European Food Safety Authority

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## GUIDANCE OF EFSA

# EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil[1]

**European Food Safety Authority**[2,3]

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## 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[4] 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 Art. 31 of Regulation (EC) No 178/2002[5] 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 is restricted to annual field crops under conventional and reduced tillage. The recommended exposure assessment procedure consists of five 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, an easy-to-use table for the fraction of the dose reaching the soil has been developed, which should be used at higher tiers 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.



## KEY WORDS

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

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[4] 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, p. 1-50.

[5] 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, p. 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 EC No 1107/2009 of the European Parliament and the Council.[6] This guidance was produced by EFSA in response to a question posed by the European Commission according to Art. 31 of Regulation (EC) No 178/2002 of the European Parliament and of the Council.[7] 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. 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, 2015).

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, 2012a). The goal is to assess the 90th percentile concentration considering all agricultural fields within a regulatory zone (North–Central–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 $kg^{-1}$) and the concentration in pore water (mg $l^{-1}$), 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 $ha^{-1}$). The current methodology is restricted to annual crops under conventional and reduced tillage (excluding crops grown on ridges). Guidance for permanent crops, no-tillage systems and crops grown on ridges will be made available at a later stage.

The recommended exposure assessment procedure consists of five 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, 2012a). 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)).


[6] 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, p. 1–50.

[7] 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, p. 1–22.

This guidance has changed the tiered assessment scheme given in EFSA PPR Panel (2012a) 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–Central–South. Simulations can be carried out with the simple analytical model PERSAM at Tier 1 or with the numerical models (PEARL and PELMO) at Tier 2A. At Tier 1, PERSAM has the advantage that the required number of inputs is very limited and thus the documentation will also require little effort. Tier 2A 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.

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. As a consequence, 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.

The predefined scenarios in Tier 1 and Tier 2A are based on the total area of annual crops 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, Tiers 2B and 2C are provided. At these tiers, 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 3. Tier 3 is also based on the area of a given crop, but uses numerical models (PEARL and PELMO). In Tier 3B crop-specific and substance-specific scenarios are used. Guidance is given on how to select and use these scenarios. This guidance document introduces an easy to use Tier 3A, which uses a refined scenario adjustment factor based on results from Tier 2A and Tier 2B.

Tiers 1 and 2B are based on the assumption that crop interception of the substance does not occur. In Tiers 2A, 2C, 3A, 3B and 4 this can be included. Interception and subsequent dissipation at the crop canopy may be based on simulations with the numerical models. To facilitate harmonisation of the regulatory process, canopy processes in PEARL and PELMO were harmonised. This guidance further introduces a table for the fraction of the dose reaching the soil surface that was created based on simulations with PEARL and PELMO. This table should be used at Tier 2C. The availability of this table simplifies the tiered approach because it is no longer necessary to run Tier 2A before Tier 2C.

The predefined scenarios used at Tier 1 and 2A are based on the 95th spatial percentile considering the total area of annual crops in each regulatory zone. However, the purpose of the exposure assessment is to consider 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, 2012a) have been included at Tier 1 and Tier 2A to ensure that these tiers are more conservative than Tiers 2B, 2C, 3A, 3B and 4.

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 Tiers 2A, 3A, 3B and 4, model adjustment factors have been included in all tiers where the analytical model is used. The model adjustment factors proposed in EFSA PPR Panel (2012a) have been reassessed for this guidance document and the number of factors has been reduced to ease their use in the regulatory process.

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.

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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 EU Member States (MSs) requested a revision of the SANCO Guidance Document on persistence in soil (SANCO/9188VI/1997 of 12 July 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, 2012a) the Commission tasked 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 Commission dated 9 October 2012. The 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, 2012a), 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 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 Commission (DG SANCO) 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, 2012a).

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 in accordance with Regulation EC No 1107/2009 of the European Parliament and the Council (Figure 1). 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 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, 2015).

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 European Food Safety Authority (EFSA) Plant Protection Products and their Residues (PPR) Panel (2010a, d, 2012a, b). Some further scientific developments have taken place after the publication of EFSA PPR Panel (2012a) with the goal to facilitate and further harmonise the exposure assessment. These scientific developments are described in the appendices to this guidance document.

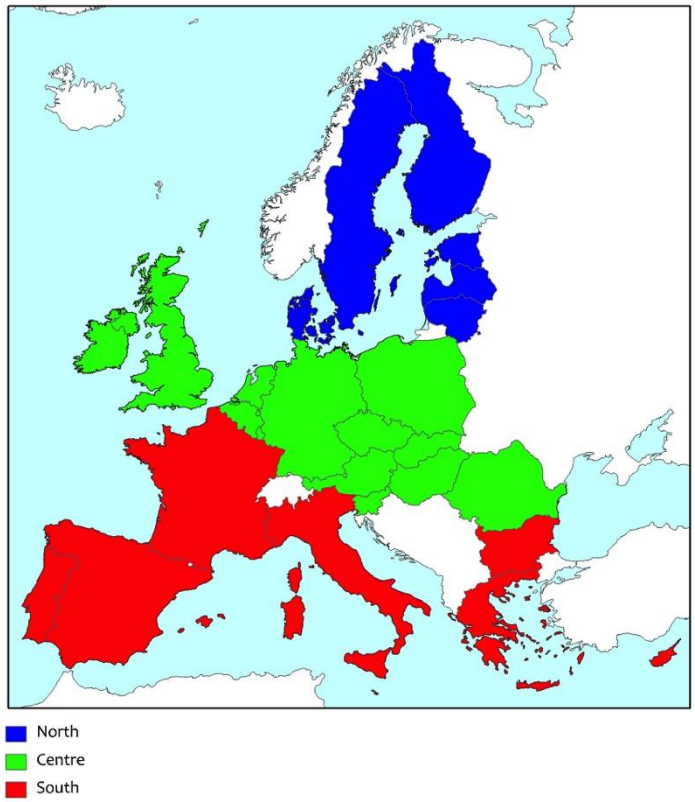


**Figure 1:** Map of the three regulatory zones according to Regulation EC No 1107/2009 of the European Parliament and the Council.

The recommended procedure consists of five tiers. The first three tiers are explained in this guidance document. This guidance document will also provide brief guidance on Tier 4 (spatially distributed

modelling with numerical models) and Tier 5 (post-registration monitoring). The scenarios in this guidance document were selected using a procedure that works well for parent substances 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 methodology also provides conservative estimates of exposure for metabolites at Tiers 1 and 2B/C. Additional analyses show that results generated at Tiers 2A, 3A and 3B may not represent the 95th spatial percentile exposure estimate for all metabolites. Despite this, it is advisable to use the exposure assessment scheme also for all metabolites.

### 1.2. The exposure assessment goal

As described in EFSA PPR Panel (2012a), the methodology is based on the goal to assess the 90th percentile concentration considering all agricultural fields within a regulatory zone (North–Central–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 pedological data to identify scenarios (e.g. Forum for Co-ordination of Pesticide Fate Models and their Use (FOCUS) Groundwater reports of 2000 and 2014, in which nine scenarios were distinguished). This 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 for assessing 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 (2009) indicated that the following types of concentrations are needed:

- The concentration in total soil (mg $kg^{-1}$) averaged over the top 1, 5 or 20 cm of soil for various time windows: peak and time-weighted averages (TWAs) for 7–56 days.
- The concentration in pore water (mg $l^{-1}$) averaged over the top 1, 5 or 20 cm of soil for the same time windows.

As indicated in EFSA PPR Panel (2012a), 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 following after the occurrence of the peak concentration.

Older soil ecotoxicological studies sometimes expressed exposure in terms of only the applied rate (in kg $ha^{-1}$). This guidance document therefore also briefly describes how to express exposure in kg $ha^{-1}$.

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 (2009)).

Based on discussions with stakeholders, it was a boundary condition that the exposure assessment methodology can be applied by taking median or average substance properties from the dossiers (so no high or low percentile values of substance properties should be used). Such substance properties are uncertain and inclusion of this uncertainty leads to probability density functions that show greater spread. As a consequence, 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 (2012a) for details). Together with the 100th percentile in time and the median or average substance properties, the overall goal (90th percentile concentration) is considered to be reached.

### 1.3. Cropping and applications systems covered by this guidance

The methodology has been developed for spray applications to annual crops under conventional and reduced tillage (excluding tillage systems with ridges and furrows; Figure 2). For both conventional and reduced tillage systems it is assumed that the soil is ploughed annually to a depth of 20 cm (EFSA PPR Panel, 2010d). It is assumed that for applications of granular products (to the soil surface or incorporated), this methodology can be used as well. With small modifications, the procedure covers row treatments to a reasonable degree.

The exposure assessment for annual crops differs from that for permanent crops (e.g. permanent crops often have a litter layer). The exposure assessment for no-tillage systems is also different because annual ploughing has a large diluting effect on the concentration in the topsoil (which, of course, does not occur in no-tillage systems). The current guidance document is therefore not applicable to permanent crops and no-tillage systems (Figure 2). The exposure assessment methodology for these cropping systems is currently under development, and guidance for these cropping systems should be available by the end of 2017. Until new guidance has been taken note of by the Standing Committee of Plant Animal Food and Feed (SCoPAFF), and a date for implementation has been set, old methods still apply.

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 guidance.

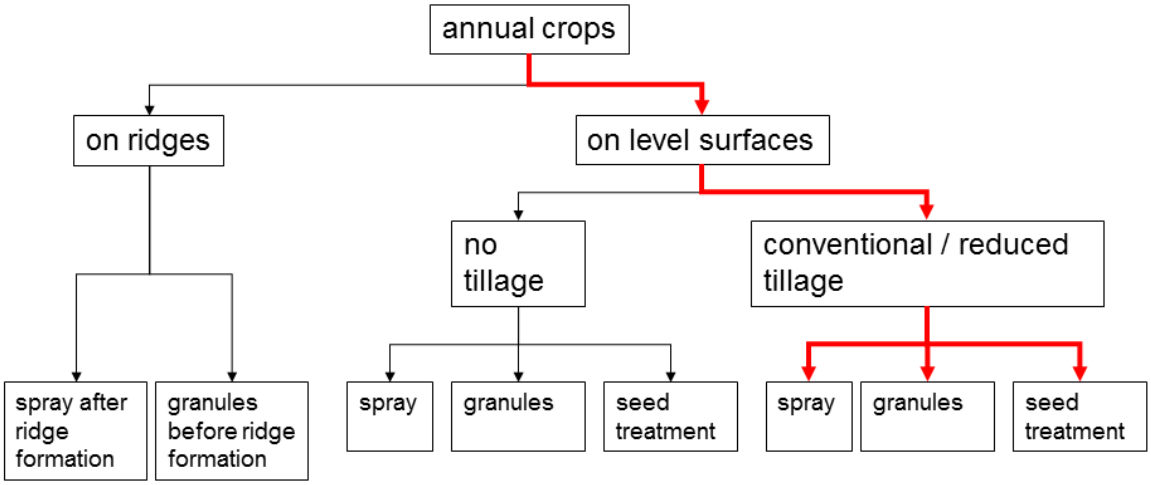


**Figure 2:** Cropping and application systems covered by this guidance are indicated by red lines

### 1.4. Software tools

To facilitate efficient use of the tiered approach in regulatory practice, user-friendly software tools have been developed. This includes the new software tool PERSAM (Persistence in Soil Analytical Model) (Decorte et al., 2014a; based on EFSA PPR Panel, 2012a) 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) 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 EFSA, 2010a). This must be performed in combination with the EFSA spatial dataset (version 1.1) as available at the Joint Research Centre (JRC) website. Applicants should demonstrate that their own software reproduces the same output as PERSAM, e.g. by comparison for the six 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 PEARL or PELMO, they should demonstrate that their model produces the

same 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)).

The software tools are operational for spray applications to annual crops under conventional and reduced tillage (excluding tillage systems with ridges and furrows). These cropping systems are indicated with solid red lines in Figure 2.

### 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, 2012a) on which this guidance document is based. Section 3 provides practical guidance on how to perform exposure assessments in soil for annual crops for active substances of PPPs and for the metabolites of these active substances. Section 3 is restricted to spray applications; the other application types (row treatments, seed treatments and granules) are described in Section 4. Section 5 briefly describes documentation requirements. Scientific backgrounds to the new developments, desirable future development and practical examples are given in the Appendices.

## 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 PPR Panel (2012a) proposed a tiered assessment scheme for the exposure assessment. This guidance has changed the tiered assessment scheme with the goal to simplify the exposure assessment for regulatory purposes. The revised scheme can be found in Figure 3. The lower tiers are more conservative and less sophisticated than the higher tiers, but all tiers aim to address the same protection goal (i.e. the 90th percentile concentration within the area of intended use of a PPP). This principle allows the direct move 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). However, in the current tiered approach, Tier 3A depends on input from lower tiers. In this case, the applicant should, of course, first carry out the lower tier assessments (see Section 3.6). For transparency, and to allow comparison between substances, applicants should in this case also submit results derived from lower tiers (see Section 5 for reporting requirements).

The exposure assessment starts with simulations for one predefined scenario per regulatory zone, North–Central–South. Simulations can be carried out with PERSAM at Tier 1 or with one of the numerical models at Tier 2A. At Tier 1, PERSAM has the advantage that the required number of inputs is very limited and thus also the documentation will require little effort. Tier 2A 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.

The predefined scenarios in Tier 1 and Tier 2A are based on the total area of annual crops in a regulatory zone. However, 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, Tiers 2B and 2C are provided. At these tiers, 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. The predefined scenarios at Tier 1 and Tier 2A are not designed for substances whose properties depend on soil properties such as pH. For such substances, the applicant should therefore go to Tier 2B/C or Tier 3B 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.

Tiers 1 and 2B are based on the assumption that crop interception of the substance does not occur. In Tiers 2A, 2C, 3A, 3B and 4, crop interception and subsequent loss processes at the plant canopy can be included. This can be carried out by simulations with the numerical models at Tier 2A, 3A or 3B, or by using a table with default soil loads depending on crop development (Table 7) at Tier 2C. Refer to Section 2.5 for details on crop interception.

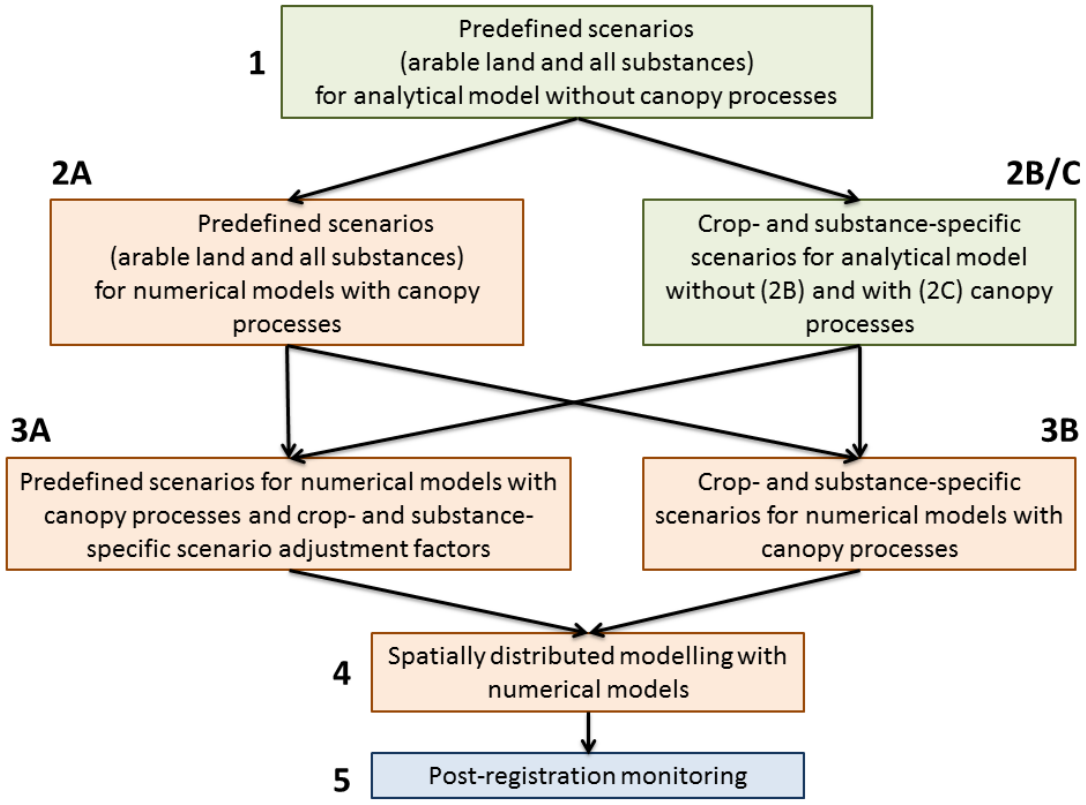


**Figure 3:** Tiered scheme for the exposure assessment of spray applications to annual crops under conventional or reduced tillage. The scheme applies to both the concentration in total soil and the concentration in pore water. Tiers 1, 2 and 3 are all based on one PEC for each of the regulatory zones, North, Central and South, and allow for one or multiple applications every one, two or three years. At Tiers 1 and 2B/C (green) the analytical model in the software tool PERSAM is used. At Tiers 2A, 3A, 3B and 4 (orange) modelling is carried out with numerical models

Should the assessment at Tier 2 still indicate an unacceptable risk to soil organisms, the applicant has the option to move to Tier 3. Tier 3 is based on the numerical models and on the area of a given crop. Tier 3 has two options:

- Tier 3A, which uses a crop- and substance-specific scenario adjustment factor to refine the exposure assessment at Tier 2A. This refined scenario adjustment factor is based on the ratio between the PEC obtained at Tier 2B and Tier 1 divided by the default scenario adjustment factor and is therefore very simple to carry out. However, this procedure is defensible only for substances whose properties do not depend on soil properties.
- Tier 3B, which uses crop- and substance-specific scenarios. In contrast to Tier 3A, the Tier 3B scenarios are also valid for substances whose properties depend on soil properties. The scenario is first identified in the PERSAM software. PERSAM then generates a file containing the geographical coordinates. This file is used by PEARL or PELMO to automatically generate the input files for the Tier 3B scenarios.

The scheme also contains a Tier 4, 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. The development of such a model is possible using the database, which is available at the European Soil Data Centre (Panagos et al., 2012); guidance is given in Section 3.8. Tier 5 is a post-registration monitoring approach, which is described in Section 3.9.

## 2.2. Properties of the six predefined soil exposure scenarios

As described in the previous section, Tiers 1, 2A and 3A are based on one predefined scenario per regulatory zone (North–Central–South) for each of the two types of Ecotoxicological Relevant Concentration (ERC) (concentration in total soil and concentration in pore water). The properties of these six scenarios are summarised in Tables 1 and 2 and their position is shown in Figure 4.

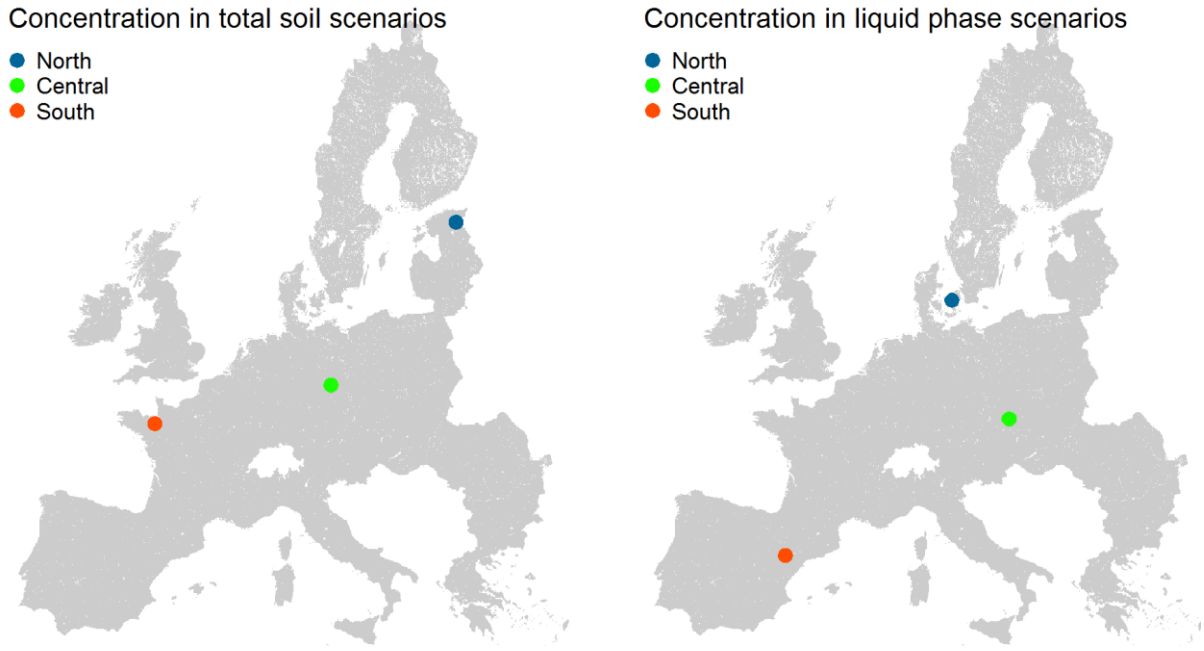


**Figure 4:** Position of the six predefined scenarios for carrying out Tier 1, 2A and 3A soil exposure assessments. Left-hand panel: Scenarios for the concentration in total soil. Right-hand panel: Scenarios for the concentration in pore water

**Table 1:** Properties of the predefined scenarios used at Tier 1, Tier 2A and Tier 3A for the concentration in total soil.

| Zone | Code | Country | $T_{arit}$ [(a)] (°C) | $T_{arr}$ [(b)] (°C) | Texture | $f_{om}$ (–) [(c)] | $\theta_{fc}$ ($m^3$ $m^{-3}$) [(d)] | ρ (kg $dm^{-3}$)[(e)] |
|---|---|---|---|---|---|---|---|---|
| North | CTN | Estonia | 4.7 | 7.0 | Coarse | 0.118 | 0.244 | 0.95 |
| Central | CTC | Germany | 8.0 | 10.1 | Coarse | 0.086 | 0.244 | 1.05 |
| South | CTS | France | 11.0 | 12.3 | Medium fine | 0.048 | 0.385 | 1.22 |

*(a):* $T_{arit}$ is the arithmetic mean annual temperature
(b): $T_{arr}$ is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012a)
(c): $f_{om}$ (–) is the organic matter content
*(d):* $\theta_{fc}$ ($m^3$ $m^{-3}$) is the water content at field capacity
(e): ρ (kg $dm^{-3}$) is the dry bulk density of the soil.
Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to EFSA PPR Panel (2012b)

CTC, scenario for the total concentration in the Central Zone; CTN, scenario for the total concentration in the North Zone; CTS, scenario for the total concentration in the South Zone.

**Table 2:** Properties of the selected predefined scenarios used at Tiers 1, 2A and 3A for the concentration in pore water.

| Zone | Code | Country | $T_{arit}$ (a) (°C) | $T_{arr}$ (b) (°C) | Texture | $f_{om}$ (–)(c) | $\theta_{fc}$ ($m^3$ $m^{-3}$) (d) | ρ (kg $dm^{-3}$) (e) |
|---|---|---|---|---|---|---|---|---|
| North | CLN | Denmark | 8.2 | 9.8 | Medium | 0.023 | 0.347 | 1.39 |
| Central | CLC | Czech Republic | 9.1 | 11.2 | Medium | 0.018 | 0.347 | 1.43 |
| South | CLS | Spain | 12.8 | 14.7 | Medium | 0.011 | 0.347 | 1.51 |

*(a):* $T_{arit}$ is the arithmetic mean annual temperature
(b): $T_{arr}$ is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012a)
(c): $f_{om}$ (–) is the organic matter content
*(d):* $\theta_{fc}$ ($m^3$ $m^{-3}$) is the water content at field capacity
(e): ρ (kg $dm^{-3}$) is the dry bulk density of the soil.
Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to EFSA PPR Panel (2012b)

CLC, scenario for the concentration in pore water for the Central 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.

## 2.3. Crops and scenario adjustment factors

The scenarios in Tables 1 and 2 were based on the 95th spatial percentile considering the total area of annual crops in each regulatory zone. However, the purpose of the exposure assessment is to consider 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 Tiers 1 and 2A default scenario adjustment factors (named crop extrapolation factors in EFSA PPR Panel, 2012a) are needed because the 95th percentile scenario for a specific crop could differ from the 95th percentile scenario for all arable land (see Table 3 for an overview of tiers where scenario adjustment factors are needed).

**Table 3:** Overview of inclusion of canopy processes, scenario adjustment factors and model adjustment factors in the different modelling tiers of Figure 3. "+" indicates that the process or factor is included, "–" indicates that it is not included and "o" indicates that a refined factor as indicated in the footnote is used

| Tier | Canopy processes | Scenario adjustment factors | Model adjustment factors |
|---|---|---|---|
| 1 | – | + | + |
| 2A | + | + | – |
| 2B | – | – | + |
| 2C | + | – | + |
| 3A | + | o (a) | – |
| 3B | + | – | – |
| 4 | + | – | – |

(a): At Tier 3A, substance- and crop-specific scenario adjustment factors are used instead of the conservative default scenario adjustment factors given in Table 4.

This guidance has slightly modified the procedure for deriving these scenario adjustment factors and therefore the values of these factors have changed as well. The spatial dataset on which the exposure scenarios are based has been replaced with a new version (see Appendix C1 for background information). The new scenario adjustment factors are listed in Table 4. For substantial future changes to spatial datasets a revision of the scenarios and the adjustment factors might again be needed. However, this is not expected to happen very often.

**Table 4:** Default scenario adjustment factors ($f_s$) to be used when performing an assessment for one of the PERSAM crops included in Table 5 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

| Zone | Default scenario adjustment factors to be used for the | |
|---|---|---|
| | Concentration in total soil | Concentration in pore water |
| North | 3.0 | 2.0 |
| Central | 2.0 | 1.5 |
| South | 2.0 | 1.5 |

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 when using one of the numerical models. In PERSAM, a crop must be specified at Tier 2B/C. As described in EFSA PPR Panel (2012a), PERSAM uses this crop as a proxy of the area of potential use of the PPP. For that reason, a PERSAM crop is also needed when performing an assessment at Tier 3B and Tier 4. The crop list in PERSAM is based on so-called Common Agricultural Policy Regionalised Impact (CAPRI) crops or crop groups (Leip et al., 2008) for which EU crop maps are available at a scale of $1 \times 1$ km$^2$. Table 5 gives the link between the two crop lists. As an example, if the user wants to carry out an assessment for the FOCUS crop "cabbage", the crop "other fresh vegetables" should be selected in PERSAM.

