, the final results are directly obtained from the model output file.

Results for pesticide A at each individual tier are given in Table G.2.

Table G.2: Results for pesticide A, applied to maize 1 day before emergence at an application rate of 1 kg/ha

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	18.6	13.0	9.9	0.48	0.60	0.91
	5	21	PERSAM	18.2	12.7	9.6	0.47	0.58	0.86
Tier-2	5	0	PERSAM	9.4	8.0	6.9	0.30	0.40	0.48
	5	21	PERSAM	9.3	7.9	6.8	0.30	0.40	0.48
Tier-3A	5	0	PEARL	4.1	3.1	2.6	0.09	0.12	0.15
	5	0	PELMO	4.3	3.1	2.7	0.09	0.12	0.14
	5	21	PEARL	4.1	3.0	2.6	0.09	0.11	0.13
	5	21	PELMO	4.3	3.0	2.6	0.08	0.10	0.12

G.2. Example 2 (annual crops, application to the crop canopy)

G.2.1 Application to the crop canopy including default crop parameter

Example 2.1 is the same as Example 1. However, in this example pesticide A is applied to maize twice, first at BBCH 10–19 and second at BBCH 20–39, each time at a rate of 1 kg/ha with an interval of 14 days. So, crop interception, canopy processes and foliar wash-off have to be taken into account. In this example, we further assume that there are no experimental data available on the behaviour of pesticide A on the crop canopy, so the default *DegT50* at crop surface of 10 days and the default wash-off factor (*w*) of 0.1/mm (EFSA, 2014a) are applied.

At Tier-1 (assessment for annual crops planted once a year), crop canopy processes are not taken into account; so, the entire load is directed to the soil. The application rates at Tier-1 are two times 1 kg/ha with an interval of 14 days. At Tier-2 (maize) crop canopy processes are included; therefore, the BBCH code and the crop interception (EFSA, 2014a) for each application have to be specified. In this example (maize), this is 1 kg/ha at BBCH 10–19 with a crop interception of 25% for the first application and 1 kg/ha at BBCH 20–39 with a crop interception of 50% for the second application, with an interval of 14 days. Based on the crop interception specified by the user and the default wash-off fractions (0.45 and 0.65 for the first and second application, respectively; Table 9), PERSAM internally calculates the soil load for these two applications in line with Equation 1. This gives 0.86 kg/ha for the first and 0.83 kg/ha for the second application. As degradation between the applications is taken into account, the final annual soil dose, which is location specific, is lower than the sum of the two applications.

At Tier-3A, the user may have to further specify the application scheme in the numerical models based on the information available in the PERSAM transfer file. In this example, we assume that the first application is 14 days after emergence. Notice that in the numerical model application 'to the crop canopy, intercepted fraction specified by the user' is already selected as this information is part of the PERSAM transfer file. The application rate is automatically set to 2 × 1 kg/ha (interval of 14 days), with crop interception fractions of 0.25 and 0.5 for BBCH 10–19 and BBCH 20–39, respectively. (Notice that the application details as specified in PERSAM are transferred to the numerical models. So normally there is no need to revise them in the numerical models apart from the setting of the first application date.) In this example, the substance parameter for processes on the crop canopy are set to EFSA default values (so *DegT50* on crop surface = 10 days, w = 0.1/mm).

Results for pesticide A at each individual tier are given in Table G.3.

Table G.3: Results for pesticide A (default crop parameter), applied to maize at BBCH 11–19 and BBCH 20–39 at 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	37.0	25.9	19.6	0.95	1.18	1.79
	5	21	PERSAM	36.1	25.2	18.9	0.93	1.15	1.69
Tier-2	5	0	PERSAM	15.7	13.4	11.6	0.51	0.67	0.81
	5	21	PERSAM	15.6	13.3	11.4	0.50	0.66	0.79
Tier-3A	5	0	PEARL	7.2	5.6	4.8	0.15	0.20	0.23
	5	0	PELMO	7.5	5.6	4.8	0.15	0.19	0.23
	5	21	PEARL	7.2	5.5	4.7	0.15	0.19	0.23
	5	21	PELMO	7.5	5.5	4.7	0.15	0.18	0.23

G.2.2 Application to the crop canopy including substance-specific crop parameter

Example 2.1 is based on pesticide A assuming EFSA default parameter for crop canopy processes. In Example 2.2, we consider pesticide B for which specific substance properties are available. Let us consider a *DT50* at the crop canopy of 2 days instead of the default value of 10 days based on experimental data. All other properties of pesticide B are assumed to be the same as pesticide A.

There is no possibility to account for non-default parameters of crop canopy processes at Tier-1 and Tier–2. So, these tiers are exactly the same as for pesticide A in Example 2.1.

At Tier-3A (applying numerical models), the default substance parameters for crop canopy processes in the model shell have to be replaced by the specific ones (in this example *DT50* on the crop surface is 2 days instead of the default value of 10 days). All other model settings, including the application scheme, are the same as in Example 2.1.

Results for pesticide B are given in Table G.4.

Table G.4: Results for pesticide B (substance-specific crop parameter), applied to maize at BBCH 11–19 and BBCH 20–39 at 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	37.0	25.9	19.6	0.95	1.18	1.79
	5	21	PERSAM	36.1	25.2	18.9	0.93	1.15	1.69
Tier-2	5	0	PERSAM	15.7	13.4	11.6	0.51	0.67	0.81
	5	21	PERSAM	15.6	13.3	11.4	0.50	0.66	0.79
Tier-3A	5	0	PEARL	6.3	4.8	4.2	0.13	0.17	0.21
	5	0	PELMO	6.5	4.9	4.2	0.13	0.17	0.21
	5	21	PEARL	6.3	4.7	4.2	0.13	0.17	0.20
	5	21	PELMO	6.5	4.8	4.2	0.13	0.16	0.20

G.3. Example 3 (application to crops grown on ridges)

G.3.1. Ridge application

In Example 3.1, we consider a dedicated ridge application of compound A to potatoes at BBCH 10–19, so before the crop canopy has been closed (14 days post-emergence). Let's assume further that the application rate is 1 kg/ha related to the soil surface area treated. In case of potatoes, predefined f_{ridge} values for North–Centre–South are 0.55, 0.72, and 0.62 (Table 12).

At Tier-1, non-uniform application is not taken into account. So, the user only specifies application to annual crops (planted once a year) and the application rate is set to 1 kg/ha (crop interception is not taken into account at Tier-1). At Tier-2 the crop ('potatoes') is selected, application rate is set to 1 kg/ha, the BBCH code is set to 10–19 and the crop interception is set to 15% (EFSA, 2014a). Next the fraction of the soil surface area treated ($f_{treated} = f_{ridge}$ in this case) is set to their respective values (0.55, 0.72, and 0.62 for North–Centre–South, Table 12). In case of non-uniform application, PERSAM internally calculates a refinement factor (f_{ref}), which is forwarded to the numerical models via the PERSAM transfer file.

At Tier-3A, the numerical models read the transfer files, so the application is also set to 1 kg/ha 'to the crop canopy, intercepted fraction specified by the user', crop interception is set to 0.15. In line with the examples given before, the user usually only has to revise the first date of application, which is 14 days after emergence in this example. Finally, the numerical models internally correct the calculation results with the respective refinement factor (f_{ref}).

Table G.5: Results for pesticide A, applied to potatoes (dedicated ridge treatment) at BBCH 10–19 at an application rate of 1 kg/ha

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	18.6	13.0	9.9	0.48	0.60	0.91
	5	21	PERSAM	18.2	12.7	9.6	0.47	0.58	0.86
Tier-2	5	0	PERSAM	9.3	7.6	6.0	0.24	0.31	0.48
	5	21	PERSAM	9.2	7.5	5.9	0.24	0.30	0.47
Tier-3A	5	0	PEARL	4.2	3.1	2.4	0.07	0.09	0.14
	5	0	PELMO	4.2	3.2	2.5	0.07	0.09	0.14
	5	21	PEARL	4.2	3.1	2.4	0.07	0.09	0.13
	5	21	PELMO	4.2	3.1	2.4	0.07	0.08	0.13

G.3.2. Furrow application

Application to the furrow in potatoes is handled in analogy with Example 3.1 replacing f_{ridge} by f_{furrow} (= $f_{treated}$), which is 0.45, 0.28 and 0.38 for North, Centre and South (Table 12). Application is assumed to be on bare soil, so crop interception as well as crop canopy processes are not taken into account.

As non-uniform application is not considered for at Tier-1, input and results for Tier-1 are the same as for Example 3.1 (ridge application). At Tier-2, 'potatoes' are selected and the application rate is set to 1 kg/ha (without crop interception). The fraction of the soil surface area treated ($f_{treated} = f_{furrow}$) is set to the respective values (0.45, 0.28, and 0.38 for North–Centre–South).

Notice that in the numerical models (Tier-3A) application has to be set 'to the soil surface'.

Table G.6: Results for pesticide A, applied to potatoes (dedicated furrow treatment) at BBCH 10–19 at an application rate of 1 kg/ha

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	18.6	13.0	9.9	0.48	0.60	0.91
	5	21	PERSAM	18.2	12.7	9.6	0.47	0.58	0.86
Tier-2	5	0	PERSAM	10.0	7.3	6.2	0.26	0.31	0.53
	5	21	PERSAM	9.9	7.2	6.2	0.26	0.31	0.51
Tier-3A	5	0	PEARL	4.2	3.0	2.5	0.08	0.09	0.16
	5	0	PELMO	4.2	3.0	2.5	0.08	0.09	0.15
	5	21	PEARL	4.2	2.9	2.4	0.08	0.09	0.14
	5	21	PELMO	4.2	3.0	2.4	0.07	0.08	0.13

G.4. Example 4 (annual crops, soil incorporation)

G.4.1. Evenly distributed incorporation of granules over a certain soil depth

This example considers evenly distributed incorporation of granules. Let's assume that granules containing pesticide A are evenly incorporated (mixed) to a soil depth (z_{inc}) of 10 cm 2 weeks before planting of maize (30 days before emergence). The application rate is 1 kg/ha.

At Tier-1, incorporation is not taken into account, so the user only specifies application to annual crops (planted once a year) with an application rate of 1 kg/ha. At Tier-2, 'potatoes' are selected, the application rate is set to 1 kg/ha as well. However, as z_{inc} (10 cm) is deeper than z_{eco} (5 cm), Equation A19b is used for the calculation of the initial concentration in PERSAM to account for 'dilution' of the pesticide over z_{inc} following application.

Notice that in the numerical models (Tier-3A) application has to be set to 'incorporation' with a soil depth of 10 cm and the date of application is set to 30 days before emergence. Everything else is identical to Example 1.

Table G.7: Results for pesticide A, applied to maize at 1 kg/ha 2 weeks before planting (evenly distributed soil incorporation)

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	18.6	13.0	9.9	0.48	0.60	0.91
	5	21	PERSAM	18.2	12.7	9.6	0.47	0.58	0.86
Tier-2	5	0	PERSAM	6.7	5.6	4.5	0.21	0.25	0.30
	5	21	PERSAM	6.7	5.5	4.5	0.21	0.25	0.30
Tier-3A	5	0	PEARL	2.6	2.1	1.7	0.05	0.06	0.07
	5	0	PELMO	2.7	2.1	1.7	0.05	0.06	0.07
	5	21	PEARL	2.6	2.1	1.7	0.05	0.06	0.07
	5	21	PELMO	2.7	2.1	1.7	0.05	0.06	0.07

G.4.2. Placing of granules at a certain soil depth

In contrast with the example given previously, Example 4.2 considers placing granules at a certain soil depth. Let us assume that granules containing pesticide A are placed at a soil depth (z_{inc}) of 10 cm

2 weeks before planting of maize (30 days before emergence). The application rate is 1 kg/ha. For granules placed at a certain soil depth, the upper layer of the ecotoxicological averaging depth (z_{eco}) is 'moved' from the soil surface to the depth of incorporation (z_{inc}) (as described in Section 4.4.2).

At Tier-1, incorporation is not taken into account, so the user only specifies the application to annual crops (planted once a year) with an application rate of 1 kg/ha. At Tier-2, 'potatoes' are selected. Notice that in the analytical model (Tier-1 and Tier-2) z_{eco} cannot be 'moved', so only the soil depth for calculating the mean annual water flux (f_q) is internally set to z_{inc} + z_{eco} instead of z_{eco}, which gives 15 cm in this case. So, at Tier-2, z_{inc} (10 cm) has to be additionally specified.

In the numerical models (Tier-3A), application is set to 'injection' and the date of application is set to 30 days before emergence. Notice that for technical reasons the incorporation depth in these PEARL calculations was set 0.5 cm below the 'true' incorporation depth (so 10.5 cm in this case) to adequately cover the peak concentration after placing of the granules. Next, z_{eco} is 'moved' from the soil surface to 10 cm by setting the top and bottom layer of the evaluation depth in the numerical models to 10 and 15 cm, respectively. Other settings are identical to Example 1.

Table G.8: Results for pesticide A, applied to maize at 1 kg/ha 2 weeks before planting (evenly distributed soil incorporation)

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	18.6	13.0	9.9	0.48	0.60	0.91
	5	21	PERSAM	18.2	12.7	9.6	0.47	0.58	0.86
Tier-2	5	0	PERSAM	9.5	8.2	7.0	0.31	0.41	0.49
	5	21	PERSAM	9.4	8.1	6.9	0.31	0.40	0.48
Tier-3A	5	0	PEARL	3.6	3.1	2.6	0.08	0.11	0.13
	5	0	PELMO	4.8	3.6	2.9	0.09	0.09	0.11
	5	21	PEARL	3.6	3.0	2.5	0.07	0.10	0.12
	5	21	PELMO	4.8	3.6	2.8	0.08	0.09	0.10

G.5. Example 5 (air blast application to crops)

G.5.1. In-row exposure assessment

Example 2.1 considers a single air blast application of substance A in apples at BBCH 71–75 (around 15 September). Let us first consider that we are interested in the in-row soil exposure assessment. The application rate given in the GAP is 1 kg/ha related to the whole field (which is at current usually the case in GAP tables). In this case, the EFSA guidance recommends applying a default dose rate assessment factor (f_{dose}) of 2.9 to account for non-uniform spray distribution in permanent crops. (Notice that if the application rate is already related to the soil surface area treated no dose rate assessment factor has to be applied.)

At Tier-1, the user enters a single application rate of 2.9 kg/ha, crop canopy processes are not taken into account. Further, the user has to specify that application is intended for permanent crops without further specifying the crop. At Tier-2 the user selects 'apples – in-row exposure'. The rate is still 2.9 kg/ha, but further information on the crop development stage (BBCH 71–75) and the crop interception (65% for this BBCH code in apples according to EFSA, 2014a) have to be provided. Based on the default wash-off fraction of 0.60 for BBCH 71–75 in apples (Table 10), PERSAM internally calculates the fraction of the dose reaching the soil (f_{soil} = 0.74) and the final soil load, which gives 2.15 kg/ha in this example.

In the numerical models (Tier-3A), the application is automatically set to the same as in PERSAM (2.9 kg/ha 'to the crop canopy, intercepted fraction specified by the user', crop interception 65%), the user only has to reconsider the application date, which is 15 September in this case, for all regulatory zones (HA and SE as the dominant FOCUS zones).

Table G.9: Results for pesticide A (in-row exposure), applied to apples (air blast) at BBCH 71–75 at an application rate of 1 kg/ha related to the whole field

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	191	105	65.5	1.57	1.74	2.05
	5	21	PERSAM	186	102	63.2	1.52	1.68	1.94
Tier-2	5	0	PERSAM	75.9	47.9	26.9	0.77	0.79	0.81
	5	21	PERSAM	75.3	47.3	26.5	0.76	0.78	0.79
Tier-3A	5	0	PEARL	33.4	20.9	8.0	0.21	0.22	0.16
	5	0	PELMO	30.4	19.4	8.2	0.19	0.20	0.16
	5	21	PEARL	33.1	20.7	7.9	0.21	0.22	0.15
	5	21	PELMO	30.1	19.2	8.1	0.18	0.19	0.15

G.5.2. Between-row exposure assessment

Let us now consider the situation for a between-row soil exposure-assessment resulting from air blast spray drift as given in the example above (Example 2.1b). In this case, the guidance recommends assuming uniform overspray, applying the application rate related to the whole field, which is 1 kg/ha in this example.