**Table 5:** PERSAM crop that a user has to select when performing an assessment for a specific FOCUS crop. The table further indicates for each of the six predefined scenarios which FOCUS–PERSAM combinations are possible and which FOCUS groundwater scenario is used by the numerical models for the crop parameterisation (see EFSA, 2012b). Note that the latter selection is done internally in the model shells and is added here for transparency reasons only

| FOCUS crop | PERSAM crop | CTN | CTC | CTS | CLN | CLC | CLS |
|---|---|---|---|---|---|---|---|
| Beans (field) | Pulses | HA | HA | – | HA | HA | – |
| Beans (vegetables) | Pulses | – | – | PO | – | – | TH |
| Cabbage | Other fresh vegetables | JO | CH | KR | HA | CH | SE |
| Carrots | Other fresh vegetables | – | CH | KR | HA | CH | TH |
| Cotton | Texture crops | – | – | SE | – | – | SE |
| Linseed | Texture crops | – | OK | OK | – | OK | OK |
| Maize | Maize | HA | CH | KR | HA | CH | SE |
| No crops (= fallow soil) | Fallow | JO | CH | KR | HA | CH | SE |
| Oil seed rape (summer) | Oilseed rapes | JO | OK | – | JO | OK | – |
| Oil seed rape (winter) | Oilseed rapes | HA | CH | KR | HA | CH | PI |
| Onions | Other fresh vegetables | JO | CH | KR | HA | CH | TH |
| Onions | Floriculture and flower bulbs[(a)] | JO | CH | KR | HA | CH | TH |
| Peas (animals) | Pulses | JO | CH | – | HA | CH | – |
| Potatoes[(b)] | Potatoes | JO | CH | KR | HA | CH | TH |
| Soybean | Soya beans | – | PI | PI | – | PI | PI |
| Strawberries | Other fresh vegetables | JO | HA | KR | HA | HA | SE |
| Sugar beets | Sugar beets | JO | CH | KR | HA | CH | SE |
| Sunflower | Sunflowers | – | PI | PI | – | PI | SE |
| Tobacco | Tobacco | – | – | PI | – | – | TH |
| Tomatoes | Other fresh vegetables | – | CH | PI | – | CH | SE |
| Spring cereals[(c)] | Barley | JO | CH | KR | HA | CH | PO |
| | Common wheat | JO | CH | KR | HA | CH | PO |
| | Durum wheat | – | CH | KR | – | CH | PO |
| | Oats | JO | CH | KR | HA | CH | PO |
| | Rye | JO | CH | KR | HA | CH | PO |
| Winter cereals[(c)] | Barley | JO | CH | KR | HA | CH | SE |
| | Common wheat | JO | CH | KR | HA | CH | SE |
| | Durum wheat | – | CH | KR | – | CH | SE |
| | Oats | JO | CH | KR | HA | CH | SE |
| | Rye | JO | CH | KR | HA | CH | SE |

(a): Not a FOCUS crop; therefore, onions are suggested as a surrogate in the numerical models at Tiers 2A, 3A and 3B.
(b): Potatoes are included in PERSAM; however, this guidance document does not apply to crops grown on ridges.
(c): In cases where the FOCUS crop spring or winter cereals is not represented by a PERSAM crop or is not further specified, for the concentration in the total soil, the application should use oats for the North Zone, rye for the Central Zone and common wheat for the South Zone. For the concentration in the pore water, rye should be used for the North Zone, common wheat for the Central Zone and oats for the South Zone. These crops have the largest scenario adjustment factors in their respective regulatory zones (also refer to Tables C.2 and C.3).
CH, Châteaudun; HA, Hamburg; JO, Jokioinen; KR, Kremsmünster; OK, Okehampton; PI, Piacenza; PO, Porto; SE, Seville. See EC (2014) for further details.

If a well-documented crop map is available, it is acceptable to use the Tier 2B procedure to calculate the 95th spatial percentile of the PEC using this crop map. This 95th percentile concentration can also be used to derive a crop- and substance-specific scenario adjustment factor, which can be used to refine the assessment at Tier 3A (see Section 3.6 for details). Since the current version of the PERSAM tool does not provide the option to import other crop maps, the Tier 2B assessments should be performed outside the software tool using, for example, the script in Appendix A6 of EFSA PPR Panel (2010a). "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).

## 2.4. Model adjustment factors

The simple analytical model is used in lower tiers. Since it cannot be a priori guaranteed that the simple analytical model is conservative enough when compared with the more realistic numerical models used in Tiers 2A, 3A, 3B and 4, model adjustment factors are needed in all the tiers that use the analytical model (Table 3). 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 (see Appendix C2 for details). The revised model adjustment factors are listed in Table 6. 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 (2012a) 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 as PEARL and PELMO, e.g. by comparison for the six predefined scenarios (see Section 1.4).

**Table 6:** Model adjustment factors ($f_M$) to be 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 | 2.0 | 4.0 |
| Central | 2.0 | 4.0 |
| South | 2.0 | 4.0 |

## 2.5. Crop canopy processes

Tiers 1 and 2B are based on the assumption that crop interception of the substance does not occur. In Tiers 2A, 2C, 3A, 3B and 4 this may be included (Table 3). 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. So 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 Tiers 2A, 3A, 3B and 4. 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 (see Appendix B3 for details).

The analytical model used at Tier 2C cannot simulate plant processes. For this reason, a table of the fraction of the dose reaching the soil depending on the crop development stage was created based on simulations with PEARL and PELMO. This table should be used only when performing an assessment at Tier 2C.

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 5):

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

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 fraction of the dose washed off from the canopy. The fraction of the dose intercepted was taken from EFSA (2014a). Further details on the development of the tables are given in Appendix B; the resulting calculations are summarised in Table 7. Note that this guidance uses the average fraction washed-off ($f_{soil}$) instead of the maximum fraction washed-off ($F_{soil,max}$), which was used in EFSA PPR Panel (2012a). 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 B2).

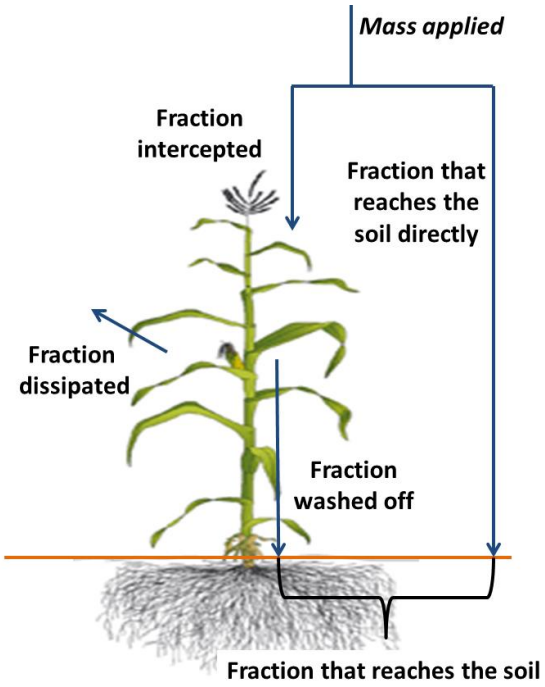


**Figure 5:** Schematic overview of the processes occurring at the crop canopy. The fraction of the dose reaching the soil is the sum of wash-off from the canopy and the fraction of the dose that reaches the soil directly

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.

**Table 7:** Fraction of the dose reaching the soil ($f_{soil}$) to be used at Tier 2C considering crop interception and canopy dissipation processes as a function of crop development stage. The figures are rounded to the nearest 0.05. Please note that this table is based on the weather conditions in the current six scenarios and should therefore not be used for groundwater assessments

| Crop | BBCH code[(a)(b)] | | | | |
|---|---|---|---|---|---|
| | **00–09** | **10–19** | **20–39** | **40–89** | **90–99** |
| Beans (vegetable and field) | 1.00 | 0.85 | 0.85 | 0.70 | 0.50 |
| Cabbage | 1.00 | 0.90 | 0.85 | 0.60–1.00[(c)] | 1.00[(c)] |
| Carrots | 1.00 | 0.85 | 0.75 | 0.45–1.00[(c)] | 1.00[(c)] |
| Cotton | 1.00 | 0.90 | 0.90 | 0.55 | 0.30 |
| Linseed | 1.00 | 0.80 | 0.70 | 0.70 | 0.70 |
| Maize | 1.00 | 0.85 | 0.80 | 0.65 | 0.40 |
| Onions | 1.00 | 0.95 | 0.90 | 0.80–1.00[(c)] | 1.00[(c)] |
| Peas | 1.00 | 0.75 | 0.70 | 0.65 | 0.60 |
| Oil seed rape (summer) | 1.00 | 0.75 | 0.65 | 0.65 | 0.55 |
| Oil seed rape (winter) | 1.00 | 0.75 | 0.60 | 0.65 | 0.40 |
| Sugar beets | 1.00 | 0.90 | 0.75 | 0.55–1.00[(c)] | 1.00[(c)] |
| Soybeans | 1.00 | 0.85 | 0.80 | 0.75 | 0.65 |
| Strawberries | 1.00 | 0.80 | 0.80 | 0.65 | 0.45 |
| Sunflowers | 1.00 | 0.90 | 0.80 | 0.75 | 0.40 |
| Tobacco | 1.00 | 0.70 | 0.70 | 0.70 | 0.60 |
| Tomatoes | 1.00 | 0.80 | 0.80 | 0.70 | 0.70 |
| **Crop** | **BBCH code[(d)]** | | | | |
| | **00–09** | **10–19** | **20–39** | **40–89** | **90–99** |
| Spring cereals | 1.00 | 0.90 | 0.70 | 0.65 | 0.60 |
| Winter cereals | 1.00 | 0.90 | 0.65 | 0.60 | 0.60 |

(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): Since these crops are harvested at BBCH 50, the higher value of 1.00 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.
BBCH, Biologische Bundesanstalt, Bundesortenamt und Chemische Industrie.

## 2.6. Applicability of the tiered assessment scheme for soil metabolites

The scenarios in this guidance document were selected using a simple analytical model, which does not consider dissipation processes such as leaching and plant uptake. It was proven that this procedure works well for parent substances (EFSA PPR Panel, 2012a). Appendix A shows that, in most cases, the exposure assessment methodology also generates suitable estimates of the exposure concentrations of soil metabolites. This appendix also shows, however, that the scenario selection procedure that forms the basis of Tiers 2A, 3A and 3B is not completely appropriate for certain metabolites (i.e. metabolites that do leach significantly from the top 20 cm of soil and metabolites that do not accumulate over the years). So for these compounds, it cannot be guaranteed that the results generated at Tiers 2A, 3A and 3B are close to the 95th percentile of the spatial concentration distribution. Despite this, it is advised to use the exposure assessment scheme for all soil metabolites (including soil metabolites that show considerable leaching and for non-accumulating metabolites) until a commonly agreed alternative becomes available.

## 2.7. Exposure assessment based on the total amount in soil

If a robust Regulatory Acceptable Concentration (RAC) can be calculated in mg $kg^{-1}$ it should be compared with the PEC in mg $kg^{-1}$ 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 $ha^{-1}$). If such studies have to be used in the risk assessment, it is proposed to perform the exposure assessment on the basis of the concentration in the top 20 cm of soil (i.e. to recalculate the PEC in total soil given in mg $kg^{-1}$ into kg $ha^{-1}$ exposure estimate to allow comparison

with the ecotoxicological endpoint). 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, 2012a) since 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$^{-1}$), is calculated from the PEC in total soil (in mg kg$^{-1}$) for an ecotoxicological averaging depth ($z_{eco}$) of 20 cm and the dry bulk density ρ (in kg dm$^{-3}$) with:

$$Z = a\rho PEC \quad (2)$$

where $a$ = 2 kg dm$^3$ ha$^{-1}$ mg$^{-1}$ (parameter $a$ is needed to convert the concentration in the top 20 cm into the total amount in kg ha$^{-1}$). Therefore, if ρ = 1.05 kg dm$^{-3}$ and the PEC is 1 mg kg$^{-1}$ then $Z$ = 2 × 1.05 × 1 = 2.1 kg ha$^{-1}$.

The procedure in this section may not be applied to tiers that use predefined scenarios (Tiers 1, 2A and 3A) because an inappropriate value of the bulk density would be applied. The applicant should therefore start at Tier 2B/C and apply Tier 3B when a risk is identified. The value of ρ should be obtained from the PERSAM output.

## 3. Exposure assessment in soil for spray applications to annual crops

This section provides practical guidance on how to perform exposure assessments in soil for annual crops for active substances of PPPs and for the metabolites of these active substances. This section is restricted to spray applications; guidance on row treatments, seed treatments and granules is given in Section 4. This section starts with the tiers using the simple analytical model (Tiers 1, 2B and 2C) and then describes the tiers based on the numerical models (Tiers 2A, 3A, 3B and 4) and post-registration monitoring (Tier 5).

### 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 http://eusoils.jrc.ec.europa.eu/library/data/efsa/. Applicants might want to use the analytical model outside the PERSAM software. Applicants should demonstrate that their own software reproduces the same output as PERSAM, e.g. by comparison for the six predefined scenarios (see Section 1.4).
- An appropriate version of the numerical models PEARL or PELMO[8]. These models can be downloaded from their website (respectively, www.pearl.pesticidemodels.eu and http://server.ime.fraunhofer.de/download/permanent/mk/EFSA/PELMO/).

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–Central–South for each of the two types of PECs (i.e. the concentration in total soil and the concentration in the liquid phase). The scenarios were selected based on the total area of annual crops. The scenarios at Tier 1 are not designed for substances whose properties depend on soil

[8] The model versions at the websites of PEARL and PELMO are not under FOCUS version control and should not be used for regulatory submissions. Please refer to the website of PEARL and PELMO for information on the latest available version.

properties, such as pH. For such substances, the applicant should therefore go to Tier 2B/C or Tier 3B directly.

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 being 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 Decorte et al. (2014b). 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 include the model adjustment factor and the default scenario adjustment factor (Tables 4 and 6). 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 annual rate of application (expressed as mass applied per surface area of field) (kg $ha^{-1}$), i.e. the sum of the application rates within one growing season in case of multiple applications;
- the application cycle (years);
- the organic matter/water distribution coefficient ($K_{om}$) or the organic carbon/water distribution coefficient $K_{oc}$ ($dm^3$ $kg^{-1}$). 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 $mol^{-1}$);
- the molar mass of the molecule (g $mol^{-1}$);
- in the case of a transformation product: the molar fraction of formation (–) of the metabolite as formed from its precursor.

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 ground water assessments (Anonymous, 2014). This guidance document has further incorporated the following amendments (EFSA, 2007, 2014a; EFSA PPR Panel, 2012a):

- 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 $mol^{-1}$ (EFSA, 2007) and should be changed only when based on experimental evidence.
- The geomean $K_{om}$ or $K_{oc}$ of dossier values should be used since the geomean is the best estimator of the median value of a population (EFSA, 2014a). This guidance holds for all sample sizes, and thus also holds for sample sizes larger than nine, for which currently the median value is used.
- 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 section 3.2.1 below.

### 3.2.1. 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. Tiers 1, 2, 3 and 4):

- 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, thus the formation fraction should be set to two).
- The second step is to take the maximum of all relevant formation fractions in the dossier.
- The third step is to take the arithmetic average of all relevant formation fractions in the dossier, thus also including zero values derived from relevant soil metabolism experiments in which this soil metabolite was not detected. Use of arithmetic means is consistent with the recommendations by FOCUS (2006, p. 235). "Relevant" in this context means that there are no indications that the soil metabolism study in the dossier is invalid for the soil of the selected scenario.

## 3.3. Tier 2B: Spatially distributed modelling using PERSAM without canopy processes

Tier 2B provides the option of an exposure assessment with the simple analytical model for a particular crop and a particular substance. Tier 2B 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 pixel and therefore the 95th spatial percentile can be directly obtained from the spatial frequency distribution of the exposure concentration. At Tier 2B, the default scenario adjustment factors as listed in Table 4 are not applied; therefore, Tier 2B simulates less conservative values than Tier 1.

Tier 2B 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. (2014b). 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 6). This factor was added to account for differences between PERSAM and the numerical models (EFSA PPR Panel, 2012a).

The PERSAM tool offers the option to show maps of the concentration distribution. The user may wish to generate a more detailed map. Therefore, the tool 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 PERSAM crop for which the exposure assessment will be carried out. The PERSAM crop has to be based on one of the FOCUS crops listed in Table 5. PERSAM contains crops that are not linked to any of the FOCUS crops; however, these should not be used for regulatory purposes.

The other model inputs are exactly the same as those in Tier 1 with the exception of substance properties that depend on soil properties such as pH. 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 text below).
- The $K_{om}$ or *DegT50* depend on soil properties according to other mathematical rules. When this option is used, the applicant should provide statistical evidence that such a relationship exists. Please note that the current version of PERSAM is not capable of handling negative

*DegT50* or $K_{om}$ values, which may occur based on such a relationship. Therefore, this option should be used with due care.

### 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):

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

where $K_{om,acid}$ ($m^3$ $kg^{-1}$) is the coefficient for sorption on organic matter under acidic conditions, $K_{om,anion}$ ($m^3$ kg-1) is the coefficient for sorption on organic matter under basic conditions, $M$ (kg $mol^{-1}$) is the molar mass, *p*Ka 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. 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 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 dataset (i.e. $pH_{H2O}$). This is performed using the two equations below (Boesten et al., 2012):

$$pH_{H2O} = 0.982\,pH_{CaCl2} + 0.648 \quad (4a)$$

$$pH_{H2O} = 0.860\,pH_{KCl} + 1.482 \quad (4b)$$

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). Since the equations in EC (2014) were based on preliminary figures, Equations 3a and 3b 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).

## 3.4. Tier 2C: Spatially distributed modelling using PERSAM with canopy processes

Tier 2C offers the possibility of incorporating the effect of crop interception in the PEC calculation with the simple analytical model carried out for Tier 2B. In Tier 2C, the effect of crop interception is lumped into a single parameter, i.e. the fraction of the dose reaching the soil (see Section 2.5 for details). This parameter can be read from Table 7. Table 7 is based on simulations with PEARL and PELMO using a half-life for the decline of the dislodgeable residue of 10 days and a wash-off factor of 10 days. Should the applicant wish to refine these parameters, an assessment with the numerical models should be carried out at Tier 2A, 3A, 3B or 4.

The inputs at Tier 2C are exactly the same as the inputs at Tier 2B. The only exception is the fraction of the dose that reaches the soil surface ($f_{soil}$), which should be taken from Table 7. Using this value, the tool will simply perform the following calculation:

$$Result_{Tier\,2C} = f_{soil} Result_{Tier\,2B} \quad (5)$$

As described in Section 3.2, the applicant should input the annual rate of application (kg ha$^{-1}$), i.e. the sum of the application rates within one growing season in case of multiple applications. When crop interception is included, this annual rate should apply to the amount reaching the soil surface. This parameter can, however, not be directly input in PERSAM. Therefore, the following equation should be applied to calculate $f_{soil}$ in the case of multiple applications:

$$f_{soil} = \frac{\sum_{i=1}^{n} f_{soil,i} A_i}{\sum_{i=1}^{n} A_i} \quad (6)$$

where $f_{soil}$ (–) is the mean-weighted fraction of the dose reaching the soil, $f_{soil,i}$ (–) is the fraction of the dose reaching the soil for application $i$ and $A_i$ is the rate of application for application $i$.

Consider the following example:

- Application 1 at a rate of 2 kg ha$^{-1}$ and a fraction reaching the soil surface of 1.0;
- Application 2 at a rate of 3 kg ha$^{-1}$ and a fraction reaching the soil surface of 0.5;
- Application 3 at a rate of 5 kg ha$^{-1}$ and a fraction reaching the soil surface of 0.25.

For this example, the mean-weighted fraction of the dose reaching the soil ($f_{soil}$) to be input in PERSAM should be calculated as:
$f_{soil}$ = (1.0 × 2.0 + 0.5 × 3.0 + 0.25 × 5.0)/(2.0 + 3.0 + 5.0) = 4.75/10 = 0.475. Furthermore, a dose of 2 + 3 + 5 = 10 kg ha$^{-1}$ should be introduced.

### 3.5. Tier 2A: Predefined scenarios using the numerical models

At Tier 2A, numerical models are applied to the same predefined scenarios as those mentioned in Section 3.1. As mentioned earlier, 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)). At Tier 2A no model adjustment factor is applied and therefore it is ensured that Tier 2A delivers less conservative concentrations than Tier 1. However, since the scenarios apply to the total area of annual crops, scenario adjustment factors are needed because the 95th percentile scenario for a specific crop could differ from the 95th percentile scenario for all arable land. The scenarios are described in EFSA PPR Panel (2012a) and are included in user-friendly software shells of the numerical models 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). Please note that the scenarios at Tier 2A are not designed for substances whose properties depend on soil properties such as pH. For such substances, the applicant should therefore go to Tier 2B/C or Tier 3B directly. The exposure concentrations of soil metabolites can be calculated in the same run as the parent with the numerical models. These models will take care of the formation of these metabolites in soil.

The Tier 2A 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 (2012a), 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. It was concluded that the warming-up period ranged between 6 and 54 years, depending on the $K_{om}$ and *DegT50* of the substance (Table 8). The half-life depends on soil temperature, so the half-

lives in Table 8 refer to the half-life at the average scenario temperature. For ease of implementation it was decided to repeat the same time series of six years for this purpose (see Appendix H 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 8:** Warming-up periods (years) needed to reach the plateau concentration as a function of *DegT50* (days) and $K_{om}$ (l kg$^{-1}$). 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 ≤ $K_{om}$ < 500** | **$K_{om}$ ≥ 500** |
|---|---|---|---|
| *DegT50* < 100 | 6 | 6 | 6 |
| 100 ≤ *DegT50* < 200 | 12 | 12 | 12 |
| 200 ≤ *DegT50* < 500 | 12 | 24 | 30 |
| 500 ≤ *DegT50* < 1 000 | 18 | 30 | 30 |
| *DegT50* ≥ 1 000 | 24 | 30 | 54 |

To run the models, the following inputs are needed:

- the FOCUS crop for which the simulations are carried out,
- the application cycle (one year, two years or three years),
- the application scheme of the PPP,
- properties of the active substance and its transformation products (when applicable).

To guarantee consistency in the tiered approach, substance-specific input values that were used in Tier 1 should also be used in Tier 2A (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 ground water assessments (Anonymous, 2014). The sections below show some amendments to these guidance documents.

### 3.5.1. Application schedule and canopy processes

The application scheme entered in the numerical models should reflect an appropriate application timing (according to Good Agricultural Practice) which may be different in different regulatory zones and Member States. 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 and the rate of application (kg ha$^{-1}$). Therefore, in contrast to the analytical model, it is not necessary to sum the applications within a growing season.

When PPPs are applied to the crop canopy, the numerical models will simulate canopy processes. In these simulations, crop interception should 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 (2012a) proposed to use as default values in the exposure assessment a wash-off factor of 0.1 mm$^{-1}$ 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, 2012a, p. 59). General recommendations on how to perform such experiments can be found in Olesen and Jensen (2013, p. 48).

As mentioned in EFSA PPR Panel (2012a), the exposure assessment scheme has been developed for spray applications to annual crops under conventional or reduced tillage. It is proposed to apply the current exposure assessment scheme to also incorporated granules and treatments of small seeds (Section 4.2) that are uniformly distributed over the surface area of the field. When this option is used, the applicant should use the option "incorporation in the soil" and provide the appropriate incorporation depth.

### 3.5.2. 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 5) since 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:

$$A_{soil} = (1 - f_i)(1 - F_{field})A + f_i f_w A \quad (8)$$

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 washed off from the canopy. Detailed guidance on the use of $F_{field}$ in the regulatory process is given in Appendix G. Equation 8 implies that $F_{field}$ is an application-related parameter, i.e. a different value of $F_{field}$ may be required for each application within a year.

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). Thus, 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 (legacy studies) can be used to derive the rapidly dissipating fraction provided that a clear biphasic decline is observed (see Equation 3 in EFSA (2014a)).

### 3.5.3. The sorption coefficient under air-dry conditions

As mentioned in EFSA PPR Panel (2012a), 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 since 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 den Berg 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.

### 3.5.4. Application of scenario adjustment factors

As described in Section 2.3, default scenario adjustment factors are needed for Tier 2A. However, the PECs generated by the numerical models do not include such a factor. For regulatory submissions, the applicant should therefore multiply the PEC of Tier 2A with the corresponding default scenario adjustment factor listed in Table 4:

$$Result_{Tier\,2A} = f_S PEC \quad (9)$$

in which $Result_{Tier2A}$ is the final result of the Tier 2A simulation, PEC is the concentration generated by the numerical models and $f_S$ (–) is the default scenario adjustment factor.

### 3.6. Tier 3A: Crop- and substance-specific scenario adjustment factors

Results at Tier 2A refer to the area of annual crops and therefore default scenario adjustment factors as listed in Table 4 are applied. The applicant may therefore wish to perform an assessment for a specific PERSAM crop. This can be performed at Tier 3A using substance- and crop-specific scenario adjustment factors. Tier 3A depends on results from Tier 1, Tier 2B and Tier 2A, so these tiers must be carried out first (Figure 6). Please note that Tier 3A may not be used for substances whose properties depend on soil properties such as pH. For these substances, the applicant should go to Tier 3B.

The procedure for deriving the crop-specific and substance-specific scenario adjustment factors is as follows (Figure 6):

- Perform a calculation for Tier 2B for this crop and this substance with PERSAM.
- Divide the result of the Tier 1 calculation by the default scenario adjustment factor as given in Table 4.
- The ratio of these two values is the crop- and substance-specific scenario adjustment factor, which could be used to correct the Tier 2A PEC.

This entire approach can be summarised in the following equation:

$$Result_{Tier3A} = \frac{Result_{Tier2B}}{Result_{Tier1} / f_s} PEC_{Tier2A} \quad (10)$$

where $Result_{Tier1}$ is the result from the Tier 1 calculation, $f_s$ is the default scenario adjustment factor as taken from Table 4, $Result_{Tier2B}$ is the result from Tier 2B, $PEC_{Tier2A}$ is the PEC predicted at Tier 2A (without the scenario adjustment factor) and $Result_{Tier3A}$ is the result for the Tier 3A assessment. Results can be all types of concentrations, evaluation depths and TWAs.

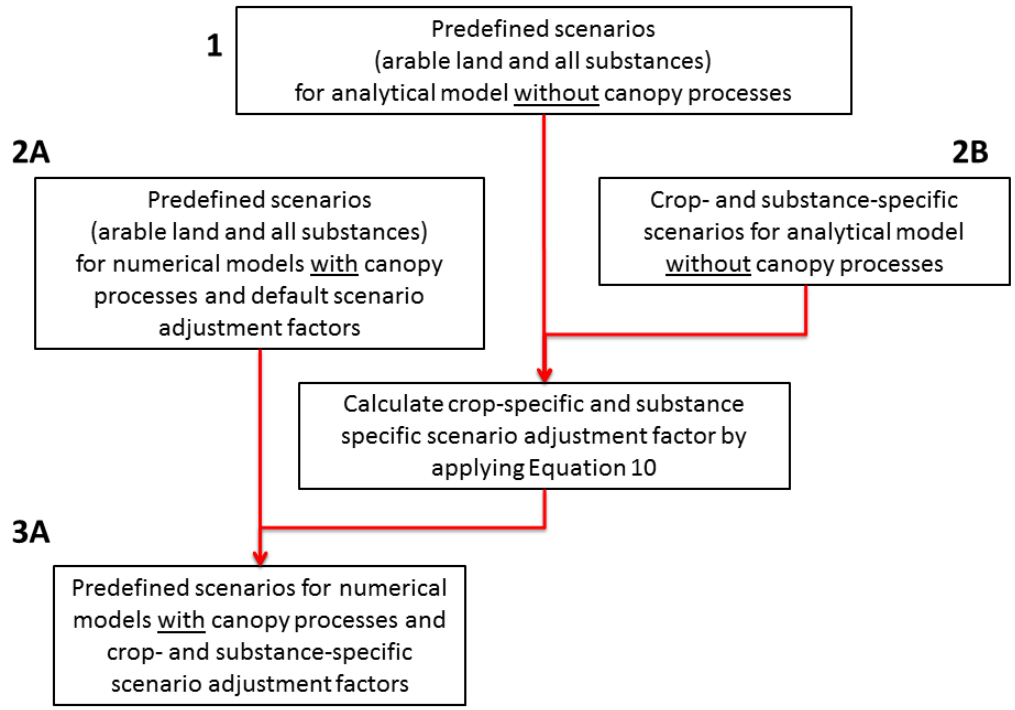


**Figure 6:** Procedure for carrying out a Tier 3A assessment. The ratio between the results obtained in Tier 2B and Tier 1 is used to obtain a crop- and substance-specific scenario adjustment factor. This factor is multiplied by the PEC from Tier 2A (see Equation 10)

### 3.7. Tier 3B: Crop- and substance-specific scenarios using the numerical models

Tier 3B 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. As a consequence, neither a model adjustment factor nor a scenario adjustment factor is needed in Tier 3B.