So, at Tier-1 and Tier-2, the application rate to be entered into PERSAM is 1 kg/ha for 'apples – between-row exposure'. Notice that the between-row area in apples is considered to be covered by grass (Table 7), so the crop interception in PERSAM has to be set to 90% according to EFSA (2014a). The BBCH code does not apply in case of grass (Table 10), instead the season (July–September in this example) is used in PERSAM to calculate the dose reaching the soil, which finally gives 0.60 kg/ha (default fraction washed off is 0.55).

Table G.10: Results for pesticide A (between-row exposure), applied to apples (air blast) at BBCH 71–75 at an application rate of 1 kg/ha related to the whole field

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	65.8	36.3	22.6	0.54	0.60	0.71
	5	21	PERSAM	64.2	35.3	21.8	0.53	0.58	0.67
Tier-2	5	0	PERSAM	21.1	13.3	8.3	0.21	0.22	0.27
	5	21	PERSAM	20.9	13.1	8.2	0.21	0.22	0.27
Tier-3A	5	0	PEARL	11.0	6.8	3.6	0.07	0.07	0.06
	5	0	PELMO	9.8	6.2	3.2	0.06	0.06	0.05
	5	21	PEARL	10.9	6.8	3.5	0.07	0.07	0.06
	5	21	PELMO	9.7	6.1	3.2	0.05	0.06	0.05

G.6. Example 6 (permanent crops, band application)

Example 6 considers a soil application in permanent crops. In this example, a dedicated in-row treatment with compound A (1 kg/ha soil surface area treated at BBCH 71–78) applied to the soil below the crop canopy is considered. As the application rate is already related to the soil surface treated, no dose rate adjustment factor is necessary in this example. As application is to bare soil (no crop cover below the crop canopy in permanent crops; Table 7), crop interception is not an issue here.

At Tier-1 and Tier-2 (PERSAM), the user selects 'apples – between-row exposure' and enters an application rate of 1 kg/ha. Neither crop interception nor crop canopy processes are taken into account.

At Tier-3A (numerical models), application has to be set by the user 'to the soil surface' with an application date of 15 September. (In analogy to this example, exposure assessments following between-row treatment are conducted; however, in case of between-row exposure, the user has to take into account that apples are considered to be covered by grass (Table 7), so crop interception and canopy processes should be accounted for in PERSAM as well as in the numerical models.)

Table G.11: Results for pesticide A, applied to apples (soil application, between-row exposure) at BBCH 71–75 with an application rate of 1 kg/ha related to the soil surface area treated

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	65.8	36.3	22.6	0.54	0.60	0.71
	5	21	PERSAM	64.2	35.3	21.8	0.53	0.58	0.67
Tier-2	5	0	PERSAM	35.4	22.3	12.5	0.36	0.37	0.38
	5	21	PERSAM	35.1	22.1	12.4	0.36	0.37	0.37
Tier-3A	5	0	PEARL	15.3	9.8	4.8	0.09	0.10	0.10
	5	0	PELMO	13.8	8.9	4.9	0.08	0.08	0.10
	5	21	PEARL	15.2	9.7	4.7	0.09	0.09	0.08
	5	21	PELMO	13.6	8.7	4.8	0.08	0.07	0.09

G.7. Example 7 (soil pH-dependent sorption)

G.7.1. Soil pH-dependent sorption, sigmoid pH–K_{om} relationship

Example 7.1 is the same as Example 2.2. However, pesticide A is now replaced by pesticide C, which shows pH-dependent sorption (all other properties are the same as for pesticide A). Let us assume that pesticide C is a weak acid with a pK_a of 4.7. Adsorption results on four soils (soil pH measured in $CaCl_2$) are available: K_{om} at pH 4 = 184 L/kg, K_{om} at pH 5.5 = 62 L/kg, K_{om} at pH 7 = 22 L/kg and K_{om} at pH 8 = 20 L/kg. Let us further assume that pesticide C has a molar mass of 300 g/mol, the anion a molar mass of 299 g/mol.

The predefined scenarios at Tier-1 are not designed for substances whose properties depend on soil properties, such as pH. For such substances, the user therefore has to directly go to Tier-2 or Tier-3A.

At Tier-2, the soil pH–K_{om} relationship for pesticide C has to be implemented in PERSAM. As the soil *p*H in PERSAM is based on measurements in H_2O, pH values measured in $CaCl_2$ for pesticide C have to first be converted into pH_{H2O} according to Equation 4a given in this guidance (Section 3.3). Fitting of the final pH_{H2O}–K_{om} data sets to the sigmoid relationship (Equation 3 in this guidance, Section 3.3), applying, for example, SOLVER in Microsoft Excel (minimum squared residue method), reveals for pesticide C a $K_{om,acid}$ of 202.5 L/kg, a $K_{om,anion}$ of 20.0 L/kg and a Δ*p*H of 0.82. These parameters have to be entered into PERSAM at Tier-2. Notice that it is not necessary to specify the soil pH–K_{om} relationship in the numerical models as PERSAM already provides the scenario-specific K_{om} value in the PERSAM transfer file.

At Tier-3A, crop-specific and substance-specific scenarios selected in PERSAM are implemented in the numerical models in the same way as in the examples mentioned before. The soil pH is part of the scenario definition and the respective K_{om} is already accounted for in the PERSAM transfer file used by the numerical models. All other settings (substance properties other than K_{om} and application scheme) are the same as in Example 2.2.

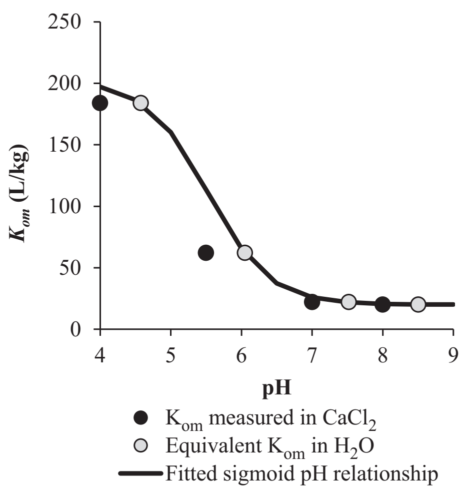

Figure G.1: Fitted sigmoid pH_{H2O}–K_{om} relationship for pesticide C

Results for pesticide C are given in Table G.12.

Table G.12: Final results for pesticide C (pH-dependent sorption, sigmoid pH–K_{om} relationship), applied to maize at BBCH 11–19 and BBCH 20–39 at 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	Not applicable			Not applicable		
	5	21	PERSAM						
Tier-2	5	0	PERSAM	12.7	10.7	9.2	8.5	15.9	17.3
	5	21	PERSAM	12.6	10.5	9.0	8.4	15.6	16.8
Tier-3A	5	0	PEARL	6.3	5.1	4.0	2.8	4.7	5.5
	5	0	PELMO	5.9	5.0	3.9	2.4	3.3	4.5
	5	21	PEARL	6.2	5.0	3.9	2.6	3.4	5.0
	5	21	PELMO	5.7	4.9	3.8	2.2	2.1	3.7

G.7.2. Soil pH-dependent sorption, linear pH–K_{om} relationship

Example 7.2 is the same as Example 7.1. However, for Example 7.2, pesticide C, showing a sigmoid pH–K_{om} relationship, is now replaced by pesticide D with a linear pH–K_{om} relationship. Let us assume the following pH–K_{om} relationship: $K_{om} = -150 \times pH_{H2O} + 1500$.

Handling of pesticide D at Tier-2 in PERSAM is identical to pesticide C, however now the linear relationship between pH and K_{om} has to be entered in the model shell. The location-specific K_{om} value is automatically transferred to the numerical models via the PERSAM transfer file.

Results for pesticide D are given in Table G.13.

Table G.13: Results for pesticide D (pH-dependent sorption, linear pH–K_{om} relationship), applied to maize at BBCH 11–19 and BBCH 20–39 at 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	Not applicable			Not applicable		
	5	21	PERSAM						
Tier-2	5	0	PERSAM	15.5	12.9	10.9	0.89	1.81	2.09
	5	21	PERSAM	15.3	12.8	10.8	0.88	1.78	2.04
Tier-3A	5	0	PEARL	7.2	5.7	4.6	0.28	0.60	0.61
	5	0	PELMO	7.4	5.5	4.6	0.28	0.54	0.59
	5	21	PEARL	7.1	5.6	4.5	0.28	0.57	0.60
	5	21	PELMO	7.4	5.5	4.5	0.27	0.51	0.56

G.8. Example 8 (soil clay-dependent sorption)

Example 8 considers a substance (pesticide E) that is considered to show clay-dependent sorption. Based on batch experiments a linear regression was established: K_{om} (L/kg) = 1.5 × clay content (%).

Notice that Tier-1 is not designed for substances showing substances depending on soil properties. Therefore, the user has to directly move to Tier-2. Handling of pesticide E at Tier-2 in PERSAM is identical to pesticide D, however now the linear relationship between clay (%) and K_{om} has to be entered in the model shell. The location-specific K_{om} value is automatically transferred to the numerical models via the PERSAM transfer file.

Table G.14: Results for pesticide E (soil clay-dependent sorption), applied to maize at BBCH 11–19 and BBCH 20–39 at 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	Not applicable			Not applicable		
	5	21	PERSAM						
Tier-2	5	0	PERSAM	10.7	9.9	9.0	21.8	19.5	26.1
	5	21	PERSAM	10.6	9.8	8.9	21.6	19.2	25.6
Tier-3A	5	0	PEARL	3.6	4.1	3.0	8.3	6.3	9.8
	5	0	PELMO	3.4	3.4	2.7	6.7	4.5	7.7
	5	21	PEARL	3.5	3.7	2.9	7.7	4.5	8.9
	5	21	PELMO	2.8	2.9	2.2	5.4	2.7	6.2

G.9. Example 9 (parent and metabolites)

Example 9 considers pesticide G (parent) together with two metabolites, metabolites M1 and M2, formed from pesticide G in series. Let us assume that pesticide G is a short-living substance and has an average (geomean) *DegT50* of 25 days (at 20°C and soil moisture related to field capacity, pF2) and an average (geomean) K_{om} of 1,000 L/kg. Metabolite M1 and metabolite M2 have average *DegT50* values of 100 and 250 days, respectively, and K_{om} values of 10 and 100 L/kg, respectively. The molar mass of pesticide G is 300 g/mol, metabolite M1 has a molar weight of 200 g/mol and metabolite M2 has a molar weight of 100 g/mol. The average (arithmetic mean) molar formation fraction of metabolite M1 from pesticide G is 0.7, the average (arithmetic mean) molar formation fraction of metabolite M2 from metabolite M1 is 1.0. The application scheme of pesticide G (to maize) is the same as in Example 2.1.

In PERSAM (Tier-1 and Tier-2) all three substances, pesticide G (*DegT50* = 25 days, K_{om} = 1,000 L/kg), metabolite M1 (*DegT50* = 100 days, K_{om} = 10 L/kg) and metabolite M2 (*DegT50* = 250 days, K_{om} = 100 L/kg), are entered in the model shell. For metabolite M1, the molar formation fraction from the parent has to be set to 0.7, and for metabolite M2, the molar formation fraction from metabolite M1 has to be set to 1.0. Results for the parent (pesticide G) and the metabolites M1 and M2 at Tier-1 and Tier-2 are directly obtained from PERSAM. Results are already corrected with the model and default scenario adjustment factors.

At Tier-3A, crop-specific and substance-specific scenarios obtained by PERSAM differ between the individual substances. For this reason, individual model runs are necessary for each individual substance and for each individual averaging depth (z_{eco}). Note that results for individual averaging times (t_{avg}) may be obtained from the t_{avg} = 0 scenario. Of course, parent and metabolites have to be linked together in the same way as at Tier-1 and Tier-2. However, final results for pesticide G have to be obtained from model runs with specific scenarios for pesticide G, whereas final results for metabolite M1 or metabolite M2 have to be obtained from model runs based on specific scenarios for metabolite M1 or metabolite M2. No model or scenario adjustment factors are needed at Tier-3A.

Table G.15: Results for pesticide G applied to maize at BBCH 11–19 and BBCH 20–39 at an application rate of 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	22.7	16.9	13.8	0.70	0.90	1.44
	5	21	PERSAM	18.1	12.9	9.9	0.53	0.66	0.86
Tier-2	5	0	PERSAM	10.2	9.2	8.2	0.37	0.55	0.65
	5	21	PERSAM	9.3	8.3	7.3	0.33	0.47	0.54
Tier-3A	5	0	PEARL	3.6	3.4	2.9	0.09	0.14	0.16
	5	0	PELMO	3.5	3.4	2.9	0.08	0.14	0.14
	5	21	PEARL	3.3	3.1	2.7	0.08	0.12	0.13
	5	21	PELMO	3.3	3.1	2.6	0.07	0.11	0.12

Table G.16: Results for metabolite M1, released from pesticide G, applied to maize at BBCH 11–19 and BBCH 20–39 at an application rate of 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	10.9	8.3	6.9	17.0	19.3	23.0
	5	21	PERSAM	10.3	7.7	6.3	15.8	17.7	20.0
Tier-2	5	0	PERSAM	4.9	4.5	4.1	9.1	10.4	11.6
	5	21	PERSAM	4.8	4.4	3.9	8.8	10.0	11.2
Tier-3A	5	0	PEARL	0.9	0.5	0.8	1.6	0.9	2.4
	5	0	PELMO	0.8	0.4	0.7	1.1	0.8	1.7
	5	21	PEARL	0.9	0.4	0.7	1.5	0.6	2.3
	5	21	PELMO	0.8	0.4	0.7	1.1	0.5	1.6

Table G.17: Final results for metabolite M2, released from pesticide G (via metabolite M1), applied to maize at BBCH 11–19 and BBCH 20–39 at an application rate of 1 kg/ha each

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	6.5	4.7	3.7	1.60	2.04	3.16
	5	21	PERSAM	6.3	4.6	3.6	1.56	1.98	2.98
Tier-2	5	0	PERSAM	2.7	2.4	2.2	0.85	1.21	1.45
	5	21	PERSAM	2.7	2.4	2.2	0.84	1.19	1.43
Tier-3A	5	0	PEARL	0.3	0.2	0.2	0.03	0.02	0.10
	5	0	PELMO	0.3	0.2	0.2	0.03	0.03	0.03
	5	21	PEARL	0.2	0.2	0.1	0.03	0.02	0.09
	5	21	PELMO	0.3	0.2	0.2	0.03	0.03	0.03

G.10. Example 10 (accounting for the rapidly dissipation fraction, F_{field})

Example 10 is the same as Example 1 (application to maize 1 day before emergence). However, in this example, pesticide A is replaced by pesticide F, which exhibits a rather high vapour pressure (10^{-4} Pa) and shows fast initial decline on the soil surface (as demonstrated in field dissipation experiments). Let us further assume that the observed fast decline is considered relevant for the required soil exposure assessment. For this example, five field dissipation studies showing F_{field} values of 30%, 40%, 60%, 60% and 80% for studies in France, the UK, Germany, Hungary and Spain under normal agricultural use conditions are available. As these are more than four values, the guidance in Appendix F proposes to use the 12.5th percentile of these values, which is 35% in this case.

Note that F_{field} may be used only in combination with the numerical models. However, Tier-2 (without accounting for F_{field}) is used to select the crop-specific and substance-specific scenarios for Tier-3A.

Input into PERSAM at Tier-2 is exactly the same as in Example 1. Consequently, there are no changes in the crop-specific and substance-specific scenarios at Tier-3A.

As stated in Appendix F, the more sophisticated procedure generally consists of two steps for each individual scenario. In the first step the model shells for PEARL and PELMO are used for an ordinary model run with F_{field} switched on for each application. However, to avoid double counting of rapid dissipation processes at the soil surface (when performing a model run with F_{field} switched on), the volatilisation of the substance (in this example pesticide E) has to be switched off (vapour pressure set to 0 Pa). As in this example, only one application to the soil surface (1 day before the crop emergence) is considered, 'application to the soil surface' is selected, the application rate is set to 1 kg/ha (with no crop interception) and F_{field} is set to 0.35.