Scenario development at Tier 3B 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. Guidance on performing these two steps is given below; a full description of the applied procedure is given in Appendix E. 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)).

#### 3.7.1. Selection of the Tier 3B scenarios

The scenario can be selected by running Tier 3 in the PERSAM tool (note that the current version of PERSAM does not make a distinction between Tier 3A and Tier 3B). The PERSAM tool will return the geographical coordinates (X and Y) and properties of the selected pixel but will not run the numerical models. PERSAM can write these coordinates to a comma-separated value (csv) file. This file can be read by the PEARL and PELMO shells, which then use this information to automatically build the scenario. Please refer to the PERSAM manual for practical guidance on scenario selection at Tier 3B. As described in EFSA PPR Panel (2012a), the selected pixel is dependent on the selected substance, the selected evaluation depth (1, 5 or 20 cm) and the selected type of concentration (pore water or concentration in total soil). For this reason, different Tier 3B scenarios are needed for each substance, for each evaluation depth and for each type of concentration. However, we consider it justified to base the scenario selection solely on the peak concentration, so it is not necessary to select different scenarios for each TWA window.

#### 3.7.2. Building and running the Tier 3B scenarios

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

- Specify the csv file generated by PERSAM to get the geographical coordinates of the Tier 3B scenarios.
- Specify the FOCUS crop, application schedule, application cycle and substances.
- Run the scenarios and generate reports.

All scenarios included in the csv file will be stored 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.

#### 3.7.3. Model inputs and outputs

To guarantee consistency in the tiered approach, all model inputs (i.e. substance-specific input values, the FOCUS crop, application schedule, crop interception, wash-off and application cycle) that were used in Tier 2A and Tier 2B/C should also be used in Tier 3B.

Since at Tier 3B neither a model adjustment factor nor a scenario adjustment factor is needed, the PECs generated by the numerical model do not need further processing.

### 3.8. Tier 4: Spatially distributed modelling with the numerical models

A further tier may be considered (Tier 4) which would consist of spatially distributed modelling with numerical models. Spatially distributed modelling has the advantage that the spatial 95th percentile of the PEC for all types of concentrations (pore water or concentration in total soil) of either the parent substance or any soil metabolite can be derived by statistical analysis of the output of the model runs, thus avoiding the need for simplifications in the scenario selection procedure.

Using the procedure described in Section 3.7, it is, in principle, possible to parameterise each $1 \times 1$ 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 certain groups. 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.

#### 3.8.1. Setting up the spatial schematisation

A spatial schematisation may be obtained by overlaying maps with spatially distributed parameters. The maps available in EFSA spatial dataset version 1.1 (Hiederer, 2012) should be used for this purpose. Before creating the overlay, grid cells with land uses other than annual 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.

Because the last three 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.

#### 3.8.2. 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 and temperature should be derived for each unique combination. This may be carried out by applying the zonal mean function in a GIS package. Once the mean values of topsoil organic matter, temperature and pH are known, the Tier 3B procedure can be applied to each individual unique combination (refer to Appendix E for details). With respect to the soil parameters, the procedure in Appendix E follows the procedure in Section 2.7 of EFSA PPR Panel (2010b). However, with respect to weather, crop and irrigation data, the procedure has been slightly modified to ensure consistency in the tiered approach:

- The weather file of the Tier 2A scenario is used for the whole regulatory zone and only the temperature is scaled.

- The crop–irrigation combination used in Tier 2A should be used for the whole regulatory zone.

The consequence is that the model for the concentration in total soil has to use a different parameterisation than the model for the concentration in pore water.

### 3.8.3. 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 dataset (see Appendix D for file names).

Since at Tier 4 neither a model adjustment factor nor a scenario adjustment factor is needed, the PECs generated in this procedure do not need further processing.

## 3.9. Tier 5: Post-registration monitoring

The PPR Panel proposes to include post-registration monitoring as Tier 5 (EFSA PPR Panel, 2012a). 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 3, 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 5, 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 on the basis of 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 procedure and crop management practices. Monitoring sites that do not meet these conditions should be excluded from the analysis. As described in EFSA PPR Panel (2012a), the scenario selection procedure is targeted mainly at applications of substances in crops where most of the substance penetrates into the soil. Thus, monitoring problems for substances that are dissipated to a large extent on plant or soil surfaces cannot be tackled using this alternative approach.

In line with the procedure that was used to simulate the overall 90th percentile of the PEC, the median value of the PEC at the individual monitoring sites should be used. Since the PECs at individual monitoring sites are expected to vary 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 for only PPPs that show accumulation of residues at a time scale of at least five 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 1.2).

## 4. Exposure assessment in soil for row treatments and granules

As described in Section 1.3, it is assumed that for applications of granular products (to the soil surface or incorporated), the exposure assessment methodology can be used as well. With small modifications, the procedure should also cover, reasonably well, row treatments. This section provides calculation procedures for row treatments (Section 4.1) and granules (Section 4.2).

### 4.1. Calculation procedure for applications in rows

For row treatments, 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 opinion 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 below the treated rows) and (iii) both the concentrations in the soil below the treated rows and the concentrations in the soil below the untreated part of the soil surface. The exposure assessment in Section 3 will provide appropriate concentrations for option (i) provided that the dosage used in the exposure assessment is defined as mass of active ingredient applied per surface area of the cropped field. The methodology is expected to cover, reasonably well, the background concentration for row treatments because this is calculated as a plateau after multi-year use assuming annual soil rotation and because the location of the rows is likely to change from year to year. However, the peak concentration will usually occur immediately or shortly after an application. Thus, for options (ii) and (iii) the analytical model needs to be changed as explained in Appendix F. As mentioned above, user-friendly software to perform these calculations is not yet available. For this reason, a simple conservative approach is suggested, which may be used until the user-friendly software has been updated to reflect the changes in Appendix F.

#### 4.1.1. Simple conservative assessment

As mentioned above, user-friendly software to perform the calculations in Appendix F is not yet available. It is therefore suggested that the models be run using the dose expressed per surface area of treated field:

$$DOSE_{in\_rows} = DOSE / f_{row} \quad (11)$$

where $DOSE$ (kg ha$^{-1}$) is the dosage defined as mass of active ingredient per surface area of field (i.e. averaged over the whole surface of the field), $DOSE_{in\_rows}$ (kg ha$^{-1}$) is the dosage per surface area of treated rows and $f_{row}$ is the fraction of the soil surface that is treated. Note that the fraction of the soil surface treated is not 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.

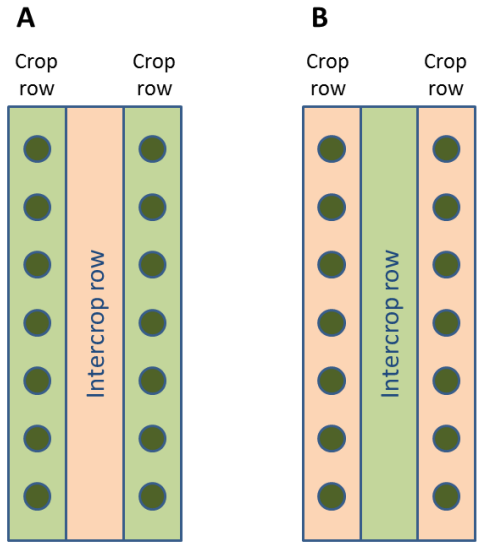


**Figure 7:** Graph showing the fraction of the soil surface treated (indicated in orange) and the fraction of the soil that is not treated (green). There are two possible situations. (A) The pesticide is applied to the intercrop row (usually herbicide treatments) so $f_{row}$ equals the relative area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

Equation 11 can be applied to all tiers of the assessment scheme (in both the analytical model and the numerical models). The underlying assumption of this simple calculation procedure is that the position of the rows does not change with time, which is a conservative assumption for both the concentration in the rows and the concentration between the rows. Selection of $f_{row}$ should be justified and supported by a thorough description of the method and rate of application. For certain crops generic values of $f_{row}$ have been provided in 2015 by EFSA procurement.

### 4.1.2. Crop interception

Crop interception should not be included in calculations for row treatments unless the spray is targeted on just the crop canopy or the crop canopy has closed between the rows. For these situations only the numerical models may be use to simulate crop interception at Tiers 2A, 3A, 3B and 4. Crop interception should in this case be derived from EFSA (2014a). In the case of Tier 2C, the default table values for the fraction of the dose reaching the soil (Table 7) should be used (see Section 2.5).

## 4.2. Calculations for granules that are incorporated and seed treatments for small seeds

The procedure for calculations for incorporated granules and treated small seeds (< 0.5 cm)[9] applies only to situations when the agricultural practice aims to result in even horizontal spatial distribution across the field, thus not when there may be uneven crop row spacing and the active substance will have higher concentrations within the crop row, which can be the case for, for example, *Brassica* vegetables. The procedure also applies to only tillage systems with a level soil surface (i.e. not to systems with ridges and furrows). Note, as for spray applications to the soil surface, the calculation method described below includes the assumption that there is even vertical redistribution of the test substance within the evaluation depth $z_{eco}$.

It is assumed that the incorporation depth of the granules or treated seeds is not deeper than 20 cm (i.e. the depth of annual ploughing assumed in the calculations). The definition of the ecotoxicologically relevant type of concentrations in this guidance is based on the concept that concentrations are

[9] Definition of small seeds is taken from draft Directorate General for Health and Consumer Affairs (DG SANCO) guidance on seed treatments. For this EFSA guidance it is proposed that maize seeds and pelleted seeds be handled as small seeds.

averaged over the evaluation depth, $z_{eco}$ (ranging between 1 and 20 cm). The consequence is that the procedure for calculations for incorporated granules and treated small seeds is identical to that for spray applications unless the incorporation depth is deeper than $z_{eco}$. Please note that this remark is valid for both the analytical model and the numerical models.

If the incorporation depth is greater than 20 cm (or less than 1 cm) the current version of PERSAM cannot be used. The reason being that the increased concentration resulting from the last application has to be based on averaging over the incorporation depth instead of averaging over the evaluation depth (Appendix F, Section F.2). Since the numerical models can handle this, the applicant should in these specific cases go to Tier 2A directly. Should it be necessary to build a Tier 3B scenario, we consider it acceptable to select the corresponding scenario with PERSAM using an evaluation depth of 20 cm.

## 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 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 to existing software tools (see also EFSA PPR Panel (2014) for guidelines on model development and model documentation).

The substance properties and the application regime (i.e. application rate, type of application, frequency of application and fraction of the dose reaching the soil) determine the outcome of a regulatory assessment to a large extent and should therefore be well documented. Whenever possible, harmonised approaches, as described in this or earlier 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 the PERSAM (Tiers 1, 2B and 2C) or the numerical models (Tiers 2A, 3A, 3B and 4).
- A document describing all manual calculations, including (i) the fraction of the dose in the case of multiple applications at Tier 2C, (ii) the scenario adjustment factors at Tier 2A and (iii) the crop- and substance-specific scenario adjustment factors at Tier 3A.

The applicant may move directly to higher tiers without performing assessments for lower tiers. Only in those cases where higher tiers depend on lower tiers should the applicant report results from lower tiers. Results from parallel tiers do not need to be submitted. Table 8 summarises reporting requirements for each individual tier of the assessment scheme.

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 PEC for regulatory submissions (this procedure is in line with EC (2014)).

**Table 9:** Reporting requirements for each tier of the exposure assessment scheme. Only tiers marked with "X" need to be reported

| Tier | Report needed from tier | | | | | | |
|---|---|---|---|---|---|---|---|
| | **1** | **2A** | **2B** | **2C** | **3A** | **3B** | **4** |
| 1 | X | | | | | | |
| 2A | | X | | | | | |
| 2B | | | X | | | | |
| 2C | | | | X | | | |
| 3A | X | X | X | | X | | |
| 3B | | | | | | X [(a)] | |
| 4 | | | | | | | X |

(a): Results from both the scenario selection procedure in PERSAM and the numerical model should be reported.

## 6. Exposure assessment in soil for permanent crops

The exposure assessment in soil for permanent crops is currently under development. Until new guidance has been taken note of by the Standing Committee on Plants Animal, Food and Feed (SCoPAFF), and a date for implementation has been set, current methods still apply.

## 7. Exposure assessment in soil for crops grown on ridges

Exposure assessment in soil for crops grown on ridges, such as potatoes, is currently under development. Until new guidance has been taken note of by the Standing Committee on Plants Animal, Food and Feed (SCoPAFF), and a date for implementation has been set, current methods still apply.

## CONCLUSIONS OR RECOMMENDATIONS

### RECOMMENDATIONS

- The current guidance document is restricted to annual crops under conventional and reduced tillage (excluding crops grown on ridges). Methodologies for performing exposure assessments for permanent crops, crops grown on ridges and for no-tillage systems are currently being developed. It is recommended that guidance for these cropping systems be developed as soon as these methodologies become available.
- This guidance has changed the tiered assessment scheme given in EFSA PPR Panel (2012a) with the goal to simplify the exposure assessment for regulatory purposes. Many of these changes could not yet be included in the user-friendly software tool PERSAM. It is recommended that these changes be included in an update of PERSAM as soon as possible. This includes:
  - exposure assessments for applications of granular products and row treatments;
  - calculation of the fraction of the dose reaching the soil in the case of multiple applications;
  - implementation of well-defined crop lists based on Appendix D of this guidance document;
  - generation of an output file with the purpose to ease the automated generation of crop- and substance-specific scenarios at Tier 3B;
  - possibility to import crop maps for higher tier assessment.
- For regulatory purposes, applicants must use commonly agreed versions of the software tools. It is therefore recommended that a procedure for version control and updating the software tools be developed, including PERSAM, PEARL and PELMO.
- For certain applications (for example metabolites), spatially distributed versions of the numerical models are needed for correct estimation of the 95th percentile of the concentration distribution. It is therefore recommended that commonly agreed versions of such spatially distributed models be made available.

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## GLOSSARY AND ABBREVIATIONS

| | |
|---|---|
| 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 |
| CLC | scenario for the concentration in pore water for the Central 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 |
| CTC | scenario for the total concentration in the Central Zone |
| CTN | scenario for the total concentration in the North Zone |
| CTS | scenario for the total concentration in the South Zone |
| *DOSE* | the mass of substance applied per unit surface area of the field (kg $ha^{-1}$). Substances may be applied uniformly or be applied in rows. In both cases, the mass is expressed per surface area of the entire field (both treated and untreated) |
| $DOSE_{in\_rows}$ | the mass of substance applied per unit surface area of treated rows (kg $ha^{-1}$). See further definition of $f_{row}$ |
| EFSA | European Food Safety Authority |
| ERC | Ecotoxicological Relevant Concentration |
| $F_{field}$ | rapidly dissipating fraction that is not related to degradation in the soil matrix (EFSA PPR Panel, 2010c) |
| $f_{row}$ | fraction of the surface area of the field that is occupied by the treated rows (–). This fraction may refer to the intercrop row or the crop row, depending on where the pesticide is applied |
| FOCUS | Forum for Co-ordination of Pesticide Fate Models and their Use |
| $f_{soil}$ | fraction of the dose that reaches the soil |
| 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 |
| 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 |
| PPR | Plant Protection Products and their Residues |
| PPP | Plant Protection Product |
| 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 |

# APPENDICES

## Appendix A. Applicability of the exposure assessment scheme for soil metabolites

### A.1. Introduction

The guidance opinion (EFSA PPR Panel, 2012a, p. 64) indicated that the exposure assessment for soil metabolites was not based on the specified exposure assessment goals because the scenario selection procedure (based on the simple analytical model) was developed only for parent substances. In this appendix it is explored under which circumstances parts of the proposed exposure assessment methodology can nevertheless be used to assess the exposure of soil metabolites.

### A.2. Applicability of the scenario selection procedure for Tiers 1 and 2B/C

Let us first consider Tier 2B/C. In this tier the 95th spatial percentile of the exposure concentration of soil metabolites can be calculated with the simple analytical model based on the conservative assumption that each metabolite is applied at the application time of the parent at a dose that is corrected for the kinetic formation fraction and the molar mass of the metabolite (see EFSA PPR Panel, 2012a, p. 24). A correct way of calculating this 95th spatial percentile would be to derive it from calculations for all pixels in the area of use with one of the numerical models, i.e. Tier 4 of the exposure assessment as proposed by EFSA PPR Panel (2012a). This is impossible because the required spatially distributed modelling tools are as yet not available; see EFSA PPR Panel, 2012a. However, let us assume that these calculations with such a tool would be available. Let us compare for a single pixel the metabolite concentration calculated with the numerical model within Tier 4 and that calculated with the simple model in Tier 2B/C (including the model adjustment factor that is part of Tier 2B/C). For each pixel the concentration calculated with the simple model of Tier 2B/C is very likely to be higher than that calculated with the numerical model because (i) a model adjustment factor is used in Tier 2B/C to account for differences between the numerical and analytical models, (ii) the calculation for the metabolite in the simple model is based on the conservative assumption that its total amount formed is applied at the application time of the parent and (iii) metabolites may also leach from the topsoil in the numerical model whereas this is impossible in the simple model. If for each pixel the Tier 2B/C calculation generates higher concentrations for metabolites than the Tier 4 calculation with the numerical model, the 95th spatial percentile as derived from Tier 2B/C has to be higher than the 95th spatial percentile as derived from Tier 4. Thus, Tier 2B/C is likely to give conservative estimates for concentrations of soil metabolites.

The tiered approach ensures that Tier 1 generates higher concentrations than Tier 2B/C, so if Tier 2B/C is conservative for soil metabolites, this also has to be the case for Tier 1. Therefore, it is concluded that both Tiers 1 and 2B/C can be used to assess the exposure of soil metabolites with the simple model.

### A.3. Applicability of the scenario selection procedure for Tiers 2A and 3

#### A.3.1. Introduction

The above considerations do not apply to Tiers 2A and 3 because these tiers require that the scenario selection procedure selects a pixel that corresponds to the 95th spatial percentile. There is no such guarantee that the ranking of concentrations based on the simple model is correct for metabolites because this ranking has not been tested for metabolites. Nevertheless, there may be circumstances in which this ranking based on the simple models is also correct for metabolites. The simple model is based on two assumptions that may not be valid for metabolites: (i) there is no significant leaching from the top 20 cm and (ii) the temperature dependence of the plateau concentration follows the Arrhenius equation. These aspects are discussed in more detail in the following sections.

### A.3.2. Restrictions resulting from the requirement of no significant leaching from the top 20 cm

The basis of the use of the simple analytical model for the scenario selection is that this model gives the same ranking of soil exposure concentrations for the 1 × 1 km$^2$ grid cells of the EU-wide databases as a more realistic numerical model (for further explanation see EFSA PPR Panel, 2012a, p. 29). For parent substances this was checked by performing calculations for 1 051 scenarios with both the simple analytical model and the PEARL model for three substances (*DegT50* = 15 days and $K_{om}$ = 15 l kg$^{-1}$, *DegT50* = 50 days and $K_{om}$ = 200 l kg$^{-1}$, *DegT50* = 200 days and $K_{om}$ = 1 000 l kg$^{-1}$). These calculations showed good correspondence between the ranking by the two models for both the concentration in total soil and the concentration in pore water for peak concentrations and TWA concentrations for time windows up to 56 days (EFSA PPR Panel, 2012a, p. 31). This ranking can be expected to only be good for substances that do not leach significantly from the top 20 cm because the simple analytical model assumes no leaching from this layer. This restriction was not considered to be a problem for parent substances because it is unlikely that these substances leach significantly below 20 cm in view of the groundwater protection goal of the EU regulatory process. Therefore, the ranking was also tested for only substances with limited leaching from the top 20 cm. Thus, use of the simple analytical model is a priori unlikely to be acceptable for soil metabolites that show significant leaching below 20 cm depth for a considerable fraction of these grid cells of the EU-wide databases; the same restriction applies, of course, to any precursor of a metabolite. As described before, it is unlikely that parent substances show significant leaching below 20 cm depth but a soil metabolite may also be formed from another soil metabolite.

It would be useful to have a criterion for "no significant leaching". This was assessed based on calculations for the FOCUS groundwater scenario Okehampton (EC, 2014. This is one of the EU scenarios with the highest leaching concentrations, likely making it suitable for assessment of a criterion for the assessment of significant leaching. Calculations were made for winter cereals and application of 1 kg ha$^{-1}$ just before emergence (17 October at Okehampton). Calculations were made for a range of $K_{om}$–*DegT50* combinations using default values for all other parameters assuming annual applications. This gives a 20-year evaluation period. Both total leaching from the top 20 cm (in kg ha$^{-1}$) and the total transformation in this top 20 cm over these 20 years (in kg ha$^{-1}$) were calculated. The contour diagram in Figure A.1 shows the quotient of total leaching divided by total transformation.

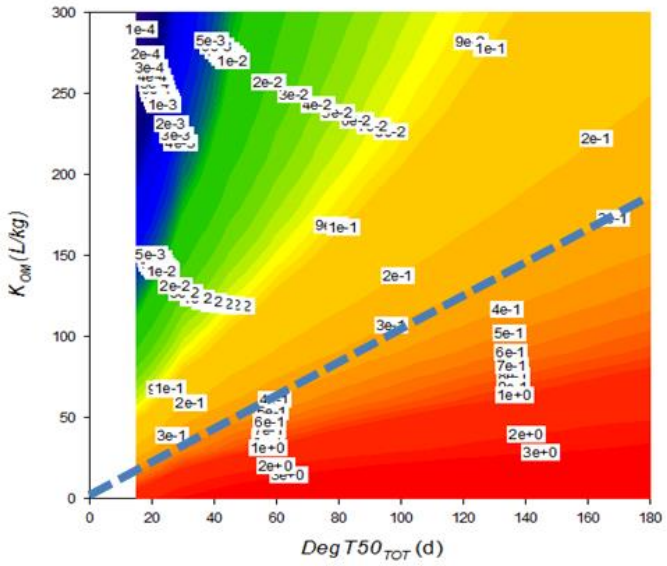


**Figure A.1:** The quotient of total leaching (kg ha$^{-1}$) from the top 20 cm of soil divided by total transformation (kg ha$^{-1}$) in the top 20 cm of soil over a 20-year simulation period as calculated for the FOCUS groundwater scenario Okehampton, UK, for winter cereals and annual application of 1 kg ha$^{-1}$ one day before emergence. The dashed line is the 1:1 line, i.e. $K_{om}$ = *DegT50*

Because this is a quite conservative leaching scenario, it is considered sufficient to require that the total transformation is at least two times leaching. Therefore, the ratio shown in Figure A.1 has to be less than 0.5, thus the area above the "5e-1" line in Figure A.1. This figure shows that this leads, approximately, to the criterion $K_{om}$ (l kg$^{-1}$) > *DegT50* (days), i.e. the dashed line in the contour diagram. Thus, the requirement of no significant leaching is likely to be met if the ratio $K_{om}$/*DegT50* is above 1 for both the soil metabolite and all his precursors.

## A.4. Temperature dependence of peak concentrations of soil metabolites in soil

### A.4.1. Introduction

Another complication of the use of the simple analytical model for soil metabolites is that this model calculates a plateau concentration in soil for parent substances based on first-order degradation. However, the plateau concentration of soil metabolites is the result of a combination of first-order formation and degradation. The simple analytical model is based on the Arrhenius equation for the description of the temperature dependency of the plateau concentration. This temperature dependency is an important element of the ranking of the scenarios. Therefore, the simple analytical model may not be suitable for the scenario selection of soil metabolites if the temperature dependency of the peak concentration of soil metabolites in the numerical models would differ significantly from the temperature dependency of peak concentrations of parent substances in these models.

There are, qualitatively, two possible cases for soil metabolites: (i) their degradation is so slow that a plateau develops (at a time scale of many years) as a result of repeated applications and (ii) the degradation is so fast that the concentration of the metabolite has decreased again considerably before the first application in the next year (or in later years) takes place. Both cases are considered below.

### A.4.2. Assessment of temperature dependency of the plateau value of an accumulating soil metabolite

The simple analytical model is used as a starting point for the assessment of the temperature dependency of the plateau value of an accumulating soil metabolite. The simple analytical model calculates the plateau level of a parent substance based on the analytical solution of a single application and by summing up the solution for all the applications via the sum of an infinite geometric series (EFSA PPR, 2010d, p. 23). This summing up is impossible for a soil metabolite because the analytical solution of a single application for a metabolite is too complex an equation. Therefore, a more simplified approach is used: it is assumed that there is a continuous application to the soil surface which mimics the single application as much as possible. Thus, let us assume that in reality there is an application at a rate $A$ (mg dm$^2$), which takes place at time interval $t_{cycle}$ (days). Then the corresponding continuous application rate equals $A/t_{cycle}$. Let us consider a soil layer of $z_{til}$ in which the substance is perfectly mixed. The rate of increase of the concentration in this layer, $\alpha$ (mg kg$^{-1}$ day$^{-1}$), is then defined as:

$$\alpha \equiv \frac{A}{\rho\, z_{til}\, t_{cycle}} \tag{A1}$$

Thus, for such a continuous application rate the rate equation for the parent substance reads:

$$\frac{d\, C_{parent}}{dt} = \alpha - k_{parent}\, C_{parent} \tag{A2}$$

where $C_{parent}$ (mg kg$^{-1}$) is the concentration of the parent in total soil, $t$ is time (days) and $k_{parent}$ is the degradation rate coefficient of the parent in soil (day$^{-1}$). This gives the steady-state solution:

$$C_{parent} = \frac{\alpha}{k_{parent}} = \frac{A}{\rho\, z_{til}\, t_{cycle}\, k_{parent}} \tag{A3}$$

Please note that this equation is valid for only relatively small values of $t_{cycle}$ because it is assumed that the application rate is continuous.

Equation A3 can be compared with the steady-state solution (for the plateau concentration) of the simple analytical model as described by EFSA PPR (2012a, p. 23) which can be rewritten as:

$$C_{parent} = \frac{A}{\rho\, z_{til}} \frac{\exp(-t_{cycle}\, k_{parent})}{1-\exp(-t_{cycle}\, k_{parent})} \tag{A4}$$

It can be shown mathematically that Equation A4 reduces to Equation A3 if $t_{cycle}\, k_{parent}$ goes to zero (which mimics a continuous application rate).

The rate equation for the metabolite is:

$$\frac{d\, C_{metabolite}}{dt} = +F_f \frac{M_{metabolite}}{M_{parent}}\, k_{parent}\, C_{parent} - k_{metabolite}\, C_{metabolite} \tag{A5}$$

where $C_{metabolite}$ (mg kg$^{-1}$) is the concentration of the metabolite in total soil, $F_f$ (–) is the formation fraction of the metabolite (i.e. the stoichiometric coefficient of the formation of this metabolite from the parent substance), $M_{metabolite}$ is the molar mass of the metabolite (g mol$^{-1}$), $M_{parent}$ is the molar mass of the parent substance and $k_{metabolite}$ is the degradation rate coefficient of the metabolite. The steady-state solution can be obtained by requiring that d $C_{metabolite}$/d $t$ is zero. Combination with Equation A3 then gives:

$$C_{metabolite} = +F_f \frac{M_{metabolite}}{M_{parent}} \frac{\alpha}{k_{metabolite}} \tag{A6}$$

Thus, $k_{parent}$ has vanished from Equation A6; the consequence is that the plateau value of the metabolite does not depend on the rate of formation of the metabolite. Comparison of Equations A3 and A6 shows that the plateau concentrations of parent and metabolite are both inversely proportional to their degradation rate coefficient, not only qualitatively but also quantitatively the temperature dependence of their plateau values is expected to be the same. The conclusion is, that for accumulating soil metabolites, there are no reasons to assume that the temperature dependency of the transformation rate in the simple model will lead to inappropriate ranking of scenarios.

The prediction based on Equation A6 was compared with a numerical solution of the rate equations for parent and metabolite assuming an annual application (so Equation A2 but without $\alpha$ combined with Equation A5). The rate equations were integrated with Euler's rectangular method and the time step was one day. A metabolite was considered with a half-life of 800 days leading to clear accumulation (see Figure A.2). Equation A6 predicted in this case a plateau concentration for the metabolite of (100/365)(800/ln(2)) = 316 mg kg$^{-1}$, which is quite close to the numerical result.

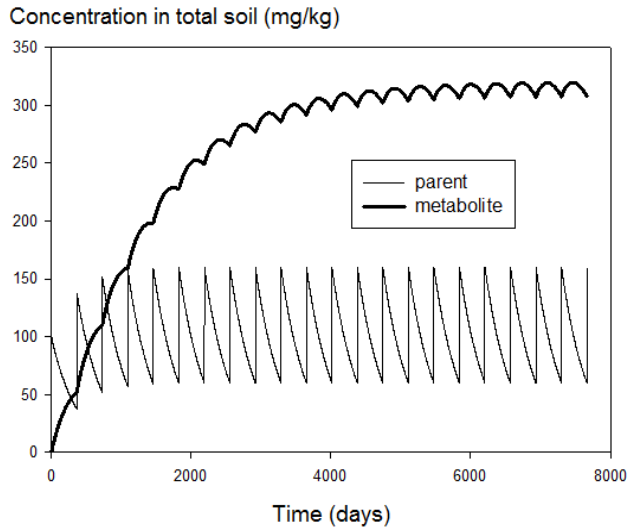


**Figure A.2:** Numerical solution of the simple analytical model for a parent and a metabolite for an annual dose corresponding to $A/(\rho\, z_{til})$ of 100 mg kg$^{-1}$, a half-life of the parent of 258 days, a half-life of the metabolite of 800 days, a formation fraction of 100 % and equal molar masses of parent and metabolite

### A.4.3. Assessment of the temperature dependency of the peak concentration if the metabolite does not accumulate

If the metabolite does not accumulate, the steady-state solution based on a continuous application of the substance as described in the previous section does not give a meaningful approximation of the time course of the concentration of the metabolite. This is illustrated in Figure A.3. Equation A6 predicts for this case a plateau of 16 mg kg$^{-1}$, which is clearly not a meaningful result.

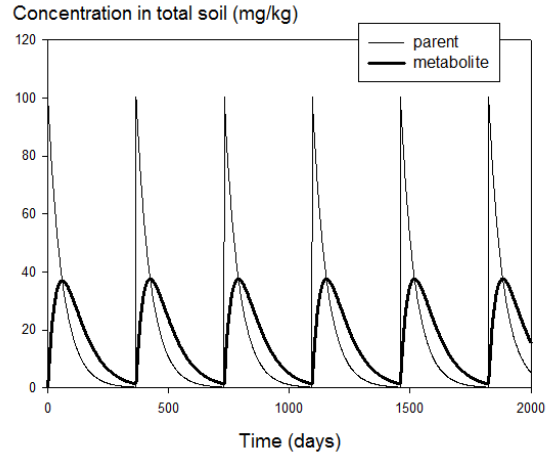


**Figure A.3:** Numerical solution of the simple analytical model for a parent and a metabolite for an annual dose corresponding to $A/(\rho\, z_{til})$ of 100 mg kg$^{-1}$, for half-lives of the parent and metabolite of 10 days at 20 ºC, Q10 = 2.58, a temperature of 5 ºC (corresponding to a half-life of parent and metabolite of 41 days), a formation fraction of 100 % and equal molar masses of parent and metabolite

Adriaanse et al.(2014) analysed the maximum in time for a parent–metabolite system with first-order transformation and formation after a single application. The time course of the concentration of the metabolite for such a system can be described with:

$$C_{metabolite} = F_f \, C_{0,parent} \frac{M_{metabolite}}{M_{parent}} \frac{k_{parent}}{k_{metabolite} - k_{parent}} \left[\exp(-k_{parent}\, t) - \exp(-k_{metabolite}\, t)\right] \quad \text{(A7)}$$

where $C_{metabolite}$ (mg kg$^{-1}$) is the concentration of this metabolite in total soil, $F_f$ (–) is the formation fraction of this metabolite (i.e. the stoichiometric coefficient of the formation of this metabolite from the parent substance), $M_{metabolite}$ is the molar mass of this metabolite (g mol$^{-1}$), $M_{parent}$ is the molar mass of the parent substance (g mol$^{-1}$), $k_{parent}$ is the degradation rate coefficient of the parent (day$^{-1}$), $k_{metabolite}$ is the degradation rate coefficient of this metabolite (day$^{-1}$), $C_{0,parent}$ (mg kg$^{-1}$) is the concentration in total soil of the parent at the application time and $t$ is the time elapsed since application (days).

Adriaanse *et al.* (2014) showed that the maximum of the concentration of the metabolite in time is given by:

$$C_{metabolite,\max} = F_f \, C_{0,parent} \frac{M_{metabolite}}{M_{parent}} \, Y^{\frac{Y}{1-Y}} \quad \text{(A8)}$$

where $Y = k_{metabolite}/k_{parent}$. This ratio of these two rate coefficients does not depend on temperature if their Arrhenius activation energy is the same. It is, of course, possible that activation energies for parent and metabolites differ but the consequence of Equation A8 is that a much lower temperature dependency is expected for a maximum concentration of a metabolite that does not accumulate.

This is illustrated by calculations with a numerical solution of the simple analytical model in which the maximum concentration in time was calculated for annual applications as a function of temperature, assuming equal Arrhenius activation energies for parent and metabolite. Figure A.4 shows that, for such a case, the maximum level of the metabolite does decrease between 0 and 5 °C but thereafter remains constant with temperature. The background of the decrease between 0 and 5 °C is that at 0 °C there is still overlap between the pulses of the different years (leading to an accumulation effect) but this overlap does not occur at 5 °C anymore (this is the calculation shown in Figure A.3). If there is no longer an overlap, the maximum concentration does not depend on temperature as is predicted by Equation A8. In this case, Equation A8 predicts a maximum concentration of 36.8 mg kg$^{-1}$, which corresponds well with the result shown in Figure A.4 (in this case, $Y$ happens to 1; therefore, the calculation of Equation A8 is not straightforward but has to be based on the limit for Y going to 1; this can be calculated by, for example, using Y = 0.99999).

Therefore, as a consequence, the scenario selection procedure is expected to not work well for soil metabolites that do not accumulate.

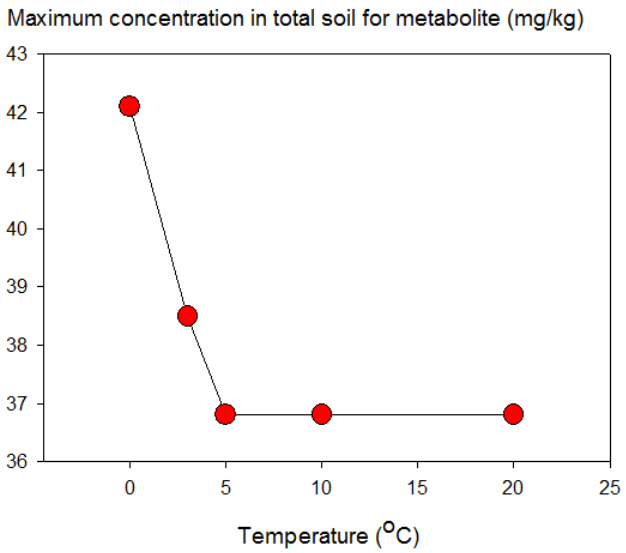


**Figure A.4:** Maximum concentration in total soil as a function of temperature calculated with a numerical solution of the simple analytical model for a parent and a metabolite for an annual dose corresponding to $A/(\rho\ z_{til})$ of 100 mg kg$^{-1}$, for half-lives of the parent and metabolite of 10 days at 20 °C, Q10 = 2.58, a formation fraction of 100 % and equal molar masses of parent and metabolite. Note that the vertical axis does not start at 0.

## A.5. Accumulation criterion for metabolites

The scenario selection procedure is likely to work well for only soil metabolites that accumulate over the years (and do not leach significantly below 20 cm depth as described before). It is then useful to have a criterion for the *DegT50* that checks whether a metabolite accumulates to such an extent that concentration increases due to formation have only a limited effect on the peak concentration (such as in the example in Figure A.1).

Let us consider the maximum increase in the metabolite concentration resulting from a single application in an ecotoxicological averaging layer with depth $z_{eco}$. This equals $[A/(\rho\ z_{eco})] \times F_f$ $(M_{metabolite}/M_{parent})$. This is the concentration increase in cases where the degradation of the parent substance would be extremely fast. This increase has to be small compared with the plateau level of the metabolite (Equation A6). Under the stipulation that the plateau concentration level is at least equal to this maximum increase, this leads to the requirement:

$$\frac{A}{\rho\ z_{til}\ t_{cycle}\ k_{metabolite}} \geq \frac{A}{\rho\ z_{eco}} \tag{A9}$$

This leads to the following requirement for the *DegT50* of the metabolite:

$$DegT50_{metabolite} \geq \frac{z_{til}}{z_{eco}}\ t_{cycle}\ \ln(2) \tag{A10}$$

Note that Equation A10 refers to the *DegT50* under field conditions, thus not to the reference temperature of 20 °C. Table 9 of EFSA PPR (2012a) shows that the *DegT50*s for the six scenarios are expected to be 1.7 to 3.4 times longer than the *DegT50* at 20 °C based on the average temperature of the scenarios.

Equation A10 leads, in general, to long *DegT50* values for the metabolites. The value of $t_{cycle}$ is at least one year and the ratio $z_{til}/z_{eco}$ ranges from 1 to 20. Therefore, the minimum *DegT50* value is 0.7 years for application every year and an ecotoxicological averaging depth of 20 cm, but it may become as high as 42 years for application every three years and an ecotoxicological averaging depth of 1 cm.

This poses considerable restrictions to the use of the selected scenarios as appropriate 95th percentile scenarios for soil metabolites.

To illustrate the above analysis, calculations were made with the PEARL model. This was carried out for the scenario for the concentration in total soil in the North Zone for $z_{eco}$ = 20 cm and an annual application in winter wheat and for a soil metabolite with *DegT50* = 200 days at 20 °C and $K_{om}$ = 1 000 l kg$^{-1}$. Calculations were made for the case where this soil metabolite was formed from a parent substance (with a parent *DegT50* of 50 days at 20 °C) and for a hypothetical case where the soil metabolite was applied as the parent substance (assuming 100 % formation and no difference in molar mass between parent and metabolite to facilitate the comparison). The latter case would approximate the case of a soil metabolite that is very rapidly formed from a parent substance (see Figure A.5 for details).

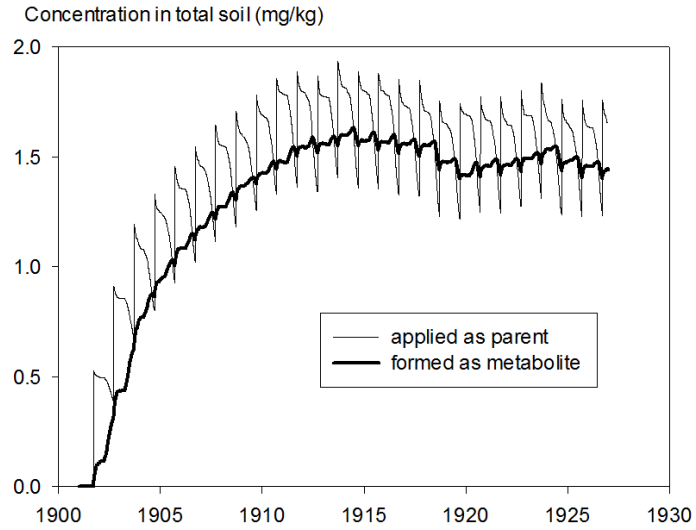


**Figure A.5:** Average concentration in total soil in the 20-cm top layer for a substance with *DegT50* = 200 days at 20 °C and $K_{om}$ = 1 000 l kg$^{-1}$ ("substance A") as calculated with PEARL for the scenario "concentration in total soil" in the North Zone and winter wheat. Results are shown for application of this substance A itself and for application of another substance ("substance B") that degrades into substance A with a formation fraction of 100 %. Substances A and B have equal molar masses. Substance B has a *DegT50* of 50 days at 20 °C and a $K_{om}$ of 1 000 l kg$^{-1}$. Both substances A and B were applied each year at a dose of 1 kg ha$^{-1}$ one day before emergence

In this case, Equation A10 requires that the *DegT50* ≥ 0.69 years. This criterion is fulfilled because the *DegT50* of 200 days at 20 °C corresponds to a *DegT50* of 694 days, so 1.9 years under field conditions for the scenario for the concentration in total soil in the North Zone (see Table 9 of EFSA, 2012a. The result in Figure A.5 shows that, in this case, accumulation dominates over the annual fluctuations so the selected scenario is also likely to be a valid 95th percentile case for this metabolite.

Figure A.5 shows a plateau concentration of about 1.5 mg kg$^{-1}$. This result can be used to check the applicability of Equation A6 for this scenario. The dry bulk density of the top 20 cm for this scenario was 0.95 kg l$^{-1}$ (EFSA, 2012a p. 37) and the effective DegT50 was 1.9 year as described above. This gives a predicted plateau concentration of 1.44 mg kg$^{-1}$ which corresponds well with the numerical result in Figure A.5.

Figure A.6 shows the results of the same calculations but now for an ecotoxicological mixing depth of 1 cm. For this case, Equation A10 requires that the *DegT50* ≥ 14 years whereas it is about 1.9 years. The figure clearly shows that the effects of formation cannot be ignored when assessing the peak concentrations. When applied as a parent (mimicking a very rapidly degrading metabolite) the peak concentrations are about four times higher than when formed as a soil metabolite.

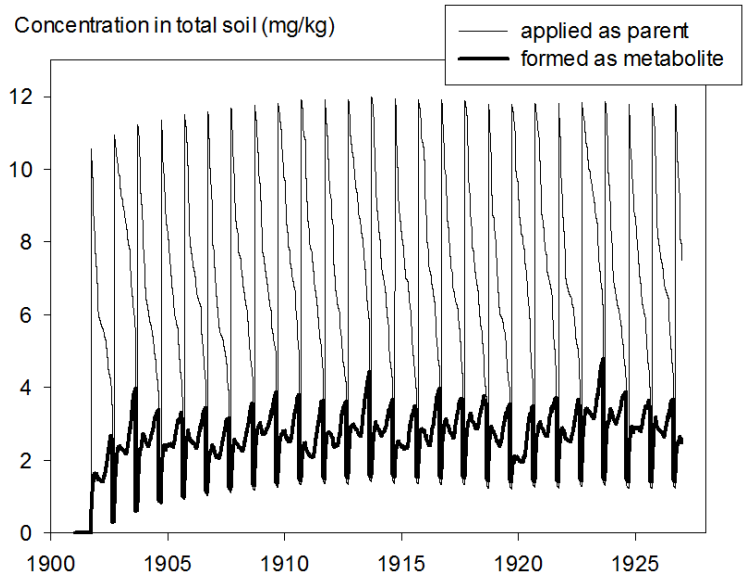


**Figure A.6:** Average concentration in total soil in the 1-cm top layer for a substance with *DegT50* = 200 days at 20 °C and $K_{om}$ = 1 000 l /kg$^{-1}$ ("substance A") as calculated with PEARL for the scenario "concentration in total soil" in the North Zone and winter wheat. Results are shown for application of this substance A itself and for application of another substance ("substance B") that degrades into substance A with a formation fraction of 100 %. Substances A and B have equal molar masses. Substance B has a *DegT50* of 50 days at 20 °C and a $K_{om}$ of 1 000 l kg$^{-1}$. Both substances A and B were applied each year at a dose of 1 kg ha$^{-1}$ one day before emergence

## A.6. Conclusions

Tiers 1 and 2B/C are expected to generate exposure concentrations for soil metabolites that are conservative enough given the exposure assessment goal.

The scenario selection procedure that forms the basis of Tiers 2A and 3 is considered inappropriate for soil metabolites that do leach significantly from the top 20 cm of soil or have precursors that do leach significantly from this top 20 cm of soil. The requirement of no significant leaching of a substance is considered to be met if the ratio $K_{om}$/*DegT50* is above 1 L/(kg d). Furthermore, this selection procedure is considered appropriate only for soil metabolites that show accumulation over the years (to be assessed with Equation A10).

For metabolites that do not accumulate or that penetrate significantly below a 20 cm depth (either by leaching of the metabolite itself or by leaching of one of its precursors), it cannot be guaranteed that the results generated at Tier 2A, Tier 3A and Tier 3B are close to the 95th spatial percentile of the spatial concentration distribution. Despite this, use of the exposure assessment scheme for all soil metabolites is advised (including soil metabolites that show considerable leaching) until better alternatives become available.

# Appendix B. Procedure for assessing the table of the fraction of the dose reaching the soil

## B.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 thus never reach the soil. EFSA PPR Panel (2012a) considered this approach not defensible and proposed to use, as defaults in the exposure assessment, 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. Crop canopy processes and foliar wash-off can be simulated by PEARL and PELMO. However, for Tier 2C this would require running one of the numerical models before running PERSAM. For this reason, tables of the fraction of the dose reaching the soil 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 FOCUS 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 $ha^{-1}$ was applied to the plant surface.
- For each year, the annual wash-off (kg $ha^{-1}$) 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 $ha^{-1}$).

Calculations were made with PELMO and PEARL with applications on the 5th, 15th and 25th 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 FOCUS tables are based on crop development stages using so-called BBCH codes (Meier, 2001). How these two tables are linked is described in Section B4.

## B.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 CTN sugar beets, substance P3 ($DegT50$ = 200 days, $K_{om}$ = 1 000 l $kg^{-1}$), annual application of 1 kg $ha^{-1}$ 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 $ha^{-1}$ to the soil, 0.9 kg $ha^{-1}$ on the crop and simulation of wash-off by PEARL using the wash-off factor of 0.1 $mm^{-1}$ 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 $ha^{-1}$ 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 $ha^{-1}$ 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$^{-1}$ was based on the equation:

$$A_{soil} = ((1 - f_i) + f_i f_w) A \quad \text{(B1)}$$

where $A_{soil}$ is the soil load (kg ha$^{-1}$), $A$ is the dosage (kg ha$^{-1}$), $f_i$ is the fraction of the dose that is intercepted by the crop (–) and $f_w$ is the fraction (–) washed off.

The time course for the concentration in total soil averaged over the top 20 cm in Figure B.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.

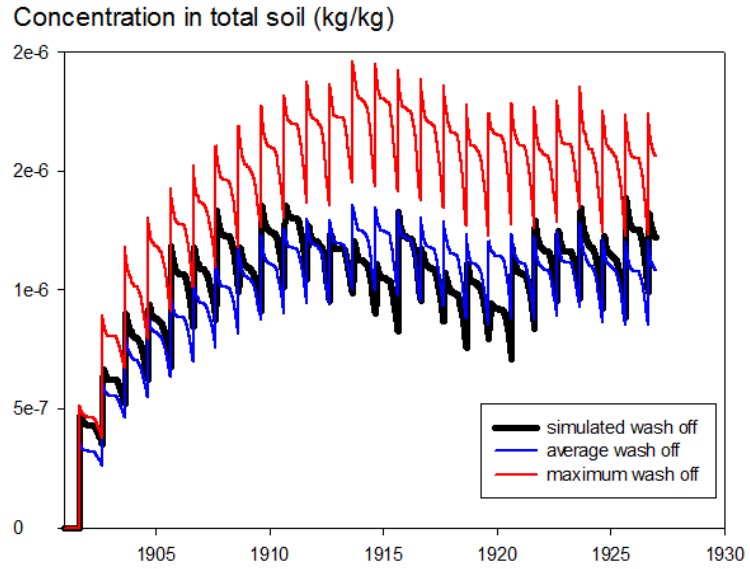


**Figure B.1:** Concentration in total soil (average over top 20 cm) as a function of time as calculated with PEARL for the scenario CTN and sugar beets, substance P3 (*DegT50* = 200 days, $K_{om}$ = 1 000 l kg$^{-1}$), annual application of 1 kg ha$^{-1}$ on 25 August for the three types of PEARL calculations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

The results for the concentration in total soil in the top 1 cm (Figure B.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 endpoint 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 B.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 B.2) show that the annual peak concentrations vary by a factor near to 3. Comparison of the different runs in Figure B.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 (2012a) 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, 2012a, p. 31). The line for the simulated wash-off in Figure B.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. Thus, for uses that lead to a high fraction intercepted by the crop, the exposure assessment goal of an overall 90th percentile should, in principle, 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, 2012a). 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.

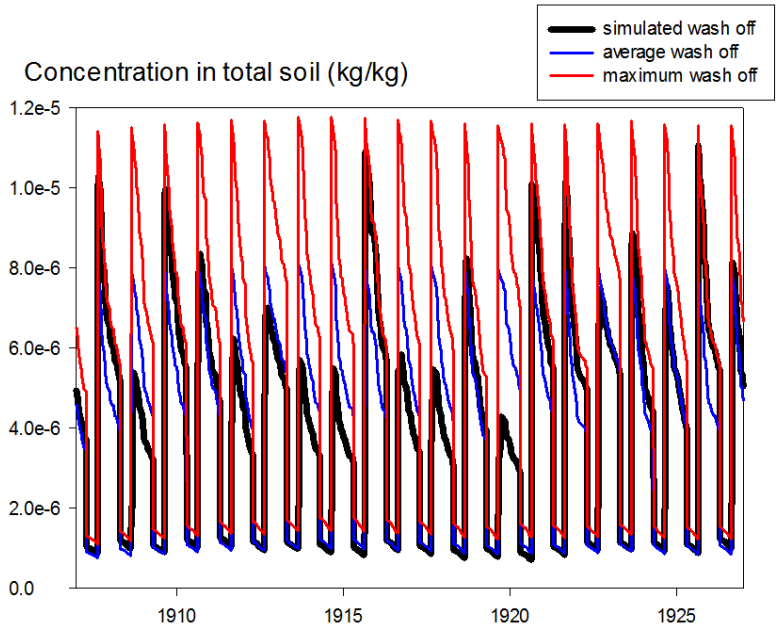


**Figure B.2:** Concentration in total soil (average over top 1 cm) as a function of time as calculated with PEARL for the scenario CTN and sugar beets, substance P3 (*DegT50* = 200 days, $K_{om}$ = 1 000 l kg$^{-1}$), annual application of 1 kg ha$^{-1}$ on 25 August for the three types of PEARL calculations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

In view of the foregoing, and because the wash-off factor of 0.1 mm$^{-1}$ is considered a conservative default value (EFSA PPR Panel, 2012a), it is proposed to base the approach on the annual average wash-off fraction; so the maximum annual wash-off will not be considered.

## B.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 crop cover fraction. The description of crop development was therefore harmonised. In both PEARL and PELMO, it is now assumed that the Leaf Area Index (LAI) increases linearly between emergence date and the date at which the maximum LAI occurs. Furthermore, it was decided to base the crop cover needed in the wash-off calculations on Beer's law:

$$SC = 1 - e^{-\kappa LAI} \qquad \text{(B2)}$$

in which κ is the extinction coefficient for diffuse solar radiation (set to 0.39 based on Kroes et al., 2008).

Figures B3 and B4 show the results of the harmonisation process. The figures show calculations with PELMO and PEARL for the six scenarios as a function of application time. Differences between PEARL and PELMO are, generally, small, indicating that the harmonisation process has been successful. However, there are systematic differences between PEARL and PELMO for early development stages in winter wheat and winter oil seed rapes (note that the sequence of the 10-day periods is based on the calendar year so crops that grow from autumn to summer show a bimodal pattern in Figures B3 and B4). This systematic difference is caused by the spring point that is implemented in PEARL but not in PELMO.

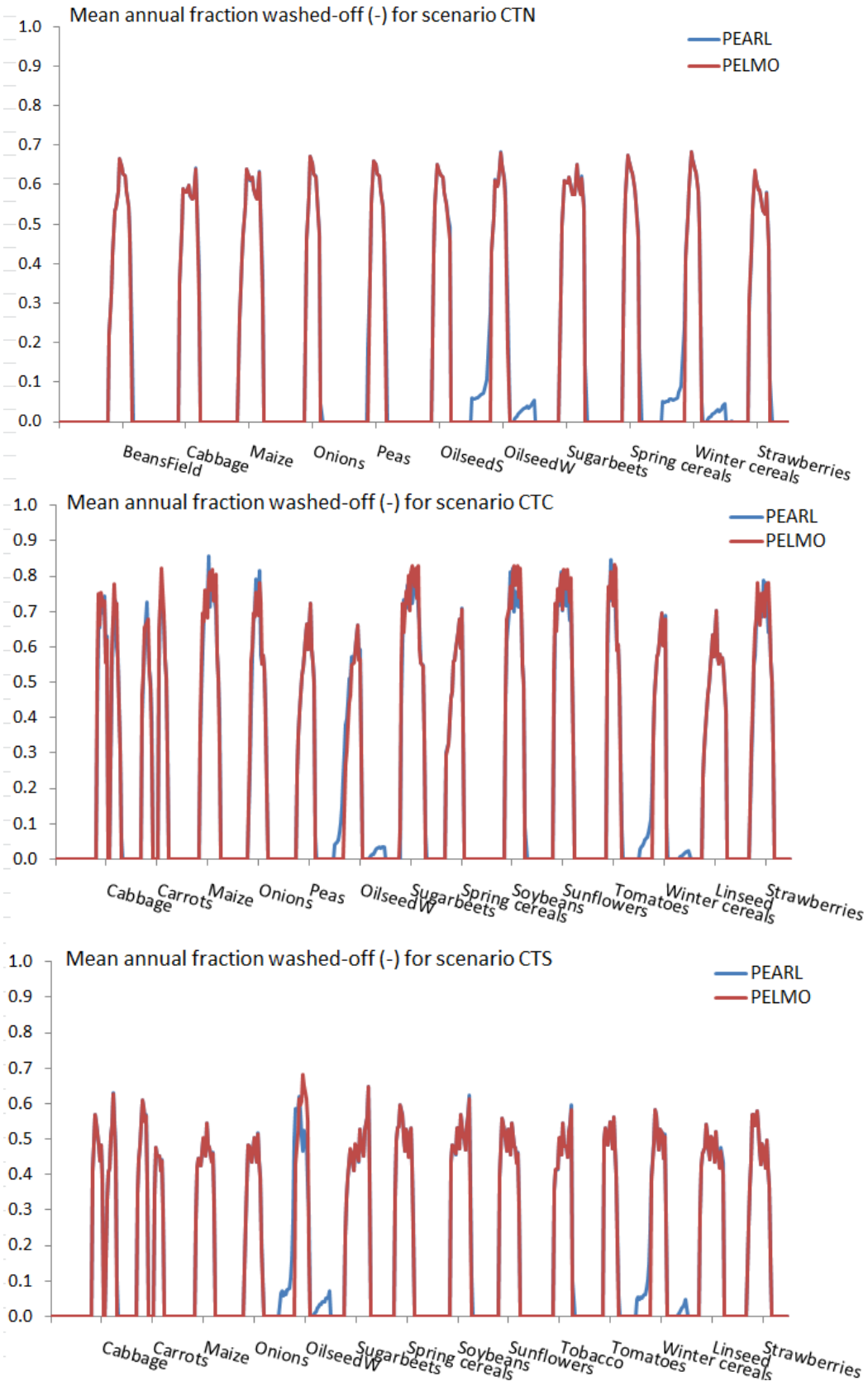


**Figure B.3:** Average annual fraction washed off as a function of application time for the three scenarios for the concentration in total soil as calculated with PELMO and PEARL