For the second step, the year in which the all-time-high concentration occurs is obtained for each individual scenario from the first model run (obtained from the summary reports). Subsequently, the input files for the numerical models are edited outside of the model shells to enable an irregular application scheme (i.e. the application is specified for each individual year). Once this irregular application scheme is established with F_{field} set to 0.35 for each individual application, F_{field} is reset to zero for the last application in the year in which the all-time-high concentration occurs and the model is run once again. The final result is obtained from this second run.

In line with the other examples, Tier-3A is based on the crop-specific and substance-specific scenarios, which are selected using PERSAM (as in Example 1).

Table G.18: Final results for pesticide F (accounting for the rapidly dissipating fraction from field dissipation studies, F_{field}), applied to maize 1 day before emergence at an application rate of 1 kg/ha

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Pore soil water (mg/L)		
				North	Centre	South	North	Centre	South
Tier-1	5	0	PERSAM	Not applicable[(a)]			Not applicable[(a)]		
	5	21	PERSAM						
Tier-2	5	0	PERSAM	Not applicable[(a)]			Not applicable[(a)]		
	5	21	PERSAM						
Tier-3A	5	0	PEARL	3.4	2.7	2.3	0.08	0.11	0.14
	5	0	PELMO	Not calculated			Not calculated		
	5	21	PEARL	3.4	2.6	2.3	0.07	0.10	0.12
	5	21	PELMO	Not calculated			Not calculated		

(a): Note that PERSAM is not capable of handling the rapidly dissipating fraction F_{field}.

G.11. Example 11 (exposure assessment based on the total amount in soil)

Example 11 is the same as Example 1. However, in this case, the end-point concentration in the ecotoxicology study is expressed in terms of the applied rate (kg/ha) only. Therefore, the soil exposure assessment has to be performed on the basis of the concentration in the top 20 cm of soil. So, z_{eco} has to be set to 20 cm. As stated in Section 2.9 of this guidance, the procedure in this example may not be applied at Tier-1 that use predefined scenarios because an inappropriate value of the bulk density would be applied. So, to apply Equation 2 of this guidance (Section 2.9) scenario-specific soil density (ρ) values at Tier-2 and Tier-3A are obtained from PERSAM output.

Table G.19: Scenario-specific ρ (kg/L) values needed to convert the final PEC given in mg/kg into kg/ha

Tier	z_{eco} (cm)	t_{avg} (days)	Total soil			Pore soil water		
			North	Centre	South	North	Centre	South
Tier-1	Not applicable					Not applicable		
Tier-2	20	0	0.94	0.99	1.10			
Tier-3A	20	0	0.94	0.99	1.10			

Results for pesticide A expressed in terms of the total concentration in soil (mg/kg), as well as the applied rate (kg/ha), are given in Table G.20.

Table G.20: Results (total soil only) for pesticide A, applied to maize at 1 kg/ha 1 day before emergence, expressed in terms of the total concentration in soil (mg/kg) and the applied rate (kg/ha)

Tier	z_{eco} (cm)	t_{avg} (days)	Model	Total soil (mg/kg)			Total soil (kg/ha)		
				North	Centre	South	North	Centre	South
Tier-1	Not applicable								
Tier-2	20	0	PERSAM	5.5	4.4	3.4	10.3	8.7	7.5
	20	21	PERSAM	5.4	4.3	3.3	10.2	8.6	7.4
Tier-3A	20	0	PEARL	2.1	1.7	1.3	3.9	3.3	2.8
	20	0	PELMO	2.2	1.7	1.3	4.1	3.4	2.8
	20	21	PEARL	2.0	1.6	1.3	3.8	3.2	2.8
	20	21	PELMO	2.1	1.7	1.3	4.0	3.3	2.8

Appendix H – Results of simulations for example scenarios and application of one example substance

H.1. Procedure

Experience with releases of the FOCUS Groundwater scenarios has shown that it is desirable (as a basic quality check) to run all models for all scenarios and to compare annual average water balances and output for an example substance. Calculations were performed for all crop–scenario combinations with PEARL and PELMO for one strongly adsorbing and persistent example substance 'P' using an ecotoxicological averaging depth of 5 cm (considering only the peak concentration, no TWA values). It was assumed that this substance P was applied annually at a rate of 1 kg/ha 1 day before emergence in case of annual crops and at 1 May in case of permanent crops (the substance was applied to the soil surface). Calculations were performed for the six predefined Tier-1 scenarios.

The K_{om} of substance P at reference conditions was 1,000 L/kg and its *DegT50* in topsoil at 20°C and field capacity was 730 days. The K_{om} under air-dry conditions was assumed to be 100,000 L/kg (i.e. 100 times the K_{om} value at reference conditions). The log K_{ow} of substance P is 3.8, so the transpiration stream concentration factor (*TSCF)* was set at 0.15 according to EC (2014).

Furthermore, the conversion factor of 1.724 was used for the relationship between K_{om} and K_{oc}. In line with EFSA, (2008), the molar activation energy E_{Act} was assumed to be 65.4 kJ/mol (Q_{10} = 2.58). Other substance properties were set as equal to substance D as defined by EC (2014).

A warming-up period of 54 years was used for all scenarios, because the *DegT50* value at the average scenario temperature was greater than 1,000 days for all six scenarios.

Calculations were done with the model versions that were available at the time of publication of this Guidance Document and may change when updated model version are released. The model versions at the time of publication were PERSAM version 1.0.2, PEARL kernel version 3.2.8 (16 June 2017) and PELMO version 4.10 (February 2017). Results may change when updated models are released.

H.2. Results for pesticide P

Tables H.1–H.3 show that differences between PELMO and PEARL were usually less than 20% for the concentration in total soil. For winter cereals in the northern zone, differences were larger. The reason for this is not clear. For the pore water concentrations, differences are sometimes larger. This may be due to the different hydrological concepts of the two models, resulting in different moisture contents at the time of maximum concentration.

Table H.1: Concentration in pore water (mg/L) and the concentration in total soil (mg/kg) for pesticide P in the top 5 cm of soil in regulatory zone **North**. The percentage difference (%) was calculated by dividing the difference by the value of PEARL.

Crop	Concentration in total soil (mg/kg)			Concentration in pore water (mg/L)		
	PEARL	PELMO	Difference (%)	PEARL	PELMO	Difference (%)
Apples (between-row, grass)	45.56	38.14	−16.3	0.16	0.12	−23.5
Apples (in-row)	43.77	38.10	−12.9	0.15	0.12	−20.4
Beans (field, veg.)	10.37	10.94	5.5	0.14	0.13	−4.0
Bush berries (between-row, grass)	45.56	37.76	−17.1	0.16	0.12	−24.8
Bush berries (in-row)	43.89	37.78	−13.9	0.15	0.12	−21.0
Cabbage	20.25	19.02	−6.1	0.27	0.21	−22.5
Carrots	19.88	18.84	−5.2	0.26	0.21	−19.8
Fallow	9.72	10.56	8.6	0.13	0.13	1.8
Grass (pasture)	45.56	37.76	−17.1	0.16	0.12	−24.8
Linseed	10.62	10.74	1.1	0.14	0.13	−7.7
Maize	10.21	10.86	6.3	0.13	0.13	−1.9
Oilseed rape (summer)	10.54	10.75	2.0	0.14	0.13	−7.2

Crop	Concentration in total soil (mg/kg)			Concentration in pore water (mg/L)		
	PEARL	PELMO	Difference (%)	PEARL	PELMO	Difference (%)
Oilseed rape (winter)	9.95	11.20	12.5	0.13	0.14	4.0
Onions	10.34	10.77	4.2	0.14	0.13	−4.0
Peas (animal)	10.42	11.08	6.3	0.14	0.13	−3.6
Potatoes	10.50	10.99	4.7	0.14	0.13	−5.5
Spring cereals	10.23	10.80	5.6	0.14	0.13	−5.3
Strawberries	10.30	10.62	3.2	0.14	0.13	−6.0
Sugar beets	10.45	11.00	5.3	0.14	0.13	−3.6
Tomatoes	10.25	10.98	7.1	0.14	0.13	−3.0
Winter cereals	10.04	11.21	11.7	0.13	0.14	3.1

Table H.2: Concentration in pore water (mg/L) and the concentration in total soil (mg/kg) for pesticide P in the top 5 cm of soil in regulatory zone **Centre**. The percentage difference (%) was calculated by dividing the difference by the value of PEARL