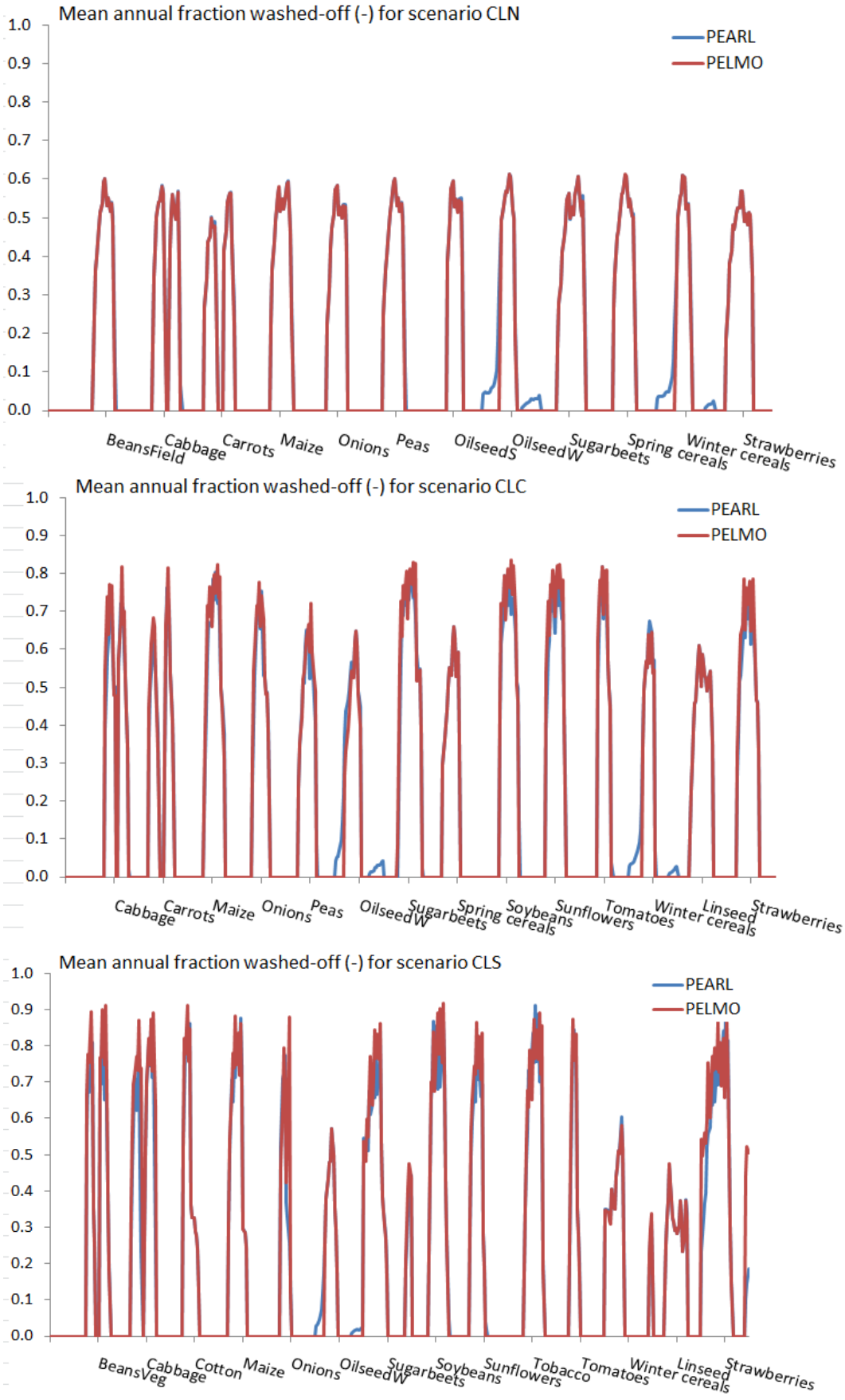


**Figure B.4:** Average annual fraction washed off as a function of application time for the three scenarios for the concentration in pore water as calculated with PELMO and PEARL

For the irrigated crops (most crops in the CTC, CLC and CLS scenarios), wash-off is, generally, higher than for the non-irrigated crops (all crops in the CTN, CTS and CLN scenarios and some crops in the other scenarios). Typically, in irrigated crops, the fraction of the dose reaching the soil is between 0.8 and 0.9; for non-irrigated scenarios, these fractions are between 0.5 and 0.6. The high wash-off in irrigated scenarios is caused by the relatively short time interval between the time of application and the next irrigation or rainfall event (and hence less dissipation at the crop canopy). Note that the figures are based on spray irrigation. The fractions washed off are generally in line with those reported in the manual of the Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) model (http://www.tifton.uga.edu/sewrl/gleams/glm30pst.pdf).

## B.4. Development of the table for the fraction of the dose reaching the soil

The table that is needed in the regulatory exposure assessment should consider the fraction of the dose that reaches the soil ($f_{soil}$). This fraction considers crop interception at the time of application as well as wash-off in the following days (where the latter is, of course, affected by dissipation processes at the plant canopy). Crop interception is based on the tables provided in EFSA (2014a). Wash-off fractions are calculated with PEARL and PELMO following the recommendations in EFSA PPR Panel (2012a) (i.e. using a default wash-off factor of 0.1 $mm^{-1}$ and a half-life of 10 days for the decline of pesticide residues on plants).

The wash-off factors are based on calculations with PELMO and PEARL over 26 years, of which the last 20 years were used considering annual applications for every scenario–crop combination. For each of these scenarios, 36 simulations were performed with different application dates (always on the 5th, 15th or 25th of every month). In the simulations it was assumed that crop interception was 100 %. However, as PELMO and PEARL consider 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 PELMO and PEARL for the last 20 years of the simulations (see Section B.2 for a justification for taking the average wash-off fraction). Though the calculations were somewhat different in both computer models (e.g. a spring point was used for winter crops by PEARL but not by PELMO), their results were found to be identical in most situations (Section B.3). Therefore, this table was based on the arithmetic mean of the PELMO and PEARL results.

In order 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 9) and ending at the date of harvest (i.e. BBCH 99 in the case of annual crops or BBCH 50 in the case of biennial crops, such as onions, sugar beet or cabbage). However, to improve the link for winter crops with their dormancy shortly after emergence, BBCH stage 9 was attached to the spring point rather than to the date of emergence.

The actual wash-off fraction was calculated according to following equation:

$$W_{act} = \frac{W_{100}\, CI}{100} \tag{B2}$$

where $W_{act}$ (–) is the actual wash-off fraction (i.e. the wash-off fraction considering the appropriate crop interception), $W_{100}$ is the wash-off fraction considering 100 % interception (i.e. the results of the above simulations) and $CI$ (%) is the actual crop interception according to the EFSA crop interception tables. Finally, $f_{soil}$ (i.e. the value that should be used in the exposure assessment) was calculated according to following equation:

$$f_{soil} = \frac{(100 - CI)}{100} + W_{act} \qquad \text{(B3)}$$

where $f_{soil}$ (–) is the fraction of the dose reaching the soil.

As mentioned above, simulations were carried for each crop–scenario combination. Since wash-off depends on the weather conditions (and therefore on the scenario), the fraction of the dose reaching the soil is also dependent on scenario. However, the variability of these fractions between the scenarios is, generally, less than 10 % (only in some cases is the coefficient of variation higher; refer to Table B.1). We therefore judged it defensible to use one average fraction of the dose reaching the soil for all six scenarios. Using such an average avoids too much complexity in the regulatory process.

**Table B.1:** Fraction of the dose reaching the soil ($f_{soil}$) considering crop interception and canopy dissipation processes as a function of crop development stage. Figures are averages for the six scenarios. Figures between brackets refer to the coefficient of variation (i.e. the standard deviation divided by the mean)

| | **BBCH code**[(a)(b)] | | | | |
|---|---|---|---|---|---|
| **Crop** | **00–09** | **10–19** | **20–39** | **40–89** | **90–99** |
| Beans (vegetable and field) | 1.00 (0.00) | 0.86 (0.06) | 0.83 (0.07) | 0.71 (0.02) | 0.50 (0.13) |
| Cabbage[(c)] | 1.00 (0.00) | 0.88 (0.02) | 0.85 (0.04) | 0.61 (0.07) | 1.00 (0.00) |
| Carrots[(c)] | 1.00 (0.00) | 0.87 (0.02) | 0.73 (0.07) | 0.46 (0.09) | 1.00 (0.00) |
| Cotton | 1.00 (0.00) | 0.92 (0.00) | 0.89 (0.00) | 0.55 (0.00) | 0.32 (0.00) |
| Linseed | 1.00 (0.00) | 0.79 (0.01) | 0.68 (0.03) | 0.63 (0.08) | 0.61 (0.04) |
| Maize | 1.00 (0.00) | 0.85 (0.01) | 0.80 (0.06) | 0.67 (0.12) | 0.38 (0.04) |
| Onions[(c)] | 1.00 (0.00) | 0.94 (0.02) | 0.90 (0.02) | 0.78 (0.03) | 1.00 (0.00) |
| Peas | 1.00 (0.00) | 0.77 (0.03) | 0.71 (0.11) | 0.63 (0.18) | 0.58 (0.17) |
| Oil seed rape (summer) | 1.00 (0.00) | 0.77 (0.01) | 0.66 (0.04) | 0.66 (0.03) | 0.56 (0.17) |
| Oil seed rape (winter) | 1.00 (0.00) | 0.76 (0.04) | 0.60 (0.06) | 0.64 (0.05) | 0.38 (0.14) |
| Sugar beets[(c)] | 1.00 (0.00) | 0.91 (0.03) | 0.75 (0.10) | 0.55 (0.07) | 1.00 (0.00) |
| Soybeans | 1.00 (0.00) | 0.84 (0.02) | 0.82 (0.07) | 0.73 (0.09) | 0.65 (0.09) |
| Strawberries | 1.00 (0.00) | 0.81 (0.02) | 0.78 (0.04) | 0.77 (0.06) | 0.61 (0.06) |
| Sunflowers | 1.00 (0.00) | 0.90 (0.02) | 0.82 (0.04) | 0.73 (0.10) | 0.40 (0.11) |
| Tobacco | 1.00 (0.00) | 0.71 (0.02) | 0.70 (0.10) | 0.69 (0.19) | 0.58 (0.08) |
| Tomatoes | 1.00 (0.00) | 0.79 (0.02) | 0.79 (0.09) | 0.69 (0.07) | 0.69 (0.07) |
| | **BBCH code**[(d)] | | | | |
| **Crop** | **00–19** | **20–29** | **30–39** | **40–69** | **70–99** |
| Spring cereals | 1.00 (0.00) | 0.90 (0.01) | 0.70 (0.14) | 0.64 (0.06) | 0.61 (0.06) |
| Winter cereals | 1.00 (0.00) | 0.91 (0.02) | 0.63 (0.08) | 0.61 (0.10) | 0.61 (0.07) |

(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 1 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.

# Appendix C. Procedure on how the scenario and model adjustment factors have been derived

## C.1. Derivation of scenario adjustment factors

In EFSA PPR Panel (2012a), the assessment of the Tier 1 and Tier 2A scenarios (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 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 European Commission JRC.[10] Subsequently, the updated version has also been implemented in PERSAM. The issues addressed in the updated version of the EFSA spatial data are (Hiederer, 2012):

- enlargement of spatial frame to include all EU-27 Member States and candidate countries;
- country boundaries adjusted to Eurostat GISCO Country 2010;
- EU Regulatory Zones layer enlarged to EU-27;
- land use based on CLC2000, V16. CLC map reprocessed;
- General Land Use map reprocessed;
- EFSA data mask reprocessed;
- mean monthly temperature data reprocessed;
- mean annual temperature recalculated;
- mean monthly precipitation data reprocessed;
- mean annual precipitation recalculated;
- Arrhenius-weighted mean annual temperature recalculated;
- FOCUS zones recalculated;
- all soil data reprocessed and extended to EU-27;
- Topsoil Water Content at Field Capacity reprocessed;
- CAPRI2000 data reprocessed and adjusted to new EFSA spatial data frame;
- units of CAPRI2000 dataset to per cent;
- background value set consistently for integer (0) and real (–9 000.0) data.

In principle, these changes in the EFSA spatial data introduced with version 1.1 would require a full reassessment of the location and properties of the Tier 1 and Tier 2A scenarios as well as the crop extrapolation factors. This can be seen in Table C.1, which shows that the current exposure scenarios partly represent a lower spatial percentile if based on the updated dataset. This is, in particular, true for the concentration in the total soil. For that reason, the crop extrapolation factors, as given in EFSA PPR Panel (2012a), are not sufficiently conservative to also cover the updated EFSA spatial data. However, the working group decided to not change the Tier 1 and Tier 2A scenarios but to reassess the crop extrapolation factors in order to keep the non-revised Tier 1 and Tier 2A scenarios sufficiently conservative.

**Table C.1:** Ranges of spatial percentiles of the current Tier 1 and Tier 2A scenarios in respect to the updated dataset (based on the total annual crops). Example calculations were made for the standard

[10] http://eusoils.jrc.ec.europa.eu/library/data/efsa/

substances 1, 9 and 19, for an evaluation depth $z_{eco}$ of 1 and 20 cm considering the peak concentration only. The area of total annual crops is considered equal to the sum of all CAPRI crops or crop groups

| | $C_{T,peak}$ | | $C_{L,peak}$ | |
|---|---|---|---|---|
| | **Minimum** | **Maximum** | **Minimum** | **Maximum** |
| North | 69 | 76 | 94 | 99 |
| Central | 79 | 82 | 94 | 95 |
| South | 84 | 86 | 93 | 97 |

In EFSA PPR Panel (2012a), the 95th percentile crop ratio is defined as follows:

$$\zeta = \frac{P_{95,x}}{P_{95,annual}} \quad \text{(C1)}$$

where $P_{95,x}$ is the spatial 95th percentile of the concentration for the area of crop $x$ and $P_{95,annual}$ is the spatial 95th percentile of the concentration for the total area of annual crops, both values based on the EFSA spatial data version 1.0. The magnitude of $\xi$ was assessed in EFSA PPR Panel (2012a) based on calculations with the simple analytical model for most of the CAPRI crops and crop groups and for the substances P1, P2 and P3. Finally, the PPR Panel proposed to use the maxima of the crop extrapolation factors to be used in Tiers 1 and 2A (Table C.2).

Following the update of the EFSA spatial data from version 1.0 to version 1.1 the Panel decided to replace the crop extrapolation factors by so-called scenario adjustment factors, which are based on a revised 95th percentile crop ratio as follows:

$$\zeta = \frac{P_{95,x}}{P_{Tier1}} \quad \text{(C2)}$$

where $P_{95,x}$ is the spatial 95th percentile of the concentration for the area of crop $x$ based on the EFSA spatial data version 1.1 and $P_{Tier1}$ is the PEC calculated at Tier 1 (calculated with the simple analytical model without any adjustment factors) based on the EFSA spatial data version 1.0. As with the original factor, this ratio applies to either $C_{T,peak}$ or $C_{L,peak}$ and to a specific substance in a certain regulatory zone.

To assess the possible magnitude of the revised $\xi$, the working group made calculations with the simple analytical model for all CAPRI crops or crop groups that are in Table 5. This was carried out for the standard substances 1 to 19 (refer to EFSA PPR Panel (2012a) for substance properties) for all regulatory zones and for an evaluation depth $z_{eco}$ of 1 and 20 cm considering the peak concentration only.

**Table C.2:** Minimum and maximum scenario adjustment factors for concentration in the total soil ($C_{T,peak}$) based on the standards substances 1 to 19

| CAPRI crop or crop group | $z_{eco}$ 1 cm | | | | | | $z_{eco}$ 20 cm | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | North | | Central | | South | | North | | Central | | South | |
| | Min | Max | Min | Max | Min | Max | Min | Max | Min | Max | Min | Max |
| Barley | 1.78 | 1.80 | 1.16 | 1.18 | 1.09 | 1.12 | 1.78 | 1.81 | 1.16 | 1.29 | 1.09 | 1.17 |
| Common wheat | 1.25 | 1.29 | 1.10 | 1.13 | 1.10 | 1.13 | 1.21 | 1.29 | 1.10 | 1.19 | 1.10 | 1.20 |
| Durum wheat | NC | NC | 1.06 | 1.12 | 0.93 | 0.98 | NC | NC | 1.06 | 1.22 | 0.87 | 0.98 |
| Fallow | 1.83 | 1.91 | 1.24 | 1.26 | 1.07 | 1.07 | 1.72 | 1.91 | 1.24 | 1.31 | 1.07 | 1.09 |
| Floriculture and flower bulbs | 0.80 | 0.84 | 0.97 | 0.98 | 1.11 | 1.13 | 0.75 | 0.84 | 0.96 | 0.98 | 1.11 | 1.19 |
| Maize | 1.04 | 1.13 | 1.07 | 1.11 | 1.09 | 1.09 | 0.93 | 1.13 | 1.07 | 1.13 | 1.09 | 1.12 |
| Oats | 2.28 | 2.50 | 1.35 | 1.36 | 1.01 | 1.03 | 2.28 | 2.77 | 1.35 | 1.41 | 1.00 | 1.03 |
| Other fresh vegetables | 1.42 | 1.49 | 1.26 | 1.29 | 1.04 | 1.04 | 1.42 | 1.52 | 1.22 | 1.29 | 1.04 | 1.07 |
| Pulses | 1.22 | 1.27 | 1.19 | 1.20 | 1.09 | 1.13 | 1.17 | 1.27 | 1.19 | 1.23 | 1.09 | 1.18 |
| Oilseed rapes | 1.26 | 1.29 | 1.14 | 1.17 | 1.12 | 1.15 | 1.24 | 1.29 | 1.14 | 1.28 | 1.12 | 1.23 |
| Rye | 1.32 | 1.36 | 1.42 | 1.46 | 1.10 | 1.12 | 1.28 | 1.36 | 1.42 | 1.51 | 1.10 | 1.16 |
| Soya beans | NC | NC | 0.96 | 0.98 | 0.90 | 0.94 | NC | NC | 0.95 | 0.98 | 0.83 | 0.94 |
| Sugar beets | 1.10 | 1.14 | 1.33 | 1.33 | 1.10 | 1.14 | 1.11 | 1.14 | 1.33 | 1.35 | 1.10 | 1.21 |
| Sunflowers | NC | NC | 0.92 | 0.97 | 1.04 | 1.05 | NC | NC | 0.86 | 0.97 | 1.01 | 1.05 |
| Texture crops | 1.77 | 1.77 | 1.06 | 1.13 | 0.94 | 1.01 | 1.77 | 1.77 | 1.06 | 1.22 | 0.94 | 1.01 |
| Tobacco | NC | NC | 1.05 | 1.06 | 1.05 | 1.05 | NC | NC | 1.05 | 1.07 | 1.03 | 1.05 |

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

**Table C.3:** Minimum and maximum scenario adjustment factors for the concentration in the liquid phase ($C_{L,peak}$) based on the standards substances 1 to 19

| CAPRI crop or crop group | $z_{eco}$ 1 cm | | | | | | $z_{eco}$ 20 cm | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | North | | Central | | South | | North | | Central | | South | |
| | Min | Max | Min | Max | Min | Max | Min | Max | Min | Max | Min | Max |
| Barley | 0.96 | 0.98 | 0.94 | 0.98 | 1.00 | 1.03 | 0.96 | 1.02 | 0.94 | 1.02 | 0.95 | 1.03 |
| Common wheat | 0.96 | 0.98 | 1.00 | 1.03 | 0.87 | 0.97 | 0.96 | 1.03 | 1.00 | 1.03 | 0.87 | 1.00 |
| Durum wheat | NC | NC | 0.97 | 0.99 | 1.04 | 1.11 | NC | NC | 0.97 | 1.01 | 0.94 | 1.11 |
| Fallow | 0.96 | 0.98 | 0.93 | 1.02 | 1.03 | 1.08 | 0.96 | 1.03 | 0.93 | 1.03 | 0.99 | 1.08 |
| Floriculture and flower bulbs | NC | NC | 0.63 | 0.80 | 0.99 | 1.08 | NC | NC | 0.63 | 0.80 | 0.98 | 1.08 |
| Maize | 0.94 | 0.98 | 1.02 | 1.18 | 0.90 | 0.97 | 0.94 | 1.01 | 0.99 | 1.18 | 0.90 | 1.03 |
| Oats | 0.63 | 0.84 | 0.89 | 1.00 | 1.11 | 1.20 | 0.63 | 0.86 | 0.89 | 1.01 | 0.98 | 1.20 |
| Other fresh vegetables | 0.94 | 0.97 | 1.02 | 1.05 | 1.13 | 1.25 | 0.94 | 0.99 | 1.00 | 1.05 | 0.97 | 1.25 |
| Pulses | 0.89 | 0.97 | 0.94 | 0.98 | 1.01 | 1.04 | 0.89 | 0.97 | 0.94 | 1.02 | 0.98 | 1.04 |
| Oilseed rapes | 0.96 | 0.98 | 0.92 | 0.95 | 0.84 | 0.92 | 0.96 | 1.04 | 0.92 | 1.01 | 0.84 | 1.00 |
| Rye | 0.94 | 0.97 | 0.87 | 0.98 | 1.08 | 1.16 | 0.94 | 1.05 | 0.87 | 1.02 | 1.05 | 1.16 |
| Soya beans | NC | NC | 1.02 | 1.23 | 0.90 | 0.99 | NC | NC | 0.99 | 1.23 | 0.90 | 0.99 |
| Sugar beets | 0.96 | 0.98 | 1.00 | 1.03 | 0.87 | 0.99 | 0.96 | 0.99 | 1.00 | 1.04 | 0.87 | 0.99 |
| Sunflowers | NC | NC | 1.02 | 1.23 | 1.01 | 1.03 | NC | NC | 0.98 | 1.23 | 0.99 | 1.03 |
| Texture crops | 0.58 | 0.74 | 0.95 | 0.96 | 1.05 | 1.12 | 0.58 | 0.76 | 0.95 | 1.03 | 0.96 | 1.12 |
| Tobacco | NC | NC | 0.98 | 1.03 | 0.91 | 1.11 | NC | NC | 0.95 | 1.03 | 0.77 | 1.11 |

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

In line with the approach taken in EFSA PPR Panel (2012a), the working group proposes to use the maxima of these values of each regulatory zone (rounded up) to be used as scenario adjustment factors in Tiers 1 and 2A (Table C.4).

**Table C.4:** Ranges (and final values) of the new scenario adjustment factors in comparison with ranges of the former crop extrapolation factors 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] | | | | | | Crop extrapolation factor [b] (EFSA PPR Panel, 2012a) | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{T,peak}$ | | | $C_{L,peak}$ | | | $C_{T,peak}$ | | $C_{L,peak}$ | |
| | **Min** | **Max** | **Final** [c] | **Min** | **Max** | **Final** [c] | **Min** | **Max** | **Min** | **Max** |
| North | 0.75 | 2.77 | **3.0** | 0.58 | 1.05 | **2.0** | 0.64 | 1.79 | 0.87 | 1.02 |
| Central | 0.86 | 1.51 | **2.0** | 0.63 | 1.23 | **1.5** | 0.74 | 1.16 | 0.93 | 1.15 |
| South | 0.83 | 1.23 | **2.0** | 0.77 | 1.25 | **1.5** | 0.86 | 1.07 | 0.86 | 1.13 |

(a): Based on the standard substances 1 to 19
(b): Based on the substances P1, P2 and P3
(c): Rounded up to ensure consistency in the tiered approach

## C.2. Derivation of model adjustment factors

The model adjustment factors, as derived in EFSA PPR Panel (2012a), were based on simulations with PEARL and PELMO for 19 substances. In these simulations, only *DegT50* and $K_{om}$ were changed. However, at Tier 2A, users can change other substance properties, such as the Freundlich adsorption coefficient (*1/n*), the molar activation energy ($E_{Act}$), the moisture dependence of degradation exponent (*B*) and the transpiration stream concentration factor (*TSCF*). 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.

To investigate the effect of these four parameters on the model adjustment factors, a simple sensitivity analysis was carried out. In this analysis, for each parameter, three runs were performed, i.e. one with the lower limit of plausible values, one with the normal value, as reported in EFSA PPR Panel (2012a), and one with the upper limit of plausible values. All parameters were varied one-by-one and 19 substances (reported in EFSA PPR Panel, 2012a) were simulated. The following range of parameters was considered:

- *1/n* was varied between 0.7 and 1.0. This range is based on Boesten et al. (2012).
- $E_{Act}$ was varied between 35 and 115 kJ $mol^{-1}$. According to EFSA (2007), 95 % of the reported values are within this range.
- *B* was varied between 0.1 and 1.5 (EFSA, 2012a).
- *TSCF* was varied between 0 and 1, i.e. the full range of possible values in the numerical models.

## C.3. Results

Results are summarised in Figures C.1 to C.4. Each figure shows the ratio between the results obtained by PEARL and the results obtained by PERSAM. The maximum of all these ratios is the required model adjustment factor.

### *Effect of the Freundlich exponent*

Figure C.1 shows that the effect of the Freundlich exponent on the concentration in total soil is negligible (only some effect is visible, which is because of slightly different mobility and hence transport of the pesticide from the top layer). The predicted ratio is always below the model adjustment factor for the scenario as reported in EFSA PPR Panel (2012a), so adaptation of this factor is not necessary.

For the concentration in pore water, a clear effect is visible. An exponent of 0.7 leads to a higher ratio PEARL/PERSAM, an exponent of 1.0 leads to a lower ratio. For the CL and CT scenarios, the ratio is higher than the original model adjustment factor for the respective scenario.

***Effect of the molar activation energy***

In the simulations, the same value for the molar activation energy was used in PEARL and PERSAM. Results are shown in Figures C.3 and C.4.

A lower value of the molar activation energy leads to a higher ratio of the predicted concentration in total soil, whereas a higher value leads to a lower ratio (Figures C.3 and C.4). This effect is most pronounced when using an evaluation layer of 20 cm. This is most probably caused by the difference in the molar activation energy used in the model and the molar activation energy used in the calculation of the Arrhenius-weighted average temperature that has been used for the scenario selection procedure (the scenarios were selected assuming $E_{Act}$ of 65.4 kJ mol$^{-1}$). For the CTN scenario and an evaluation depth of 20 cm, the original model adjustment factor is (slightly) exceeded.

For the concentration in liquid phase, the effect is generally in the same direction. However, the original model adjustment factors were not exceeded.

***Effect of the moisture dependence of degradation***

A low value of the exponent in the moisture dependence of degradation leads to higher concentrations in total soil and hence a higher ratio PEARL/PERSAM (Figures C.5 and C.6). For the lowest value (B = 0.1), the original model adjustment factor is exceeded in many cases.

For the concentration in pore water, the effect is in the same direction but less pronounced. The original model adjustment factor is slightly exceeded in one case (scenario CLS, TWA = 56 days).

***Effect of the transpiration concentration stream factor***

A lower transpiration concentration stream factor leads to higher concentrations in total soil and hence a higher ratio PEARL/PERSAM (Figures C.7 and C.8). This effect is most pronounced for the 20 cm evaluation layer. For this evaluation layer, the model adjustment is exceeded in five out of six cases.

For the concentration in pore water, no effect is observable for the 1 cm evaluation layer. For the 20 cm layer, the effect is in the same direction as for the concentration in total soil but the model adjustment factor is exceeded in only one case (scenario CLS).

## C.4. Conclusions

Based on these findings, the model adjustment factors would have to be changed to the following values (see EFSA PPR Panel (2012a), page 45 for the old values):

- $f_m$ = 1.2 (was 1.1) for the peak concentration in total soil for $z_{eco}$ = 1 cm.
- $f_m$ = 2.0 (was 1.3) for the peak concentration in total soil for $z_{eco}$ = 20 cm.
- $f_m$ = 2.0 (was 1.7) for all TWA concentrations in total soil.
- $f_m$ = 2.5 (was 2.0) for all pore water concentrations in North and Central Zones.
- $f_m$ = 4.0 (was 3.0) for all pore water concentrations in South Zone.

Note that these findings are based on only two evaluation depths, i.e. 1 cm and 20 cm. Furthermore, worst-case combinations of parameters (i.e. *TSCF* = 0 in combination with 1/*n* = 0.7) have not been studied. If such combinations had been studied, higher model adjustment factors would have been calculated. For the sake of simplicity, and to ensure consistency within the tiered approach, it is therefore proposed to use model adjustment factors that are rounded up, i.e. $f_m$ = 2 for all concentration

in total soil scenarios and $f_m$ = 4 for all concentration in pore water scenarios. These model adjustment factors should be used in all tiers where the analytical model is used.

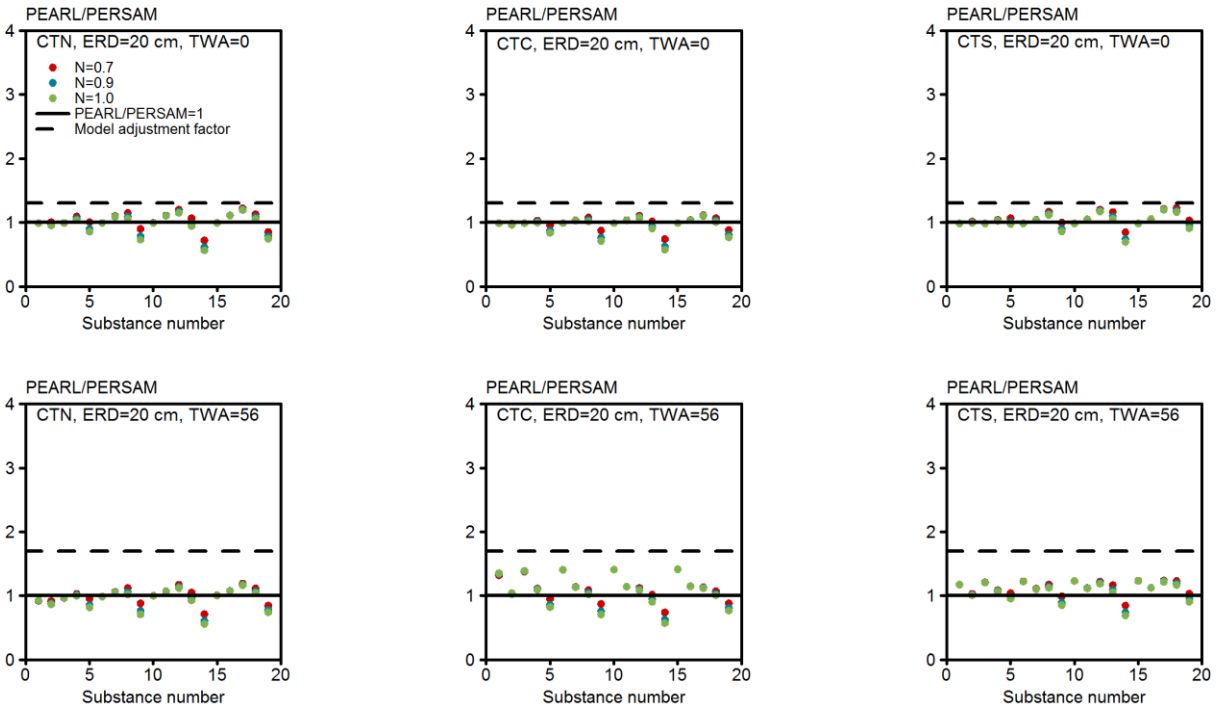


**Figure C.1:** Effect of the Freundlich exponent on the ratio between the concentration in total soil predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

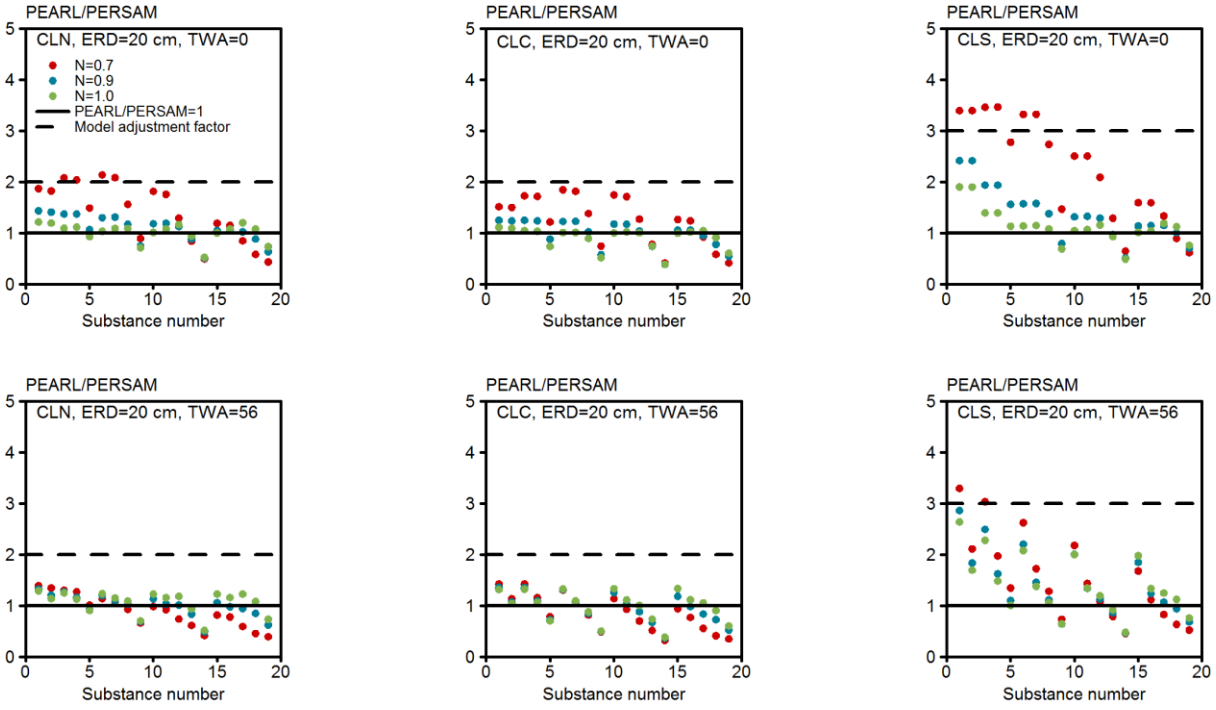


**Figure C.2:** Effect of the Freundlich exponent on the ratio between the concentration in pore water predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

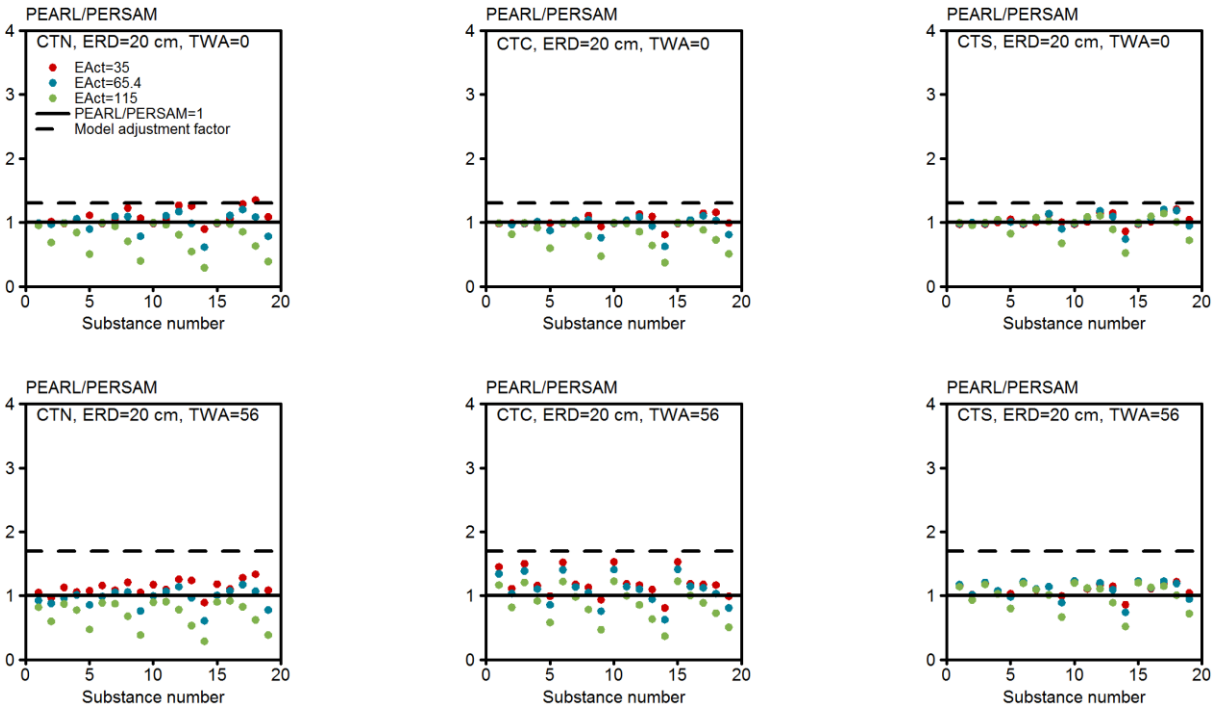


**Figure C.3:** Effect of the molar activation energy on the ratio between the concentration in total soil predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

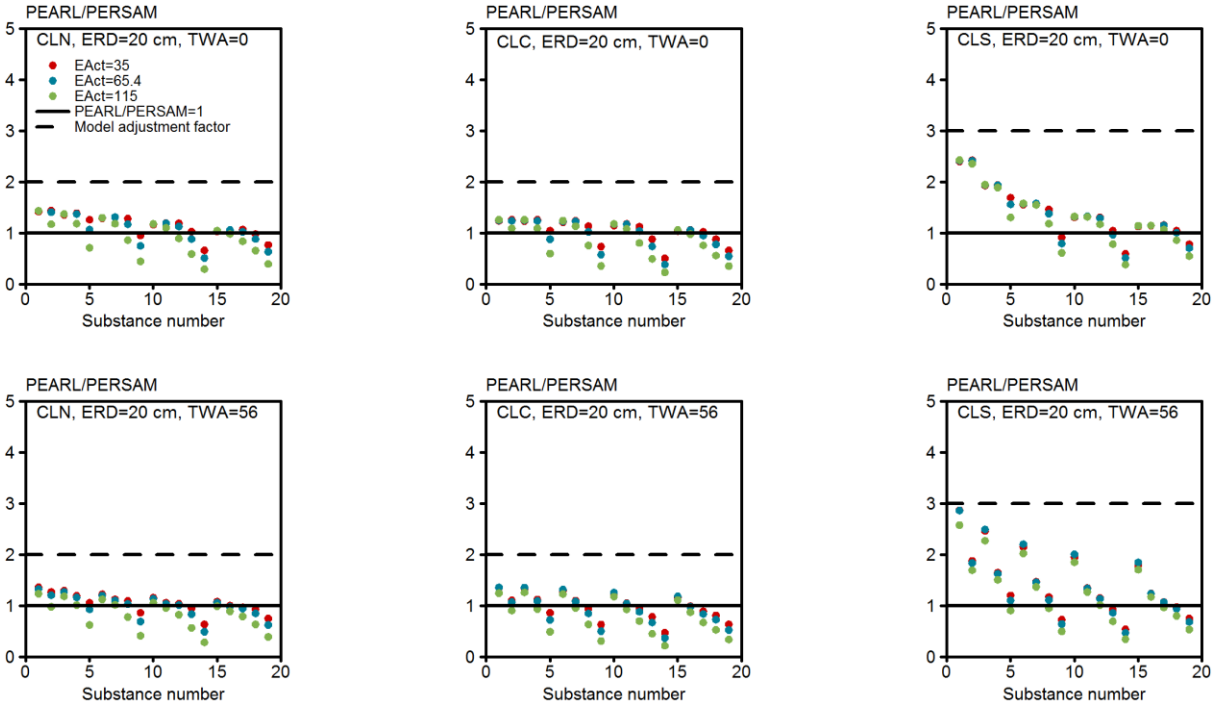


**Figure C.4:** Effect of the molar activation energy on the ratio between the concentration in pore water predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

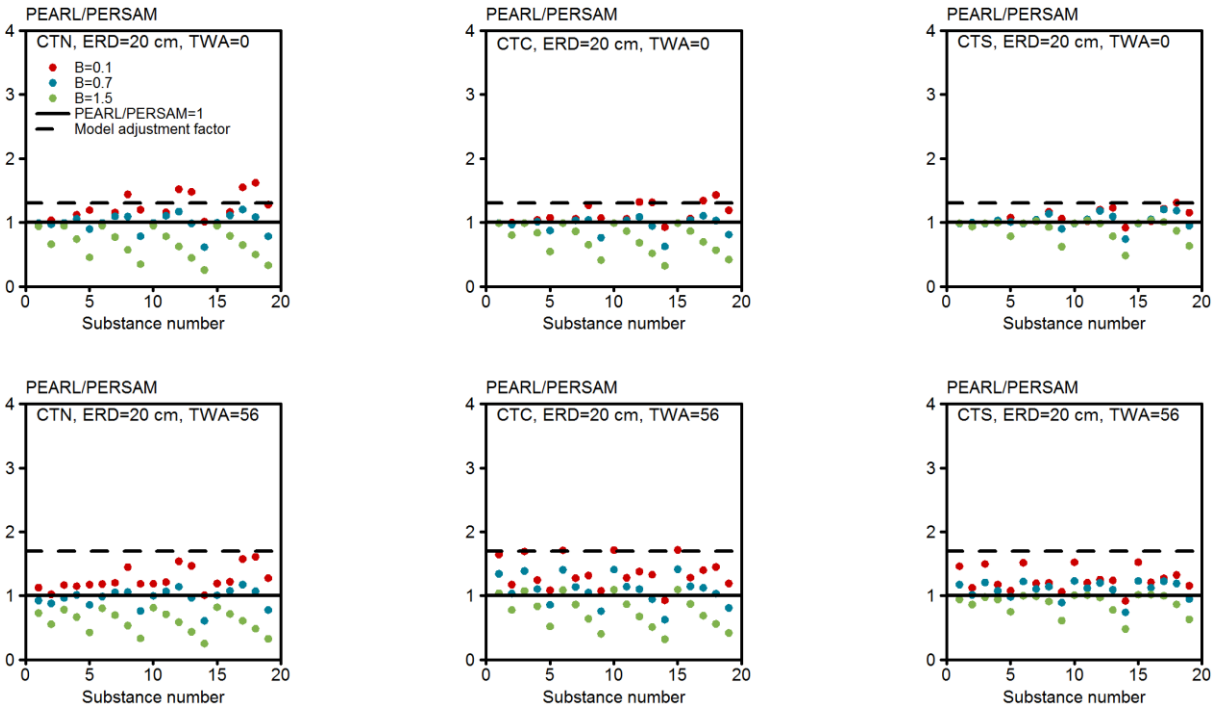


**Figure C.5:** Effect of the exponent in the equation of soil moisture on the ratio between the concentration in total soil predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

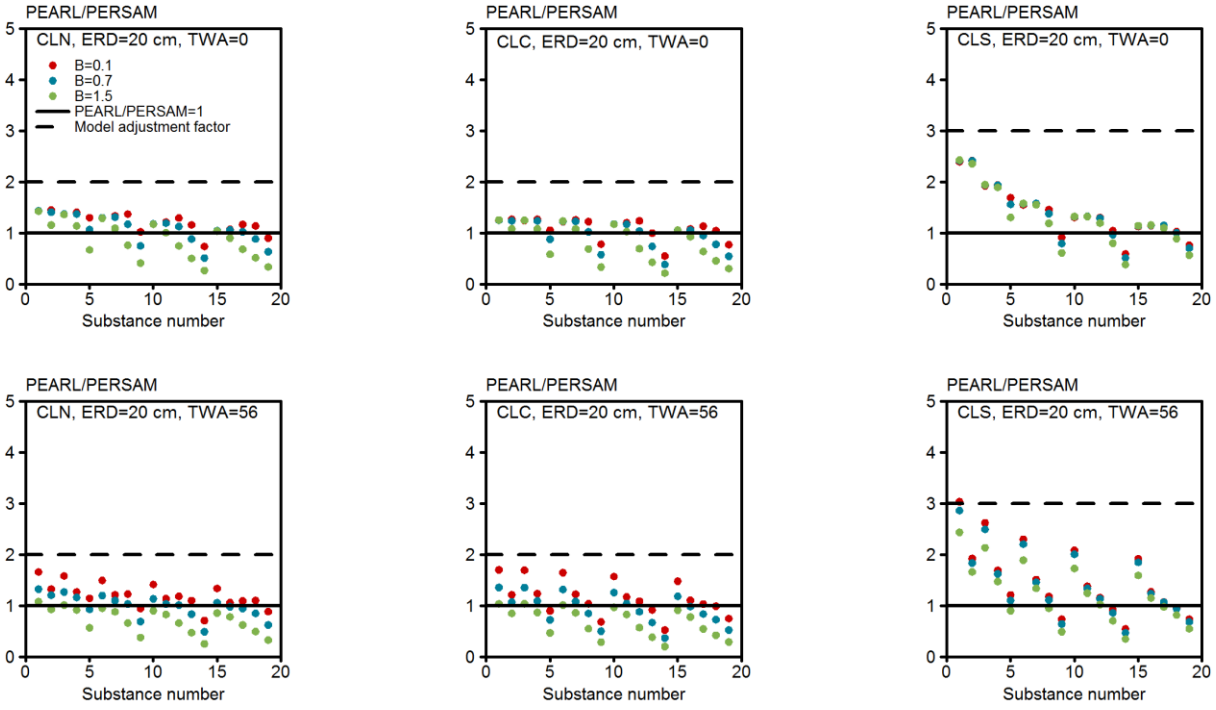


**Figure C.6:** Effect of the exponent in the equation of soil moisture on the ratio between the concentration in pore water predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

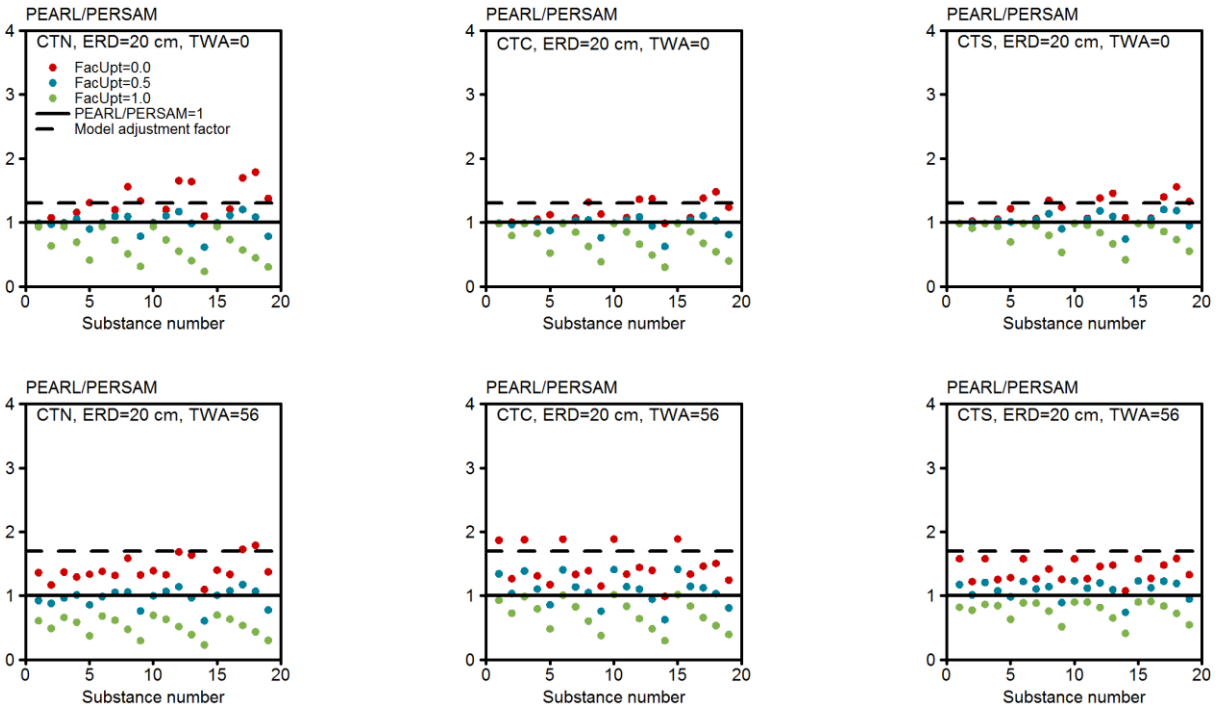


**Figure C.7:** Effect of the transpiration concentration stream factor on the ratio between the concentration in total soil predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

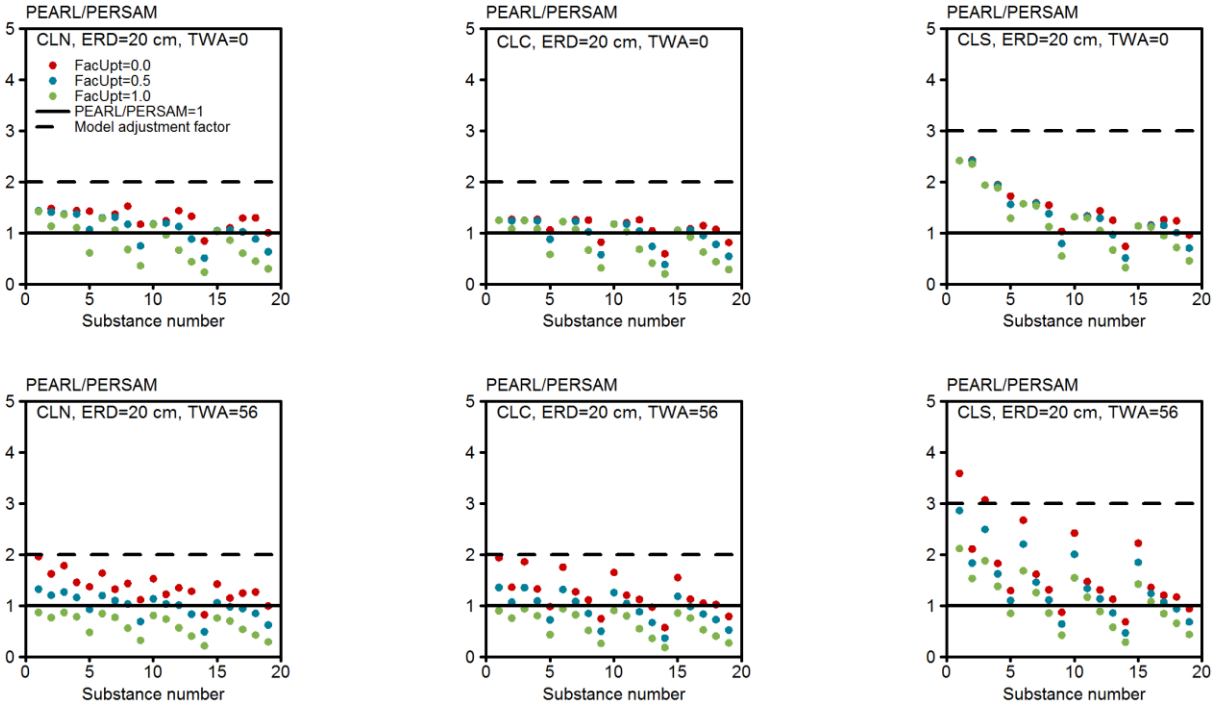


**Figure C.8:** Effect of the transpiration concentration stream factor on the ratio between the concentration in pore water predicted by PEARL and the concentration predicted by PERSAM. The evaluation layer is 20 cm. Upper panels: peak concentration. Lower panels: TWA concentration (56 days). The dashed line is the model adjustment factor reported in EFSA PPR Panel (2012a)

## Appendix D. Definition of PERSAM crops

Information on the regional distribution of annual crop or crop groups in the EU as implemented in PERSAM is based on the so-called Common Agricultural Policy Regional Impact assessment (CAPRI) database (Leip et al., 2008). This database contains official data obtained from the European statistical offices (available online: http://epp.eurostat.ec.europa.eu). In short, statistical information about agricultural production, including annual and permanent crops, was obtained at the regional level of the so-called Nomenclature of Territorial Units for Statistics (NUTS 2). Data on crop areas were downscaled to the level of the Homogeneous Spatial Mapping Units (HSMU) using a two-step statistical approach combining prior estimates based on observed behaviour with a reconciliation procedure achieving consistency between the scales (Kempen et al., 2007). The area under analysis covered 25 Member States of the European Union; Malta and Cyprus were not included. Table D.1 gives the nomenclature of the crops as stated in PERSAM in relation to the CAPRI database and the EFSA spatial data version 1.1 (Hiederer, 2012). The maps included in PERSAM show the crop area as a percentage, whereas the original CAPRI dataset described in Hiederer (2012) was at a scale of 1 to 10 000. Furthermore, only pixels with a crop area > 1 % were included.

**Table D.1:** Nomenclature of annual crops or crop groups as stated in PERSAM in relation to the CAPRI database and the EFSA spatial data version 1.1 (Hiederer, 2012)

| PERSAM | CAPRI field name | Agricultural land use 2000 field name | EFSA File Name (EFSA spatial dataset 1.1) | Crop area (1 000 km$^2$)[(a)] |
|---|---|---|---|---|
| Barley | barl | Barley | *_BARLEY | 124.9 |
| Common wheat | swhe | Common wheat | *_COMMON_WHEAT | 202.7 |
| Durum wheat | dwhe | Durum Wheat | *_DURUM_WHEAT | 31.3 |
| Fallow | lfall | Fallow land | *_FALLOW | 84.0 |
| Floriculture and flower bulbs | flow | Floriculture | *_FLOWER | 0.3 |
| Maize | lmaiz | Maize | *_MAIZE | 116.0 |
| Oats | oats | Oats | *_OATS | 40.6 |
| Oilseed rapes | lrape | Rape and turnip rape | *_RAPES | 39.3 |
| Other annual crops | ocro | Other crops | *_OTHER_CROPS | 3.4 |
| Other cereals | ocer | Other cereals | *_OTHER_CEREALS | 17.1 |
| Other fodder on arable land | ofar | Fodder other on arable land | *_OTHER_FODDER | 90.7 |
| Other fresh vegetables | oveg | Vegetables | *_OTHER_VEGETABLES | 14.2 |
| Other non-permanent industrial crops | oind | Other non-permanent industrial crops | *_OTHER_INDUSTRIAL | 2.8 |
| Other root crops | roof | Other root crops | *_OTHER_ROOTCROPS | 1.3 |
| Potatoes | pota | Potatoes | *_POTATOES | 21.0 |
| Pulses | puls | Dry pulses | *_PULSES | 15.6 |
| Rye | ryem | Rye | *_RYE | 28.1 |
| Soya beans | soya | Soya | *_SOYA | 4.0 |
| Sugar beets | sugb | Sugar beet | *_SUGARBEET | 22.4 |
| Sunflowers | sunf | Sunflower | *_SUNFLOWERS | 36.0 |
| Texture crops | ltext | Fibre crops | *_TEXTURE_CROPS | 9.1 |
| Tobacco | toba | Tobacco | *_TOBACCO | 1.3 |
| Tomatoes | toma | Tomatoes | *_TOMATOES | 0.2 |

(a): Including grid cells with general land use mask set to 1 and a crop area > 1 %.
* EFSA_CAPRI.

## Appendix E. Procedure for building the Tier 3B scenarios

The Tier 3B scenarios are automatically generated by the shells of PEARL and PELMO. This appendix provides background information on the applied procedure.

The models first read the XY-coordinates from the csv file that is generated by PERSAM (Section 3.7.1). This information is used to look up the other scenario properties from the PEARL and PELMO databases. These databases are based on the EFSA spatial data version 1.1 (Hiederer, 2012). More specifically, the following information is used:

- XY-coordinate;
- regulatory zone (1 = North, 2 = Central, 3 = South);
- arithmetic mean annual temperature (°C);
- organic matter content of the top 30 cm of the soil (kg $kg^{-1}$);
- pH of the topsoil (–);
- soil textural class (1 = course, 2 = medium, 3 = medium fine, 4 = fine, 5 = very fine, 9 = no mineral).