Crop	Concentration in total soil (mg/kg)			Concentration in pore water (mg/L)		
	PEARL	PELMO	Difference (%)	PEARL	PELMO	Difference (%)
Apples (between-row, grass)	24.85	20.68	−16.8	0.18	0.13	−23.9
Apples (in-row)	23.83	20.66	−13.3	0.17	0.14	−21.4
Beans (field, veg.)	6.99	7.35	5.2	0.18	0.16	−7.6
Bush berries (between-row, grass)	25.90	21.18	−18.2	0.20	0.14	−29.4
Bush berries (in-row)	20.43	18.00	−11.9	0.14	0.11	−21.3
Cabbage	12.14	10.77	−11.3	0.29	0.23	−22.1
Carrots	12.10	10.98	−9.2	0.30	0.23	−21.4
Cotton	6.81	6.99	2.7	0.17	0.16	−5.5
Fallow	6.38	6.85	7.4	0.16	0.16	0.9
Grass (pasture)	24.85	20.48	−17.6	0.18	0.13	−25.3
Hops (between-row, bare soil)	17.50	17.76	1.5	0.19	0.16	−12.3
Hops (in-row)	23.71	20.90	−11.8	0.17	0.14	−21.2
Linseed	6.99	6.94	−0.6	0.17	0.16	−8.8
Maize	6.12	6.26	2.3	0.15	0.15	−2.8
Oilseed rape (summer)	6.93	6.96	0.4	0.17	0.16	−8.2
Oilseed rape (winter)	6.53	7.34	12.4	0.17	0.17	4.1
Onions	6.80	6.99	2.8	0.17	0.16	−5.0
Peas (animal)	7.17	7.45	3.8	0.18	0.16	−9.3
Potatoes	6.91	7.12	3.0	0.17	0.16	−6.5
Soybean	6.11	6.26	2.4	0.15	0.15	−1.7
Spring cereals	6.93	7.45	7.5	0.18	0.17	−6.5
Strawberries	6.99	7.22	3.2	0.18	0.17	−5.7
Sugar beets	6.86	7.13	3.8	0.17	0.16	−4.5
Sunflowers	5.97	6.06	1.5	0.15	0.14	−3.3
Tobacco	6.01	6.11	1.7	0.15	0.15	−3.0
Tomatoes	6.22	6.60	6.2	0.16	0.15	−1.8
Vines (between-row, bare soil)	17.83	17.72	−0.6	0.20	0.17	−17.2
Vines (in-row)	20.80	17.70	−14.9	0.14	0.11	−21.7
Winter cereals	6.63	8.58	29.4	0.17	0.19	11.1

Table H.3: Concentration in pore water (mg/L) and the concentration in total soil (mg/kg) for pesticide P in the top 5 cm of soil in regulatory zone **South**. The percentage difference (%) was calculated by dividing the difference by the value of PEARL

Crop	Concentration in total soil (mg/kg)			Concentration in pore water (mg/L)		
	PEARL	PELMO	Difference (%)	PEARL	PELMO	Difference (%)
Apples (between-row, grass)	15.95	12.90	–19.1	0.25	0.18	–28.4
Apples (in-row)	9.45	9.36	–0.9	0.13	0.11	–9.0
Beans (field, veg.)	8.65	7.02	–18.9	0.44	0.31	–30.2
Bush berries (between-row, grass)	15.95	12.77	–19.9	0.25	0.17	–29.7
Bush berries (in-row)	10.51	10.05	–4.4	0.14	0.13	–12.3
Cabbage	8.93	7.44	–16.6	0.39	0.30	–21.9
Carrots	8.71	7.47	–14.2	0.38	0.30	–22.4
Citrus (between-row, bare soil)	10.48	10.40	–0.7	0.25	0.20	–19.6
Citrus (in-row)	10.11	8.93	–11.7	0.14	0.12	–14.4
Cotton	4.72	4.66	–1.3	0.23	0.21	–9.6
Fallow	4.50	5.07	12.8	0.23	0.24	3.2
Grass (pasture)	13.46	10.83	–19.5	0.21	0.15	–28.0
Hops (between-row, bare soil)	9.77	9.32	–4.6	0.22	0.19	–12.3
Hops (in-row)	12.76	10.96	–14.1	0.20	0.16	–23.6
Linseed	5.18	4.96	–4.2	0.26	0.23	–9.4
Maize	4.38	4.37	–0.2	0.23	0.21	–6.8
Oilseed rape (summer)	4.52	4.35	–3.8	0.23	0.21	–12.3
Oilseed rape (winter)	4.32	4.54	5.1	0.23	0.22	–3.5
Olives (between-row, bare soil)	10.48	10.40	–0.7	0.25	0.20	–19.6
Olives (in-row)	8.28	6.76	–18.4	0.17	0.12	–28.0
Onions	5.23	4.90	–6.2	0.25	0.23	–10.0
Peas (animal)	4.46	4.41	–1.1	0.23	0.21	–8.0
Potatoes	4.48	4.41	–1.6	0.23	0.21	–9.8
Soybean	4.28	4.35	1.7	0.22	0.20	–8.9
Spring cereals	4.42	4.37	–1.2	0.23	0.21	–10.2
Strawberries	4.86	4.47	–7.9	0.23	0.20	–12.7
Sugar beets	4.45	4.38	–1.5	0.23	0.21	–8.4
Sunflowers	4.35	4.33	–0.4	0.23	0.21	–8.3
Tobacco	4.23	4.39	3.8	0.21	0.20	–4.8
Tomatoes	5.01	4.97	–0.9	0.24	0.23	–4.9
Vines (between-row, bare soil)	10.48	10.40	–0.7	0.25	0.20	–19.6
Vines (in-row)	10.32	9.34	–9.5	0.14	0.12	–15.7
Winter cereals	4.36	4.54	4.2	0.23	0.22	–5.0

H.3. Water balances

The following tables contain the most important terms of the water balances as simulated by PEARL and PELMO. Tables H.4–H.6 contain the top boundary conditions, i.e. precipitation, irrigation and wash-off from the crop canopy. Tables H.7–H.9 contain evapotranspiration terms and Tables H.10–H.12 contain the leaching flux at 1 m depth.

Table H.4: Mean annual precipitation (P), irrigation and wash-off calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **North**. All balance terms are in mm/year

Crop	Concentration in pore water scenarios					Concentration in total soil scenarios				
	P	Irrigation		Wash-off		P	Irrigation		Wash-off	
		PEARL	PELMO	PEARL	PELMO		PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	602	0	0	602	602	639	0	0	639	639
Apples (in-row)	602	0	0	602	602	639	0	0	639	639
Beans (field, veg.)	602	0	0	602	602	639	0	0	639	639
Bush berries (between-row, grass)	602	0	0	602	602	639	0	0	639	639
Bush berries (in-row)	602	0	0	602	602	639	0	0	639	639
Cabbage	602	0	0	602	602	639	0	0	639	639
Carrots	602	0	0	602	602	639	0	0	639	639
Fallow	602	0	0	602	602	639	0	0	639	639
Grass (pasture)	602	0	0	602	602	639	0	0	639	639
Linseed	602	0	0	602	602	639	0	0	639	639
Maize	602	0	0	602	602	639	0	0	639	639
Oilseed rape (summer)	602	0	0	602	602	639	0	0	639	639
Oilseed rape (winter)	602	0	0	602	602	639	0	0	639	639
Onions	602	0	0	602	602	639	0	0	639	639
Peas (animal)	602	0	0	602	602	639	0	0	639	639
Potatoes	602	0	0	602	602	639	0	0	639	639
Spring cereals	602	0	0	602	602	639	0	0	639	639
Strawberries	602	0	0	602	602	639	0	0	639	639
Sugar beets	602	0	0	602	602	639	0	0	639	639
Tomatoes	602	0	0	602	602	639	0	0	639	639
Winter cereals	602	0	0	602	602	639	0	0	639	639

Table H.5: Mean annual precipitation (P), irrigation and wash-off calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **Centre.** All balance terms are in mm/year