The Tier 2A scenario of the corresponding regulatory zone is the starting point for building the Tier 3B scenario. Based on this scenario, the model shells make changes to the weather files and the soil files. All other data—including crop and irrigation data—are kept equal to the values of the corresponding Tier 2A scenarios.

### *Weather data*

The weather file of the Tier 3B scenario is based on the weather file of the Tier 2A scenario of the corresponding regulatory zone. The daily temperature is modified using the equation:

$$T_{day,Tier3B} = T_{day,Tier2A} - T_{avg,Tier2A} + T_{avg,Tier3B} \quad \text{(E1)}$$

where $T_{day,Tier3B}$ (°C) is the daily mean temperature of the Tier 3B scenario, $T_{day,Tier2A}$ (°C) is the daily mean temperature of the Tier 2A scenario, $T_{avg,Tier2A}$ (°C) is the arithmetic mean annual temperature of the Tier 2A scenario and $T_{avg,Tier3B}$ (°C) is the arithmetic mean annual temperature of the Tier 3B scenario (i.e. the temperature of the scenario location). All other parameters—including precipitation and evapotranspiration—are kept to their original values.

### *Soil data*

The PEARL and PELMO databases contain mean soil profiles for each soil textural class (Table E.1). Clay, sand and silt content are averages for all arable Soil Profile Analytical Database of Europe (SPADE) profiles (see EFSA, 2010a). Clay content of the class "very fine" is extremely high; however, this is not expected to be a major issue since clay content is used for only the heat flow model in the numerical models; the soil physical parameters are directly taken from the Hydraulic Properties of European Soils (HYPRES) database and do not show these extreme values. Variables that are not in the table, such as the number of numerical layers and the dispersion length, should be set to the values of the Tier 2A scenarios (e.g. the dispersion length must be 2.5 cm). Wilting point and field capacity for PELMO must be calculated according to Equation 3 in EFSA (2010a).

The soil profile of the Tier 3B scenario is based on the soil textural class of the Tier 3B location. All soil parameters are kept equal to the values in the six soil profiles in Table E.1, except for the organic matter content, the bulk density and pH. The organic matter content is obtained by multiplying the organic matter content of the Tier 3B scenario with $f_{z,om}$ of the individual soil horizons (the models check that in the case of no-mineral soil $f_{om}$ cannot be > 1 since the scaling factor is > 1 for that case).

The bulk density is calculated with Equation 2 in EFSA PPR Panel (2010a). The pH value in Table E.1 is assigned to all soil horizons.

***Crop and irrigation***

The crop to be simulated should be the same as the crop that was used for the Tier 2A scenario. This is a modification from EFSA PPR Panel (2012a), which was considered necessary to ensure consistency in the tiered approach

**Table E.1:** The six soil profiles that need to be added to the PEARL and PELMO databases. See EFSA PPR Panel (2010a) for further details

| **1: Coarse** | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Depth**[(a)] | **Sand** | **Silt** | **Clay** | $f_{z,om}$ | $f_z$ | $\theta_s$ | $\theta_r$ | $\alpha$ | $n$ | $K_s$ | $\lambda$ |
| 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 |
| **2: Medium** | | | | | | | | | | | |
| **Depth** | **Sand** | **Silt** | **Clay** | $f_{z,om}$ | $f_z$ | $\theta_s$ | $\theta_r$ | $\alpha$ | $n$ | $K_s$ | $\lambda$ |
| 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 |
| **3: Medium fine** | | | | | | | | | | | |
| **Depth** | **Sand** | **Silt** | **Clay** | $f_{z,om}$ | $f_z$ | $\theta_s$ | $\theta_r$ | $\alpha$ | $n$ | $K_s$ | $\lambda$ |
| 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 |
| **4: Fine** | | | | | | | | | | | |
| **Depth** | **Sand** | **Silt** | **Clay** | $f_{z,om}$ | $f_z$ | $\theta_s$ | $\theta_r$ | $\alpha$ | $N$ | $K_s$ | $\lambda$ |
| 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 |
| **5: Very fine** | | | | | | | | | | | |
| **Depth** | **Sand** | **Silt** | **Clay** | $f_{z,om}$ | $f_z$ | $\theta_s$ | $\theta_r$ | $\alpha$ | $n$ | $K_s$ | $\lambda$ |
| 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 |
| **9: Organic** | | | | | | | | | | | |
| **Depth** | **Sand** | **Silt** | **Clay** | $f_{z,om}$ | $f_z$ | $\theta_s$ | $\theta_r$ | $\alpha$ | $n$ | $K_s$ | $\lambda$ |
| 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 evaluation 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, $\theta_s$ ($m^3\ m^{-3}$) is the volume fraction of water at saturation, $\theta_r$ ($m^3\ m^{-3}$) is the residual water content in the extremely dry range, $\alpha$ ($cm^{-1}$) and n (–) are empirical parameters of the van Genuchten equation, $K_s$ ($m\ d^{-1}$) is the saturated hydraulic conductivity and $\lambda$ (–) is a shape parameter. Standard error of $f_{z,om}$ is 0 for the 0–30 cm soil layer, and 0.02 for all other soil layers.

## Appendix F. Desirable future amendments of PERSAM for row applications and granules

As described in Section 4, the current version of PERSAM cannot handle all calculation procedures for row treatments and granules. This appendix describes these missing procedures. It is recommended to include these calculation procedures in a future release of the PERSAM software.

### F.1. More realistic exposure assessment for row applications with PERSAM

Section 4 describes a simple conservative approach for applications in rows. A more realistic procedure is described below. In principle, this procedure can be implemented easily outside the PERSAM software tool. However, it is advised to base the exposure assessment for row treatments and granules on the procedure in Section 4 until user-friendly software is available; the calculation procedures described hereafter should be performed only when a risk has been identified.

***Concentration between the rows***

We describe here the procedure for calculations for spray applications in rows based on the simple analytical model. Let us assume that $A$ is the annual application rate (kg ha$^{-1}$ or mg dm$^{-2}$) defined as the mass of substance applied per surface area of the cropped field and that $f_{row}$ is the surface area of rows divided by the surface area of the cropped field ($f_{row}$ is the fraction of the surface area of the field that is occupied by the treated rows, that can be either the crop row or the intercrop row, Figure 7). It is assumed that the rows are at different locations in the different application years and that this, in the long term, leads to a plateau concentration that is constant across the surface area of the field.

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 area between the rows the maximum concentration is equal to this steady-state plateau concentration. First, the concentration in total soil is considered and thereafter the concentration in pore water. Based on EFSA PPR Panel (2012a), the plateau concentration in total soil ($C_{T,plateau}$ mg kg$^{-1}$) can, for parent substances, be calculated as:

$$C_{T,between\_rows} = F_{mo} \frac{A}{\rho\, z_{til}} \frac{X}{1-X} \qquad \text{(F1)}$$

where $\rho$ is the dry soil bulk density (kg l$^{-1}$), $z_{til}$ (dm)[11] is the plough depth (fixed at 2 dm) and $X$ is defined as:

$$X = e^{-t_{cycle}\, f_T\, k_{ref}} \qquad \text{(F2)}$$

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 and $k_{ref}$ (day$^{-1}$) 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. The coefficient $k_{ref}$ is calculated from the degradation half-life by:

$$k_{ref} = \frac{\ln(2)}{DegT50} \qquad \text{(F3)}$$

where *DegT50* (days) is the degradation half-life in soil at the reference temperature and at field capacity. The temperature factor $f_T$ is calculated as:

[11] The unit "cm" is usually used for depths in this guidance because this is more common than "dm"; here "dm" is used as the unit for $z_{til}$ and similarly for $z_{eco}$ in Equation 16 to ensure consistency of units within Equations 12 and 16 (1 dm = 10 cm).

$$f_T = \exp\left(\frac{-E}{R}\left[\frac{1}{(T_{Arr}+273.15)} - \frac{1}{(T_{ref}+273.15)}\right]\right) \quad \text{(F4)}$$

where $E$ is the Arrhenius activation energy (65.4 kJ mol$^{-1}$), $R$ is the gas constant (0.008314 kJ mol$^{-1}$ K$^{-1}$), $T_{arr}$ is the so-called Arrhenius soil temperature (°C) of the scenario and $T_{ref}$ is the temperature at reference conditions (20 °C).

***Concentration in the rows***

The maximum concentration in the rows will be highest after the last application and is the sum of the plateau concentration and the concentration generated by this last application:

$$C_{T,in\_rows} = F_{mo}\left(\frac{A}{f_{row}\,\rho\, z_{eco}} + \frac{A}{\rho\, z_{til}}\frac{X}{1-X}\right) \quad \text{(F5)}$$

where $z_{eco}$ (dm) is the ecotoxicological averaging depth (i.e. 0.1, 0.25, 0.5 or 2 dm as specified by EFSA PPR Panel, 2012a).

***Concentration in pore water***

The maximum concentration in the pore water (liquid phase) is calculated from the maximum concentrations in total soil (Equation 12 or 16) assuming a linear sorption isotherm:

$$C_L = \frac{C_T}{\theta/\rho + f_{om}K_{om}} \quad \text{(F6)}$$

where $C_L$ (mg l$^{-1}$) is the maximum concentration in the liquid phase, $\theta$ (m$^3$ m$^{-3}$) is the volume fraction of liquid in soil at field capacity, $f_{om}$ (kg kg$^{-1}$) is the mass fraction of organic matter and $K_{om}$ (l kg$^{-1}$) is the coefficient for sorption on organic matter. The values for the scenario parameters $\rho$, $\theta$, $f_{om}$ and $T_{Arr}$ can be taken from Tables 1 and 2.

***Time-weighted averages***

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

$$C_{T,TWA} = \frac{C_T}{t_{avg}\, f_T\, k_{ref}}\left[1-\exp\left(-f_T\, k_{ref}\, t_{avg}\right)\right] \quad \text{(F7)}$$

The TWA concentration in the liquid phase, $C_{L,TWA}$, is calculated from an equation akin to Equation 18 but with $C_L$ instead of $C_T$.

***Soil metabolites***

For soil metabolites, the calculation procedure is the same as described above with one exception: in Equations 12 and 16 the annual application rate $A$ is replaced by the equivalent annual application rate of the metabolite (and of course using the *DegT50* and $K_{om}$ of the metabolite instead of the parent). For a soil metabolite formed from the parent, this equivalent rate is given by:

$$A_{met,1} = F_{f,1\_p}\,\frac{M_{met,1}}{M_{parent}}A \quad \text{(F8)}$$

where $F_{f,1\_p}$ (–) is the formation fraction of this metabolite (i.e. the stoichiometric coefficient of the formation of this metabolite from the parent substance, kinetically determined), $M_{met,1}$ is the molar mass of this metabolite (g mol$^{-1}$) and $M_{parent}$ is the molar mass of the parent substance (g mol$^{-1}$). The maximum occurrence observed should not be used since this would underestimate the concentration of the metabolite.

For a second soil metabolite formed from this first soil metabolite, the equivalent application rate is given by:

$$A_{met,2} = F_{f,1\_p} \; F_{f,2\_1} \quad \frac{M_{met,2}}{M_{parent}} A \tag{F9}$$

where $F_{f,2\_1}$ is the formation fraction (–) of this second metabolite as formed from the first metabolite and $M_{met,2}$ is the molar mass of this second metabolite (g mol$^{-1}$).

## F.2. Granular applications with an incorporation depth greater than 20 cm

Section 4.2 describes that the analytical model may be used for granular applications with an incorporation depth between 1 cm and 20 cm. Thus, PERSAM cannot be used if the incorporation depth is greater than 20 cm (or less than 1 cm). The reason being that the increase of the concentration resulting from the last application has to be based on averaging over the incorporation depth instead of averaging over $z_{eco}$. It is therefore recommended to include the following calculation procedure in the next release of PERSAM:

$$C_T = \left( \frac{A}{\rho z_{inc}} + \frac{A}{\rho z_{til}} \frac{X}{1-X} \right) \qquad z_{eco} < z_{inc} \tag{F10a}$$

$$C_T = \left( \frac{A}{\rho z_{eco}} + \frac{A}{\rho z_{til}} \frac{X}{1-X} \right) \qquad z_{eco} > z_{inc} \tag{F10b}$$

where $z_{inc}$ is the incorporation depth of the granules or small seed (dm) and $A$ is the application rate of the active substance in the granules or on the seed (kg ha$^{-1}$). The concentration in the pore water can be calculated using Equation 17 based on $C_T$ from Equation 21. The values for the scenario parameters $\rho$, $\theta$, $f_{om}$ and $T_{Arr}$ can be taken from Tables 1 and 2.

## Appendix G. Use of the rapidly dissipating fraction derived from field dissipation studies in the soil exposure assessment

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 exposure scenario.

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 step A, 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: a case YES where this is indeed expected and a case NO where this is not expected. In case YES, the field dissipation study was in Germany 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.

For Step B, 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, UK, Germany and Spain under normal agricultural use conditions. If fewer or more than four such values are available, it is proposed to use an estimate of the 12.5th percentile. 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 was 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 ($F_{field}$) were 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 to include 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 5) since it is unlikely that fast dissipation processes play an important role for the fraction that is washed off from the canopy.

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:

$$A_{ism} = (1 - f_i)(1 - F_{field})A \quad \text{(G1)}$$

where $A_{ism}$ is that part of the dose (kg ha$^{-1}$) that is assumed to reach the soil surface on the day of application (the part that penetrates immediately into the soil matrix), $f_i$ is the fraction of the dose intercepted by the canopy 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 runoff of substance 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 procedure for the handling of the fast surface decline is given by 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 in case of 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 (point iii) 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 H. Justification of selection of warming-up periods

As described in Section 3.5, the warming-up period consists of a multiple of six years and each six-year period consists of the same meteorological time series. It is important that this six-year time series has an approximately "average" air temperature. If the temperature of this six-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, the six-year averages of the Arrhenius air temperatures of the meteorological time series were calculated (see Table H.1). This gives 15 possible options for six-year periods for each scenario (starting in 1907 to 1921). Next, the average Arrhenius air temperature of all 15 options was calculated (e.g. 6.99 °C for CTN as shown in Table H.1). Subsequently, the desired six-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 CTN this is the period 1912–1917 because its Arrhenius temperature of 6.95 °C is lower than the 6.99 °C average and is closer to 6.99 °C than all the other periods with an average Arrhenius temperature below 6.99 °C.

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

- CTN: 1912–1917;
- CTC: 1907–1912;
- CTS: 1907–1912;
- CLN: 1909–1914;
- CLC: 1907–1912;
- CLS: 1921–1926.

**Table H.1:** Annual average air temperatures and annual average Arrhenius air temperatures of the CTN and CTC scenarios

| Year | Scenario CTN | | | Scenario CTC | | |
|---|---|---|---|---|---|---|
| | **Annual average temperature (°C)** | **Annual average Arrhenius temperature (°C)** | **Average of Arrhenius temperature of previous 6 years (°C)** | **Annual average temperature (°C)** | **Annual average Arrhenius temperature (°C)** | **Average of Arrhenius temperature of previous 6 years (°C)** |
| 1907 | 5.13 | 6.29 | | 8.44 | 10.14 | |
| 1908 | 4.70 | 6.43 | | 7.54 | 9.53 | |
| 1909 | 5.70 | 6.98 | | 8.29 | 10.55 | |
| 1910 | 2.97 | 4.81 | | 7.31 | 9.26 | |
| 1911 | 3.90 | 6.67 | | 8.56 | 10.73 | |
| 1912 | 4.94 | 7.26 | 6.41 | 7.53 | 9.69 | **9.98** |
| 1913 | 3.28 | 6.25 | 6.40 | 5.55 | 7.71 | 9.58 |
| 1914 | 4.47 | 6.89 | 6.48 | 7.52 | 9.58 | 9.59 |
| 1915 | 4.01 | 6.14 | 6.34 | 8.05 | 9.96 | 9.49 |
| 1916 | 5.10 | 7.87 | 6.85 | 8.38 | 10.27 | 9.66 |
| 1917 | 5.66 | 7.29 | **6.95** | 9.13 | 10.98 | 9.70 |
| 1918 | 4.70 | 7.64 | 7.01 | 7.87 | 9.87 | 9.73 |
| 1919 | 4.86 | 7.77 | 7.27 | 8.42 | 10.5 | 10.19 |
| 1920 | 4.47 | 7.08 | 7.30 | 8.28 | 11.14 | 10.45 |
| 1921 | 4.59 | 6.94 | 7.43 | 7.71 | 9.35 | 10.35 |
| 1922 | 4.57 | 7.31 | 7.34 | 7.82 | 9.87 | 10.29 |
| 1923 | 5.16 | 8.29 | 7.51 | 8.35 | 10.76 | 10.25 |
| 1924 | 5.43 | 7.99 | 7.56 | 8.77 | 10.52 | 10.36 |
| 1925 | 5.87 | 7.12 | 7.46 | 8.51 | 10.36 | 10.33 |
| 1926 | 4.59 | 6.78 | 7.41 | 7.94 | 10.08 | 10.16 |
| Average | | | **6.99** | | | **10.04** |

| Year | Scenario CTS | | | Scenario CLN | | |
|---|---|---|---|---|---|---|
| | Annual average temperature (°C) | Annual average Arrhenius temperature (°C) | Average of Arrhenius temperature of previous 6 years (°C) | Annual average temperature (°C) | Annual average Arrhenius temperature (°C) | Average of Arrhenius temperature of previous 6 years (°C) |
| 1907 | 11.54 | 12.97 | | 9.12 | 10.38 | |
| 1908 | 10.15 | 11.73 | | 7.94 | 9.39 | |
| 1909 | 10.68 | 12.01 | | 8.83 | 10.58 | |
| 1910 | 10.28 | 11.39 | | 7.49 | 8.65 | |
| 1911 | 11.57 | 12.69 | | 8.24 | 9.82 | |
| 1912 | 11.34 | 12.89 | **12.28** | 7.97 | 9.81 | 9.77 |
| 1913 | 10.14 | 11.58 | 12.05 | 6.31 | 7.96 | 9.37 |
| 1914 | 11.44 | 12.81 | 12.23 | 7.82 | 9.81 | **9.44** |
| 1915 | 10.69 | 11.83 | 12.20 | 7.75 | 8.98 | 9.17 |
| 1916 | 11.59 | 12.91 | 12.45 | 8.29 | 9.95 | 9.39 |
| 1917 | 11.25 | 12.45 | 12.41 | 8.72 | 9.88 | 9.40 |
| 1918 | 11.1 | 12.54 | 12.35 | 7.88 | 9.51 | 9.35 |
| 1919 | 11.61 | 12.5 | 12.51 | 8.64 | 10.53 | 9.78 |
| 1920 | 11.78 | 13.57 | 12.63 | 7.94 | 9.78 | 9.77 |
| 1921 | 10.83 | 12.19 | 12.69 | 7.96 | 9.34 | 9.83 |
| 1922 | 10.97 | 12.56 | 12.64 | 8.07 | 9.5 | 9.76 |
| 1923 | 11.37 | 13.07 | 12.74 | 8.7 | 10.61 | 9.88 |
| 1924 | 10.85 | 11.75 | 12.61 | 8.93 | 10.28 | 10.01 |
| 1925 | 10.43 | 11.54 | 12.45 | 9.05 | 10.41 | 9.99 |
| 1926 | 10.52 | 11.79 | 12.15 | 8.36 | 10 | 10.02 |
| Average | | | **12.34** | | | **9.76** |

| Year | Scenario CTS | | | Scenario CLN | | |
|---|---|---|---|---|---|---|
| | Annual average temperature (°C) | Annual average Arrhenius temperature (°C) | Average of Arrhenius temperature of previous 6 years (°C) | Annual average temperature (°C) | Annual average Arrhenius temperature (°C) | Average of Arrhenius temperature of previous 6 years (°C) |
| 1907 | 9.8 | 11.35 | | 10.92 | 12.5 | |
| 1908 | 8.07 | 9.86 | | 11.93 | 13.86 | |
| 1909 | 9.56 | 11.81 | | 12.73 | 14.77 | |
| 1910 | 8.33 | 10.2 | | 12.61 | 14.61 | |
| 1911 | 9.62 | 11.79 | | 13.72 | 15.45 | |
| 1912 | 8.95 | 11.22 | **11.04** | 13.49 | 15.1 | 14.38 |
| 1913 | 6.77 | 9.07 | 10.66 | 12.63 | 14.2 | 14.67 |
| 1914 | 8.82 | 11.15 | 10.87 | 13.31 | 14.84 | 14.83 |
| 1915 | 9.01 | 10.78 | 10.70 | 12.91 | 14.79 | 14.83 |
| 1916 | 9.51 | 11.35 | 10.89 | 13.09 | 15.12 | 14.92 |
| 1917 | 9.85 | 11.43 | 10.83 | 13.41 | 15.2 | 14.88 |
| 1918 | 8.85 | 10.88 | 10.78 | 13.4 | 15.35 | 14.92 |
| 1919 | 9.13 | 11.21 | 11.13 | 13.24 | 14.74 | 15.01 |
| 1920 | 9.04 | 11.65 | 11.22 | 13.72 | 15.99 | 15.20 |
| 1921 | 8.91 | 10.64 | 11.19 | 12.81 | 15.28 | 15.28 |
| 1922 | 9.04 | 10.97 | 11.13 | 11.31 | 13.69 | 15.04 |
| 1923 | 9.71 | 12.08 | 11.24 | 12.35 | 14.58 | 14.94 |
| 1924 | 10.11 | 11.86 | 11.40 | 12.4 | 14.31 | 14.77 |
| 1925 | 9.68 | 11.47 | 11.45 | 12.12 | 14.17 | 14.67 |
| 1926 | 9.28 | 11.39 | 11.40 | 13.96 | 16.39 | **14.74** |
| Average | | | **11.11** | | | **14.75** |

## Appendix I. Examples on how the EFSA Guidance Document can be used

This appendix gives examples on how the EFSA Guidance Document can be used covering the following issues:

| | |
|---|---|
| Example 1: | Application to the soil |
| Example 2.1: | Application to the crop canopy, default crop parameter |
| Example 2.2: | Application to the crop canopy, substance specific crop parameter |
| Example 3.1: | Soil pH-dependent sorption (sigmoid relationship) |
| Example 3.2: | Soil pH-dependent sorption (linear relationship) |
| Example 4: | Parent and metabolites |
| Example 5: | Accounting for the rapidly dissipation fraction derived from field dissipating studies ($F_{field}$) |
| Example 6: | Exposure assessment based on the total amount in soil |

Calculations are based on PERSAM version 1.0.2, PEARL kernel version 3.2.2 (25 March 2015) and PELMO version 4.02 (28 March 2015). Note that these models are still under development. Results may change when updated models are released.

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

**Table I.1:** Summary of substance properties of pesticides and metabolites used in the examples

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

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

## I.1. Example 1 (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$^{-1}$ (Table I.1). Pesticide A is intended to be applied once each year via spraying onto winter cereals one day before emergence (application to soil surface) with an application rate of 1 kg ha$^{-1}$. 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 averaging depth ($z_{eco}$) of 5 cm and for averaging times ($t_{avg}$) of 0 and 21 days.

Input values in Tier 1 (PERSAM) are the *DegT50* (250 days), the $K_{om}$ (1 000 l kg$^{-1}$), the annual rate of application (1 kg ha$^{-1}$) and the application cycle (each year in this case) without further specifying the crop. Input parameters for Tier 2B and Tier 2C (PERSAM) are exactly the same. However, at Tier 2B and Tier 2C we additionally have to specify the crop in PERSAM. Table 5 (Section 2.3) in this guidance indicates that for the FOCUS crop winter cereals individual types of cereals may be selected in PERSAM (e.g. barley, common wheat) if specified. However, as in this example, if winter cereals are not specified we have to select for the concentration in the total soil oats for the North Zone, rye for the Central Zone and common wheat for the South Zone. For the concentration in the pore water we have to select rye for the North Zone, common wheat for the Central Zone and oats for the South zone. The final results for Tiers 1, 2B and 2C, already corrected for with the model and default scenario adjustment factors, are directly obtained from the model output tables (and respective reports). As crop canopy processes are not accounted for in this example (application to the soil one day before emergence) results for Tier 2C equal those of Tier 2B. At Tiers 1, 2B and 2C all individual combinations of averaging depths ($z_{eco}$) and averaging times ($t_{avg}$) can be directly obtained from the output tables without any recalculation.

At Tier 2A the numerical models PEARL and PELMO are used. The six predefined scenarios for Tier 2A are already implemented in the model shells. The substance properties are the same as used for Tiers 1, 2B and 2C. However, the numerical models require some more substance properties to adequately account for substance behaviour in soil. Thus, let us assume a water solubility of 0.1 mg l$^{-1}$ (at 20 °C), a vapour pressure of $10^{-8}$ Pa, a Freundlich exponent (1/*n*) of 0.9 and a crop uptake factor of 0 for pesticide A (Table I.1). The $K_{om}$ under air-dry conditions was assumed to be 100 times the $K_{om}$ under reference conditions (i.e. 100 000 l kg$^{-1}$). In this example application in the numerical models is set to "application to the soil surface" to the FOCUS crop winter cereals one day before emergence. As the numerical models at Tier 2A do not account for scenario adjustment factors, results from both numerical models, PEARL and PELMO, have to be corrected with their respective default scenario adjustment factors as given in Table 4 of this guidance (Section 2.3) to obtain the final results (Table I.2). No model adjustment factors are needed at Tiers applying numerical models. In line with Tiers 1, Tier 2B and Tier 2C each individual combination of $z_{eco}$ and $t_{avg}$ can be directly obtained from the model output without any recalculation (note that in PEARL recalculation is necessary if $z_{eco}$ changes).

**Table I.2:** Default scenario adjustment factors to be applied at Tier 2A (data taken from Table 4 in Section 2.3)

| Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|
| **North** | **Central** | **South** | **North** | **Central** | **South** |
| 3.0 | 2.0 | 2.0 | 2.0 | 1.5 | 1.5 |

Tier 3A uses almost the same information as Tier 2A. However, at Tier 3A the numerical model output has to be corrected with a crop- and substance-specific (refined) scenario adjustment factor instead of the default scenario adjustment factor used at Tier 2A. In line with Equation 10 of this guidance (Section 3.6) this refined scenario adjustment factor is simply the ratio between the results obtained at Tier 2B and Tier 1 divided by the default scenario adjustment factor (obtained from Table I.5). Note that these refined adjustment factors have to account for the specific averaging depth ($z_{eco}$)

(Table I.3). In contrast, the refined scenario adjustment factors for individual averaging times ($t_{avg}$), other than 0 days, should always be based on a $t_{avg}$ of 0 days.

**Table I.3:** Example 1: Crop- and substance-specific (refined) scenario adjustment factors for pesticide A to be applied at Tier 3A

| $z_{eco}$ (cm) | $t_{avg}$ (days) | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|---|
| | | North | Central | South | North | Central | South |
| 5 | 0 | 2.55 | 1.46 | 1.14 | 0.99 | 1.00 | 1.12 |

At Tier 3B crop- and substance-specific scenarios are used in the numerical models instead of the predefined ones. Each Tier 3B scenario selected by PERSAM is specified by its XY-coordinates, which are directly obtained from PERSAMs "Tier 3" (Table I.4). In contrast to all other Tiers mentioned before, the scenario to be selected for numerical modelling at Tier 3B has to be always based on the specific averaging depth ($z_{eco}$). 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 name and location of PERSAMs "Tier 3" export file has to be specified. The models then automatically generate the scenario-specific input files for the Tier 3B scenarios. Substance properties and the application scheme are the same as those at Tier 2A and Tier 3A. Note that at Tier 3B no adjustment factors are needed. Therefore, the final results are directly obtained from the model output file.