Crop	Concentration in total soil scenarios					Concentration in pore water scenarios				
	P	Irrigation		Wash-off		P	Irrigation		Wash-off	
		PEARL	PELMO	PEARL	PELMO		PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	589	0	0	589	589	617	0	0	617	617
Apples (in-row)	589	0	0	589	589	617	0	0	617	617
Beans (field, veg.)	589	0	0	590	589	617	0	0	617	617

Crop	Concentration in total soil scenarios					Concentration in pore water scenarios				
	P	Irrigation		Wash-off		P	Irrigation		Wash-off	
		PEARL	PELMO	PEARL	PELMO		PEARL	PELMO	PEARL	PELMO
Bush berries (between-row, grass)	589	0	0	590	589	617	0	0	617	617
Bush berries (in-row)	649	155	239	649	648	649	182	239	649	648
Cabbage	649	158	249	806	897	649	166	239	815	887
Carrots	649	111	197	759	845	649	124	191	772	840
Cotton	589	0	0	589	589	617	0	0	617	617
Fallow	589	0	0	589	589	617	0	0	617	617
Grass (pasture)	589	0	0	589	589	617	0	0	617	617
Hops (between-row, bare soil)	589	0	0	589	589	617	0	0	617	617
Hops (in-row)	589	0	0	589	589	617	0	0	617	617
Linseed	589	0	0	589	589	617	0	0	617	617
Maize	649	209	290	858	939	649	232	286	880	934
Oilseed rape (summer)	589	0	0	589	589	617	0	0	617	617
Oilseed rape (winter)	589	0	0	589	589	617	0	0	617	617
Onions	589	0	0	589	589	617	0	0	617	617
Peas (animal)	589	0	0	590	589	617	0	0	617	617
Potatoes	589	0	0	589	589	617	0	0	617	617
Soybean	649	217	293	865	942	649	235	291	884	939
Spring cereals	589	0	0	590	589	617	0	0	617	617
Strawberries	589	0	0	590	589	617	0	0	617	617
Sugar beets	589	0	0	589	589	617	0	0	617	617
Sunflowers	649	220	343	869	991	649	251	341	899	990
Tobacco	649	200	306	849	954	649	226	304	874	952
Tomatoes	649	127	190	775	839	649	141	189	789	837
Vines (between-row, bare soil)	589	0	0	590	589	617	0	0	617	617
Vines (in-row)	649	112	239	649	648	649	102	239	649	648
Winter cereals	589	0	0	590	589	617	0	0	617	617

Table H.6: Mean annual precipitation (P), irrigation and wash-off calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **South.** All balance terms are in mm/year

Crop	Concentration in total soil scenarios					Concentration in pore water scenarios				
	P	Irrigation		Wash-off		P	Irrigation		Wash-off	
		PEARL	PELMO	PEARL	PELMO		PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	526	0	0	526	526	667	0	0	667	667
Apples (in-row)	493	885	903	493	493	493	885	903	493	493

Crop	Concentration in total soil scenarios					Concentration in pore water scenarios				
	P	Irrigation		Wash-off		P	Irrigation		Wash-off	
		PEARL	PELMO	PEARL	PELMO		PEARL	PELMO	PEARL	PELMO
Beans (field, veg.)	526	0	0	526	526	668	0	0	668	668
Bush berries (between-row, grass)	526	0	0	526	526	667	0	0	667	667
Bush berries (in-row)	493	651	651	493	493	493	651	651	493	493
Cabbage	493	490	583	983	1,076	493	490	583	983	1,076
Carrots	493	509	608	1,002	1,101	493	509	608	1,002	1,101
Citrus (between-row, bare soil)	526	0	0	526	526	667	0	0	667	667
Citrus (in-row)	493	561	728	493	493	493	561	728	493	493
Cotton	500	271	322	771	822	500	271	322	771	822
Fallow	526	0	0	526	526	667	0	0	667	667
Grass (pasture)	526	0	0	526	526	668	0	0	668	668
Hops (between-row, bare soil)	526	0	0	526	526	668	0	0	668	668
Hops (in-row)	526	0	0	526	526	668	0	0	668	668
Linseed	526	0	0	526	526	667	0	0	667	667
Maize	526	0	0	526	526	668	0	0	668	668
Oilseed rape (summer)	526	0	0	526	526	668	0	0	668	668
Oilseed rape (winter)	526	0	0	526	526	668	0	0	668	668
Olives (between-row, bare soil)	526	0	0	526	526	667	0	0	667	667
Olives (in-row)	493	500	728	493	493	493	500	728	493	493
Onions	493	72	261	564	754	493	72	261	564	754
Peas (animal)	526	0	0	526	526	668	0	0	668	668
Potatoes	526	0	0	526	526	668	0	0	668	668
Soybean	500	526	578	1,026	1,078	500	526	578	1,026	1,078
Spring cereals	526	0	0	526	526	668	0	0	668	668
Strawberries	493	524	800	1,017	1,293	493	524	800	1,017	1,293
Sugar beets	526	0	0	526	526	668	0	0	668	668
Sunflowers	526	0	0	526	526	668	0	0	668	668
Tobacco	493	659	754	1,152	1,247	493	659	754	1,152	1,247
Tomatoes	493	138	180	631	673	493	138	180	631	673
Vines (between-row, bare soil)	526	0	0	526	526	667	0	0	667	667
Vines (in-row)	493	659	769	493	493	493	659	769	493	493
Winter cereals	526	0	0	526	526	668	0	0	668	668

Table H.7: Mean annual potential evapotranspiration (ET_{pot}) and mean annual actual transpiration (ET_{act}) calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **North.** All balance terms are in mm/year

Crop	Concentration in pore water scenarios				Concentration in total soil scenarios			
	ET_{pot}		ET_{act}		ET_{pot}		ET_{act}	
	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	610	610	471	420	610	610	450	424
Apples (in-row)	647	647	505	471	647	647	475	466
Beans (field, veg.)	617	615	475	452	617	615	445	447
Bush berries (between-row, grass)	610	610	471	420	610	610	450	424
Bush berries (in-row)	510	508	418	395	510	508	404	396
Cabbage	605	605	462	427	605	605	442	429
Carrots	602	601	461	438	602	601	450	438
Fallow	610	610	334	355	610	610	338	363
Grass (pasture)	610	610	471	420	610	610	450	424
Linseed	600	598	453	410	600	598	425	412
Maize	622	621	460	454	622	621	442	450
Oilseed rape (summer)	603	603	463	425	603	603	435	426
Oilseed rape (winter)	603	605	481	522	603	605	458	532
Onions	582	580	444	426	582	580	424	426
Peas (animal)	637	637	484	460	637	637	454	456
Potatoes	625	624	452	429	625	624	430	429
Spring cereals	621	619	489	459	621	619	455	453
Strawberries	610	610	482	439	610	610	455	438
Sugar beets	628	627	472	446	628	627	446	444
Tomatoes	614	614	457	442	614	614	431	441
Winter cereals	613	623	480	507	613	623	454	513

Table H.8: Mean annual potential evapotranspiration (ET_{pot}) and mean annual actual transpiration (ET_{act}) calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **Centre**. All balance terms are in mm/year

Crop	Concentration in pore water scenarios				Concentration in total soil scenarios			
	ET_{pot}		ET_{act}		ET_{pot}		ET_{act}	
	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	610	610	467	416	610	610	443	417
Apples (in-row)	647	647	501	466	647	647	469	459
Beans (field, veg.)	780	777	539	521	779	777	513	517
Bush berries (between-row, grass)	774	774	523	478	774	774	507	482
Bush berries (in-row)	639	638	575	625	639	638	588	623
Cabbage	765	765	609	661	765	765	604	651
Carrots	766	765	591	647	766	765	589	639
Cotton	613	611	452	433	613	611	424	431

Crop	Concentration in pore water scenarios				Concentration in total soil scenarios			
	ET_{pot}		ET_{act}		ET_{pot}		ET_{act}	
	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO
Fallow	610	610	331	351	610	610	334	357
Grass (pasture)	610	610	467	416	610	610	443	417
Hops (between-row, bare soil)	610	610	331	351	610	610	334	357
Hops (in-row)	505	554	400	458	505	554	400	449
Linseed	600	598	449	406	600	598	419	406
Maize	788	787	661	721	788	787	669	715
Oilseed rape (summer)	603	603	460	422	603	603	429	420
Oilseed rape (winter)	603	605	479	515	603	605	453	521
Onions	582	580	441	423	582	580	419	420
Peas (animal)	808	808	520	496	808	808	493	496
Potatoes	625	624	449	425	625	624	424	423
Soybean	778	775	661	705	778	775	665	701
Spring cereals	770	768	504	487	770	768	477	487
Strawberries	774	774	538	510	774	774	516	509
Sugar beets	628	627	469	442	628	627	440	438
Sunflowers	794	793	683	760	794	793	699	757
Tobacco	773	773	637	711	773	773	647	707
Tomatoes	777	776	623	660	777	776	617	653
Vines (between-row, bare soil)	774	774	384	427	774	774	386	433
Vines (in-row)	650	646	582	640	650	646	569	638
Winter cereals	768	782	511	526	768	782	489	533

Table H.9: Mean annual potential evapotranspiration (ET_{pot}) and mean annual actual transpiration (ET_{act}) calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **South.** All balance terms are in mm/year

Crop	Concentration in pore water scenarios				Concentration in total soil scenarios			
	ET_{pot}		ET_{act}		ET_{pot}		ET_{act}	
	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	1,494	1,494	428	385	1,494	1,494	476	433
Apples (in-row)	1,560	1,559	1,217	1,291	1,560	1,559	1,217	1,291
Beans (field, veg.)	607	605	443	394	607	605	481	440
Bush berries (between-row, grass)	1,494	1,494	428	385	1,494	1,494	476	433
Bush berries (in-row)	1,206	1,204	961	987	1,206	1,204	961	987
Cabbage	1,483	1,482	856	917	1,483	1,482	856	917
Carrots	1,500	1,497	891	959	1,500	1,497	891	959
Citrus (between-row, bare soil)	1,494	1,494	298	333	1,495	1,494	321	367
Citrus (in-row)	896	896	850	896	896	896	850	896
Cotton	1,199	1,196	673	715	1,199	1,196	673	715
Fallow	1,494	1,494	298	333	1,495	1,494	321	367

Crop	Concentration in pore water scenarios				Concentration in total soil scenarios			
	ET_{pot}		ET_{act}		ET_{pot}		ET_{act}	
	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO
Grass (pasture)	610	610	446	394	610	610	488	442
Hops (between-row, bare soil)	610	610	316	331	610	610	346	372
Hops (in-row)	505	554	394	442	505	554	405	474
Linseed	1,451	1,446	398	374	1,451	1,446	436	408
Maize	622	621	441	433	622	621	473	470
Oilseed rape (summer)	603	603	439	402	603	603	479	443
Oilseed rape (winter)	603	605	463	481	603	605	491	556
Olives (between-row, bare soil)	1,494	1,494	298	333	1,495	1,494	321	367
Olives (in-row)	896	896	767	896	896	896	767	896
Onions	1,466	1,475	438	610	1,466	1,475	438	610
Peas (animal)	637	637	460	437	637	637	498	477
Potatoes	625	624	432	406	625	624	465	446
Soybean	1,199	1,195	875	914	1,199	1,195	875	914
Spring cereals	621	619	465	438	621	619	503	475
Strawberries	1,494	1,494	884	1,057	1,494	1,494	884	1,057
Sugar beets	628	627	450	423	628	627	486	463
Sunflowers	630	629	457	444	630	629	494	484
Tobacco	1,491	1,492	987	1,080	1,491	1,492	987	1,080
Tomatoes	1,478	1,476	524	567	1,478	1,476	524	567
Vines (between-row, bare soil)	1,494	1,494	298	333	1,495	1,494	321	367
Vines (in-row)	1,206	1,202	965	1,105	1,206	1,202	965	1,105
Winter cereals	613	623	461	469	613	623	490	537

Table H.10: Mean annual water flux from the top 1 metre of the soil column calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **North**. All balance terms are in mm/year

Crop	Concentration in pore water scenarios		Concentration in total soil scenarios	
	PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	132	182	190	215
Apples (in-row)	97	133	165	174
Beans (field, veg.)	126	151	195	192
Bush berries (between-row, grass)	132	182	190	215
Bush berries (in-row)	185	208	236	243
Cabbage	140	175	198	210
Carrots	142	164	191	201
Fallow	269	247	302	277
Grass (pasture)	132	182	190	215
Linseed	150	192	215	227
Maize	142	149	198	190
Oilseed rape (summer)	139	177	205	214
Oilseed rape (winter)	121	83	182	109
Onions	159	176	216	214

Crop	Concentration in pore water scenarios		Concentration in total soil scenarios	
	PEARL	PELMO	PEARL	PELMO
Peas (animal)	118	143	186	184
Potatoes	151	174	211	211
Spring cereals	113	144	185	187
Strawberries	121	163	185	201
Sugar beets	130	157	194	195
Tomatoes	146	160	210	199
Winter cereals	122	96	186	126

Table H.11: Mean annual water flux from the top 1 metre of the soil column calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **Centre**. All balance terms are in mm/year

Crop	Concentration in pore water scenarios		Concentration in total soil scenarios	
	PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	122	173	175	200
Apples (in-row)	87	124	149	159
Beans (field, veg.)	55	69	106	101
Bush berries (between-row, grass)	69	112	111	135
Bush berries (in-row)	229	263	243	264
Cabbage	198	236	211	237
Carrots	168	199	184	201
Cotton	137	156	194	187
Fallow	258	238	285	261
Grass (pasture)	122	173	175	200
Hops (between-row, bare soil)	258	238	285	261
Hops (in-row)	189	132	218	168
Linseed	140	183	199	212
Maize	197	217	211	219
Oilseed rape (summer)	129	168	189	198
Oilseed rape (winter)	110	77	165	98
Onions	148	166	199	197
Peas (animal)	72	95	125	122
Potatoes	141	164	194	195
Soybean	205	236	219	238
Spring cereals	88	103	141	130
Strawberries	55	80	103	108
Sugar beets	120	147	178	180
Sunflowers	185	231	200	233
Tobacco	212	242	228	243
Tomatoes	154	178	172	184
Vines (between-row, bare soil)	206	162	232	185
Vines (in-row)	179	248	182	249
Winter cereals	82	65	129	86

Table H.12: Mean annual water flux from the top 1 metre of the soil column calculated by PEARL and PELMO for the concentration in total soil scenarios and for the pore water scenarios for regulatory zone **South**. All balance terms are in mm/year

Crop	Concentration in pore water scenarios		Concentration in total soil scenarios	
	PEARL	PELMO	PEARL	PELMO
Apples (between-row, grass)	102	143	190	235
Apples (in-row)	161	114	161	114
Beans (field, veg.)	83	133	187	228
Bush berries (between-row, grass)	102	143	190	235
Bush berries (in-row)	184	159	184	159
Cabbage	129	160	129	160
Carrots	115	142	115	142
Citrus (between-row, bare soil)	228	194	342	301
Citrus (in-row)	204	325	204	325
Cotton	101	110	101	110
Fallow	228	194	342	301
Grass (pasture)	80	132	180	226
Hops (between-row, bare soil)	211	195	322	295
Hops (in-row)	132	85	262	194
Linseed	131	154	230	260
Maize	85	94	195	198
Oilseed rape (summer)	86	124	189	224
Oilseed rape (winter)	61	50	177	114
Olives (between-row, bare soil)	228	194	342	301
Olives (in-row)	226	325	226	325
Onions	129	144	129	144
Peas (animal)	64	89	170	191
Potatoes	94	120	203	221
Soybean	154	165	154	165
Spring cereals	59	88	165	193
Strawberries	135	235	135	235
Sugar beets	75	103	182	204
Sunflowers	68	83	174	184
Tobacco	166	168	166	168
Tomatoes	111	110	111	110
Vines (between-row, bare soil)	228	194	342	301
Vines (in-row)	187	160	187	160
Winter cereals	63	57	178	131

Appendix I – Modelling results and water balance used for the practical examples

An Excel sheet is enclosed with the model results as supporting information. Calculations in this appendix were done with the model versions that were available at the time of publication of this Guidance Document and may change when updated model version are released. The numerical model versions at the time of publication were PEARL kernel version 3.2.8 (16 June 2017) and PELMO version 4.10 (February 2017).