**Table I.4:** Example 1: Crop- and substance-specific scenarios (X(km)/Y(km)-coordinates) obtained from PERSAMs "Tier 3" for pesticide A applied to winter cereals

| $z_{eco}$ (cm) | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|
| | North | Central | South | North | Central | South |
| 5 | 5112/4691 | 5024/3386 | 3908/2872 | 5235/4084 | 5606/2857 | 3723/1858 |

Final results for pesticide A at each individual Tier are given in Table I.5.

**Table I.5:** Example 1: Final results for pesticide A, applied to winter cereals one day before emergence at an application rate of 1 kg $ha^{-1}$

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg $kg^{-1}$) | | | Pore soil water (mg $l^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | 22.0 | 11.5 | 9.1 | 0.76 | 0.67 | 0.91 |
| | 5 | 21 | PERSAM | 21.8 | 11.4 | 9.0 | 0.75 | 0.66 | 0.90 |
| Tier 2B | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 0.37 | 0.45 | 0.68 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 0.37 | 0.44 | 0.67 |
| Tier 2C | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 0.37 | 0.45 | 0.68 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 0.37 | 0.44 | 0.67 |
| Tier 2A | 5 | 0 | PEARL | 11.9 | 9.5 | 7.4 | 0.28 | 0.34 | 0.54 |
| | 5 | 0 | PELMO | 12.8 | 10.4 | 7.5 | 0.30 | 0.37 | 0.56 |
| | 5 | 21 | PEARL | 11.8 | 9.5 | 7.3 | 0.26 | 0.32 | 0.50 |
| | 5 | 21 | PELMO | 12.7 | 10.4 | 7.4 | 0.27 | 0.34 | 0.53 |
| Tier 3A | 5 | 0 | PEARL | 10.1 | 4.6 | 2.8 | 0.09 | 0.11 | 0.20 |
| | 5 | 0 | PELMO | 10.8 | 5.1 | 2.8 | 0.10 | 0.12 | 0.21 |
| | 5 | 21 | PEARL | 10.0 | 4.6 | 2.8 | 0.08 | 0.11 | 0.19 |
| | 5 | 21 | PELMO | 10.8 | 5.1 | 2.8 | 0.09 | 0.11 | 0.20 |
| Tier 3B | 5 | 0 | PEARL | 9.1 | 4.8 | 2.8 | 0.10 | 0.12 | 0.20 |
| | 5 | 0 | PELMO | 11.9 | 5.3 | 2.9 | 0.10 | 0.12 | 0.21 |
| | 5 | 21 | PEARL | 9.0 | 4.8 | 2.8 | 0.09 | 0.11 | 0.18 |
| | 5 | 21 | PELMO | 11.8 | 5.3 | 2.9 | 0.09 | 0.12 | 0.20 |

## I.2. Example 2 (application to the crop canopy)

### I.2.1. Application to the crop including default crop parameter

Example 2.1 is the same as example 1. However, in this example pesticide A is applied to winter cereals twice, first at BBCH 10–19 and second at BBCH 40–59, each time at a rate of 0.5 kg $ha^{-1}$. Thus, 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 we apply the default *DegT50* at crop surface of 10 days and the default wash-off factor ($w$) of 0.1 $mm^{-1}$ (EFSA, 2014a).

There is no change at Tier 1 and Tier 2B with respect to example 1 as canopy processes are not taken into account at these two Tiers and the yearly application rate is still 1 kg $ha^{-1}$ (twice at 0.5 kg $ha^{-1}$). In contrast, at Tier 2C the yearly soil load has to be corrected for crop canopy processes according to the procedure given in this guidance (Section 3.4). For each individual application the fraction of the dose reaching the soil ($f_{soil}$) is obtained from Table 7 of the EFSA Guidance Document and used to correct the actual soil load for each individual application. In case of winter cereals, $f_{soil}$ for the first application (BBCH 10–19) is 1.0 and for the second application (BBCH 40–59) 0.60. Following Equation 6 of this guidance, the mean-weighted fraction of the dose reaching the soil ($f_{soil}$) to be input in PERSAM is calculated as: $f_{soil} = (1.00 \times 0.5 + 0.60 \times 0.5)/(0.5 + 0.5) = 0.8/1 = 0.8$. Furthermore, a dose of $0.5 + 0.5 = 1$ kg $ha^{-1}$ should be introduced in PERSAM at Tier 2C.

At Tiers 2A, 3A and 3B we now have to specify the application scheme in the numerical models in more detail. Let us assume that BBCH 10–19 in winter cereals refers to an application 2 days after emergence and BBCH 40–59 to an application 80 days before harvest. In contrast to example 1 (where application was before emergence) we have to specify the crop interception for each individual application in the numerical model in line with EFSA (EFSA, 2014a). In this example, crop interception for winter cereals at BBCH 10–19 is 0 % and crop interception at BBCH 40–59 is 90 %. In the numerical model, application "to the crop canopy, intercepted fraction specified by the user" has to be selected. Therefore, the application rate for each crop interception is 0.5 kg $ha^{-1}$, with crop interception fractions of 0.0 and 0.9 for BBCH 10–19 and BBCH 40–59, respectively. Note that application "to the soil surface" (following correction of the dose for crop interception) is incorrect in this case as this approach does not account for crop canopy processes. In this example the substance parameter for processes on the crop canopy are set to EFSA default values (*DegT50* on crop surface = 10 days, $w = 0.1$ $mm^{-1}$).

All other settings (substance properties) and model output corrections (default scenario adjustment factors at Tier 2A and refined scenario adjustment factors at Tier 3A) are the same as mentioned for example 1. Note that the crop- and substance-specific scenarios at Tier 3B are the same as those in example 1 because the scenario selection procedure does not account for canopy processes.

Final results for pesticide A at each individual Tier are given in Table I.6.

**Table I.6:** Example 2.1: Final results for pesticide A (default crop parameter), applied to winter cereals at BBCH 11–19 and BBCH 40–59 at 0.5 kg $ha^{-1}$ each

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg $kg^{-1}$) | | | Pore soil water (mg $l^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | 22.0 | 11.5 | 9.1 | 0.76 | 0.67 | 0.91 |
| | 5 | 21 | PERSAM | 21.8 | 11.4 | 9.0 | 0.75 | 0.66 | 0.90 |
| Tier 2B | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 0.37 | 0.45 | 0.68 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 0.37 | 0.44 | 0.67 |
| Tier 2C | 5 | 0 | PERSAM | 14.9 | 6.8 | 4.2 | 0.30 | 0.36 | 0.55 |
| | 5 | 21 | PERSAM | 14.8 | 6.7 | 4.1 | 0.30 | 0.35 | 0.53 |
| Tier 2A | 5 | 0 | PEARL | 9.0 | 7.6 | 5.9 | 0.19 | 0.21 | 0.36 |
| | 5 | 0 | PELMO | 7.5 | 6.4 | 4.4 | 0.16 | 0.19 | 0.28 |
| | 5 | 21 | PEARL | 8.9 | 7.6 | 5.8 | 0.18 | 0.21 | 0.35 |
| | 5 | 21 | PELMO | 7.5 | 6.4 | 4.4 | 0.15 | 0.18 | 0.27 |
| Tier 3A | 5 | 0 | PEARL | 7.6 | 3.7 | 2.2 | 0.06 | 0.07 | 0.13 |
| | 5 | 0 | PELMO | 6.4 | 3.1 | 1.7 | 0.05 | 0.06 | 0.10 |
| | 5 | 21 | PEARL | 7.6 | 3.7 | 2.2 | 0.06 | 0.07 | 0.13 |
| | 5 | 21 | PELMO | 6.3 | 3.1 | 1.7 | 0.05 | 0.06 | 0.10 |
| Tier 3B | 5 | 0 | PEARL | 7.0 | 3.9 | 2.3 | 0.07 | 0.07 | 0.13 |
| | 5 | 0 | PELMO | 7.3 | 3.3 | 1.7 | 0.05 | 0.06 | 0.10 |
| | 5 | 21 | PEARL | 6.9 | 3.8 | 2.2 | 0.07 | 0.07 | 0.13 |
| | 5 | 21 | PELMO | 7.2 | 3.3 | 1.7 | 0.05 | 0.06 | 0.10 |

### I.2.2. Application to the crop 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 now 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. 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 Tiers 1, 2B and 2C. Thus, these Tiers are exactly the same as for pesticide A in example 2.1.

At Tiers 2A, 3A and 3B (applying numerical models) the default substance parameter for crop canopy processes in the model shell have to be replaced by the specific ones (*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. Model output corrections (default scenario adjustment factors at Tier 2A and refined scenario adjustment factors at Tier 3A) are the same as mentioned for examples 2.1. Note that the specific scenarios (to be used at Tier 3B) are the same as in examples 2.1.

Final results for pesticide B are given in Table I.7.

**Table I.7:** Example 2.2: Final results for pesticide B (substance-specific crop parameter), applied to winter cereals at BBCH 11–19 and BBCH 40–59 at 0.5 kg ha$^{-1}$ each

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg kg$^{-1}$) | | | Pore soil water (mg l$^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | 22.0 | 11.5 | 9.1 | 0.76 | 0.67 | 0.91 |
| | 5 | 21 | PERSAM | 21.8 | 11.4 | 9.0 | 0.75 | 0.66 | 0.90 |
| Tier 2B | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 0.37 | 0.45 | 0.68 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 0.37 | 0.44 | 0.67 |
| Tier 2C | 5 | 0 | PERSAM | 14.9 | 6.8 | 4.2 | 0.30 | 0.36 | 0.55 |
| | 5 | 21 | PERSAM | 14.8 | 6.7 | 4.1 | 0.30 | 0.35 | 0.53 |
| Tier 2A | 5 | 0 | PEARL | 7.1 | 6.3 | 5.0 | 0.15 | 0.17 | 0.32 |
| | 5 | 0 | PELMO | 6.9 | 5.7 | 4.0 | 0.15 | 0.18 | 0.27 |
| | 5 | 21 | PEARL | 7.0 | 6.3 | 4.9 | 0.15 | 0.17 | 0.32 |
| | 5 | 21 | PELMO | 6.9 | 5.7 | 4.0 | 0.14 | 0.16 | 0.26 |
| Tier 3A | 5 | 0 | PEARL | 6.0 | 3.1 | 1.9 | 0.05 | 0.06 | 0.12 |
| | 5 | 0 | PELMO | 5.9 | 2.8 | 1.5 | 0.05 | 0.06 | 0.10 |
| | 5 | 21 | PEARL | 6.0 | 3.1 | 1.9 | 0.05 | 0.06 | 0.12 |
| | 5 | 21 | PELMO | 5.8 | 2.8 | 1.5 | 0.05 | 0.05 | 0.10 |
| Tier 3B | 5 | 0 | PEARL | 5.5 | 3.2 | 1.9 | 0.05 | 0.06 | 0.12 |
| | 5 | 0 | PELMO | 6.7 | 2.9 | 1.6 | 0.05 | 0.06 | 0.10 |
| | 5 | 21 | PEARL | 5.4 | 3.2 | 1.9 | 0.05 | 0.06 | 0.12 |
| | 5 | 21 | PELMO | 6.6 | 2.9 | 1.6 | 0.05 | 0.06 | 0.10 |

## I.3. Example 3.1 (soil pH-dependent sorption)

### I.3.1. Soil pH-dependent sorption, sigmoid pH–$K_{om}$ relationship

Example 3.1 is the same as example 2.1. 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 p$K_a$ of 4.7. Adsorption results on four soils (soil pH measured in $CaCl_2$) are available: $K_{om}$ at pH 4 = 184 l kg$^{-}$1, $K_{om}$ at pH 5.5 = 62 l kg$^{-}$1, $K_{om}$ at pH 7 = 22 l kg$^{-}$1 and $K_{om}$ at pH 8 = 20 l kg$^{-}$1. Let us further assume that pesticide C has a molar mass of 300 g mol$^{-}$1, the anion a molar mass of 299 g mol$^{-}$1.

The predefined scenarios at Tiers 1, 2A and 3A are not designed for substances whose properties depend on soil properties, such as pH. For such substances we therefore have to directly go to Tier 2B, 2C or 3B.

At Tiers 2B and 2C, the soil pH–$K_{om}$ relationship for pesticide C has to be implemented in PERSAM. As the soil pH in PERSAM is based on measurements in $H_2O$, pH values measured in $CaCl_2$ for pesticide C have to first be converted into p$HH_2O$ according to Equation 4a given in this guidance (Section 3.3). Fitting of the final p$H_{H2O}$–$K_{om}$ datasets 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$^{-}$1, a $K_{om,anion}$ of 20.0 l kg$^{-1}$ and a ΔpH of 0.82 (Figure I.1). These parameters have to be entered into PERSAM at Tiers 2B and 2C, as well as into the numerical models at Tier 3B (see below).

At Tier 3B, crop- and substance-specific scenarios obtained from PERSAMs "Tier 3" are implemented in the numerical models in the same way as in the example mentioned before. Note that specific scenarios in example 3.1 are, of course, different from, for example, example 2.1 (which is based on a substance with different $K_{om}$ properties). XY-coordinates for the specific scenarios for pesticide C are given in Table I.8. Note that the soil pH is part of the scenario definition and the soil pH is therefore also accounted for in the numerical models. Therefore, the sigmoid soil pH–$K_{om}$ relationship for pesticide C has to be implemented in the numerical models exactly in the same way as was carried out

in PERSAM at Tiers 2B and 2C. All other settings (substance properties other than $K_{om}$ and application scheme) are the same as in example 2.1.

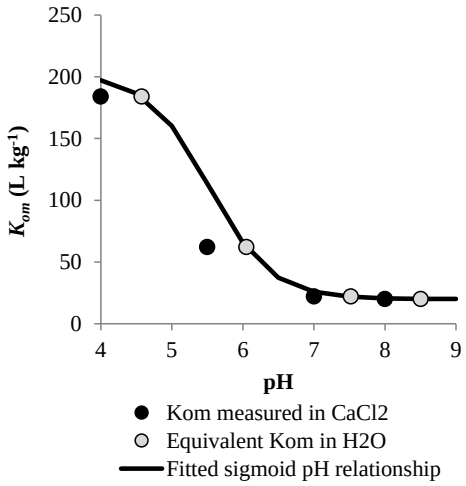


**Figure I.1:** Example 3.1: Fitted sigmoid $pH_{H2O}$–$K_{om}$ relationship for pesticide C

**Table I.8:** Example 3.1: Crop- and substance-specific scenarios (X(km)/Y(km)-coordinates) obtained from PERSAMs "Tier 3" for pesticide C

| $z_{eco}$ (cm) | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|
| | North | Central | South | North | Central | South |
| 5 | 5112/4691 | 5024/3386 | 3908/2872 | 4282/3544 | 5179/3161 | 2713/2001 |

Final results for pesticide C are given in Table I.9.

**Table I.9:** Example 3.1: Final results for pesticide C (pH-dependent sorption, sigmoid pH–$K_{om}$ relationship), applied to winter cereals at BBCH 11–19 and BBCH 40–59 at 0.5 kg $ha^{-1}$ each

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg $kg^{-1}$) | | | Pore soil water (mg $l^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | Not applicable | | | Not applicable | | |
| | 5 | 21 | PERSAM | | | | | | |
| Tier 2B | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 8.5 | 10.7 | 14.9 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 8.5 | 10.6 | 14.6 |
| Tier 2C | 5 | 0 | PERSAM | 14.9 | 6.8 | 4.2 | 6.8 | 8.6 | 11.9 |
| | 5 | 21 | PERSAM | 14.8 | 6.7 | 4.1 | 6.8 | 8.4 | 11.7 |
| Tier 2A | 5 | 0 | PEARL | Not applicable | | | Not applicable | | |
| | 5 | 0 | PELMO | | | | | | |
| | 5 | 21 | PEARL | | | | | | |
| | 5 | 21 | PELMO | | | | | | |
| Tier 3A | 5 | 0 | PEARL | Not applicable | | | Not applicable | | |
| | 5 | 0 | PELMO | | | | | | |
| | 5 | 21 | PEARL | | | | | | |
| | 5 | 21 | PELMO | | | | | | |
| Tier 3B | 5 | 0 | PEARL | 6.2 | 3.7 | 1.3 | 1.1 | 1.7 | 2.8 |
| | 5 | 0 | PELMO | 6.3 | 3.1 | 1.2 | 1.0 | 1.4 | 3.3 |
| | 5 | 21 | PEARL | 6.2 | 3.7 | 1.1 | 0.9 | 1.3 | 2.7 |
| | 5 | 21 | PELMO | 6.2 | 3.1 | 1.1 | 0.9 | 1.2 | 3.1 |

### I.3.2. Soil pH-dependent sorption, linear pH–$K_{om}$ relationship

Example 3.2 is the same as example 3.1. However, in case of example 3.2, 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: $K_{om} = -150 \times pH_{H2O} + 1\,500$.

Handling of pesticide D at Tiers 2B and 2C 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.

Neither PEARL nor PELMO are capable of handling pH–$K_{om}$ relationships, other than the implemented sigmoid one. Therefore, at Tier 3B scenario-specific $K_{om}$ values have to be calculated for pesticide D outside the model shell based on the soil pH provided by PERSAMs "Tier 3" output and the linear relationship (Table I.10). Next, these scenario-specific $K_{om}$ values have to be entered in the numerical model for each individual scenario.

**Table I.10:** Example 3.2: Crop- and substance-specific scenarios (X(km)/Y(km)-coordinates) as well as scenario-specific $K_{om}$ (l kg$^{-1}$) values (based on the soil $pH_{H2O}$) obtained from PERSAMs "Tier 3"for pesticide D

| $z_{eco}$ (cm) | Parameter | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|---|
| | | North | Central | South | North | Central | South |
| 5 | X/Y coordinates | 5112/4691 | 5024/3386 | 3908/2872 | 5028/3690 | 5637/2500 | 2725/2004 |
| | Soil $pH_{H2O}$ | 4.3 | 4.4 | 7.5 | 6.3 | 7.8 | 8 |
| | Scenario-specific $K_{om}$ | 855 | 840 | 375 | 555 | 330 | 300 |

Final results for pesticide D are given in Table I.11.

**Table I.11:** Example 3.2: Final results for pesticide D (pH-dependent sorption, linear pH–$K_{om}$ relationship), applied to winter cereals at BBCH 11–19 and BBCH 40–59 at 0.5 kg ha$^{-}$1 each

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg kg$^{-1}$) | | | Pore soil water (mg l$^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | Not applicable | | | Not applicable | | |
| | 5 | 21 | PERSAM | | | | | | |
| Tier 2B | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 0.72 | 0.99 | 2.03 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 0.71 | 0.98 | 1.99 |
| Tier 2C | 5 | 0 | PERSAM | 14.9 | 6.8 | 4.2 | 0.58 | 0.79 | 1.63 |
| | 5 | 21 | PERSAM | 14.8 | 6.7 | 4.1 | 0.57 | 0.78 | 1.59 |
| Tier 2A | 5 | 0 | PEARL | Not applicable | | | Not applicable | | |
| | 5 | 0 | PELMO | | | | | | |
| | 5 | 21 | PEARL | | | | | | |
| | 5 | 21 | PELMO | | | | | | |
| Tier 3A | 5 | 0 | PEARL | Not applicable | | | Not applicable | | |
| | 5 | 0 | PELMO | | | | | | |
| | 5 | 21 | PEARL | | | | | | |
| | 5 | 21 | PELMO | | | | | | |
| Tier 3B | 5 | 0 | PEARL | 6.9 | 3.8 | 2.1 | 0.12 | 0.16 | 0.40 |
| | 5 | 0 | PELMO | 7.2 | 3.3 | 1.7 | 0.10 | 0.16 | 0.34 |
| | 5 | 21 | PEARL | 6.9 | 3.8 | 2.1 | 0.12 | 0.16 | 0.38 |
| | 5 | 21 | PELMO | 7.2 | 3.3 | 1.7 | 0.10 | 0.14 | 0.33 |

## I.4. Example 4 (parent and metabolites)

Example 4 considers pesticide F (parent) together with two metabolites, metabolite M1 and M2, formed from pesticide F in series. Let us assume that pesticide F 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$^{-1}$. 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$^{-1}$, respectively. The molar mass of pesticide F is 300 g mol$^{-1}$, metabolite M1 has a molar weight of 200 g mol$^{-1}$ and metabolite M2 has a molar weight of 100 g mol$^{-1}$. The average (arithmetic mean) molar formation fraction of metabolite M1 from pesticide F is 0.7, the average (arithmetic mean) molar formation fraction of metabolite M2 from metabolite M1 is 1.0 (for further properties refer to Table I.1). The application scheme of pesticide F (to winter cereals) is the same as in example 2.1.

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

At Tier 2A, all substances, the parent and the two metabolites, are handled within the same predefined scenario. For that reason results for the parent and the metabolites are obtained from one and the same model run. The same is true for different combinations of zeco and tavg. Similar to PERSAM, all three substances are linked together in the model shell with a molar formation fraction of 0.7 (pesticide F to metabolite M1) and 1.0 (metabolite M1 to metabolite M2) in this example. Note that at Tier 2A results for all substances, in addition to parent and metabolites, have to be corrected with the same default scenario adjustment factors as given in Table I.2 (example 1).

At Tier 3A, crop- and substance-specific (refined) scenario adjustment factors may, of course, differ between the individual substances (parent and metabolites). Refined scenario adjustment factors for the parent F, metabolites M1 and M2, calculated in the same way as for the parent in example 1, are given in Table I.12. Similar to Tier 2A, results for parent and metabolites are obtained from one and the same numerical model run. However, results have to be corrected individually with substance-specific refined scenario adjustment factors.

**Table I.12:** Example 4: Crop- and substance-specific (refined) scenario adjustment factors for pesticide F, metabolite M1 and metabolite M2 to be applied at Tier 3A

| Substance | $z_{eco}$ (cm) | $t_{avg}$ (days) | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|---|---|
| | | | North | Central | South | North | Central | South |
| Pesticide F | 5 | 0 | 2.31 | 1.42 | 1.11 | 0.95 | 1.03 | 1.20 |
| Metabolite M1 | 5 | 0 | 2.43 | 1.44 | 1.12 | 0.99 | 0.99 | 1.11 |
| Metabolite M2 | 5 | 0 | 2.55 | 1.46 | 1.14 | 0.99 | 1.00 | 1.09 |

At Tier 3B, crop- and substance-specific scenarios obtained by PERSAMs "Tier 3" may differ between the individual substances (Table I.13). For that 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 Tiers 2A and 3A. However, final results for pesticide F have to be obtained from model runs with specific scenarios for pesticide F (Table I.13), whereas final results for metabolite M1 or M2 have to be obtained from model runs based on specific scenarios for metabolite M1 or M2 (Table I.13). No model or scenario adjustment factors are needed at Tier 3B.

**Table I.13:** Example 4: Crop- and substance-specific scenarios (X(km)/Y(km)-coordinates) obtained from PERSAMs "Tier 3" for pesticide F, metabolite M1 and metabolite M2

| Substance | $z_{eco}$ (cm) | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|---|
| | | North | Central | South | North | Central | South |
| Pesticide F | 5 | 4972/4456 | 5054/3170 | 3708/2998 | 5320/3729 | 4817/2724 | 3719/1855 |
| Metabolite M1 | 5 | 5055/4712 | 5024/3235 | 3778/2973 | 4317/3634 | 4863/2919 | 3033/1996 |
| Metabolite M2 | 5 | 5112/4691 | 5024/3386 | 3908/2872 | 5223/4085 | 5779/2473 | 2690/1845 |

Final results for pesticide P, metabolite M1 and metabolite M2 are given in Tables I.14, I.15 and I.16.

**Table I.14:** Example 4: Final results for pesticide F applied to winter cereals at BBCH 11–19 and BBCH 40–59 at an application rate of 0.5 kg ha$^{-1}$ each

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg kg$^{-1}$) | | | Pore soil water (mg l$^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | 12.8 | 7.7 | 6.6 | 0.50 | 0.46 | 0.71 |
| | 5 | 21 | PERSAM | 11.8 | 6.8 | 5.7 | 0.45 | 0.41 | 0.60 |
| Tier 2A | 5 | 0 | PEARL | 9.8 | 5.5 | 3.6 | 0.24 | 0.32 | 0.57 |
| | 5 | 0 | PELMO | 9.2 | 4.9 | 3.2 | 0.21 | 0.28 | 0.45 |
| | 5 | 21 | PEARL | 7.9 | 4.4 | 2.9 | 0.19 | 0.25 | 0.45 |
| | 5 | 21 | PELMO | 7.4 | 3.9 | 2.6 | 0.17 | 0.22 | 0.36 |
| Tier 2B | 5 | 0 | PERSAM | 3.8 | 3.8 | 2.5 | 0.09 | 0.12 | 0.21 |
| | 5 | 21 | PERSAM | 3.3 | 2.9 | 2.5 | 0.10 | 0.12 | 0.20 |
| Tier 2C | 5 | 0 | PERSAM | 3.4 | 3.6 | 2.4 | 0.08 | 0.10 | 0.19 |
| | 5 | 21 | PERSAM | 3.2 | 2.8 | 2.3 | 0.09 | 0.10 | 0.18 |
| Tier 3A | 5 | 0 | PEARL | 2.9 | 1.8 | 0.9 | 0.03 | 0.04 | 0.08 |
| | 5 | 0 | PELMO | 2.6 | 1.4 | 0.9 | 0.03 | 0.04 | 0.08 |
| | 5 | 21 | PEARL | 2.6 | 1.7 | 0.9 | 0.03 | 0.03 | 0.08 |
| | 5 | 21 | PELMO | 2.4 | 1.3 | 0.8 | 0.03 | 0.04 | 0.07 |
| Tier 3B | 5 | 0 | PEARL | 3.2 | 1.9 | 1.0 | 0.03 | 0.04 | 0.08 |
| | 5 | 0 | PELMO | 2.6 | 1.4 | 0.9 | 0.03 | 0.04 | 0.08 |
| | 5 | 21 | PEARL | 2.9 | 1.8 | 0.9 | 0.03 | 0.03 | 0.07 |
| | 5 | 21 | PELMO | 2.5 | 1.4 | 0.9 | 0.03 | 0.03 | 0.07 |

**Table I.15:** Example 4: Final results for metabolite M1, released from pesticide F, applied to winter cereals at BBCH 11–19 and BBCH 40–59 at an application rate of 0.5 kg ha$^{-1}$ each

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg kg$^{-1}$) | | | Pore soil water (mg l$^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | 7.27 | 4.08 | 3.38 | 12.93 | 10.42 | 11.66 |
| | 5 | 21 | PERSAM | 7.12 | 3.97 | 3.26 | 12.58 | 10.09 | 11.15 |
| Tier 2B | 5 | 0 | PERSAM | 5.88 | 2.95 | 1.89 | 6.39 | 6.87 | 8.59 |
| | 5 | 21 | PERSAM | 5.78 | 2.87 | 1.83 | 6.24 | 6.65 | 8.10 |
| Tier 2C | 5 | 0 | PERSAM | 4.70 | 2.36 | 1.51 | 5.12 | 5.50 | 6.87 |
| | 5 | 21 | PERSAM | 4.62 | 2.29 | 1.47 | 4.99 | 5.32 | 6.48 |
| Tier 2A | 5 | 0 | PEARL | 1.03 | 0.96 | 0.76 | 1.78 | 1.59 | 2.30 |
| | 5 | 0 | PELMO | 0.71 | 0.83 | 0.56 | 1.35 | 1.83 | 3.36 |
| | 5 | 21 | PEARL | 0.98 | 0.88 | 0.73 | 1.55 | 1.32 | 1.98 |
| | 5 | 21 | PELMO | 0.67 | 0.76 | 0.55 | 1.24 | 1.60 | 2.92 |
| Tier 3A | 5 | 0 | PEARL | 0.83 | 0.46 | 0.29 | 0.59 | 0.52 | 0.85 |
| | 5 | 0 | PELMO | 0.58 | 0.40 | 0.21 | 0.44 | 0.60 | 1.24 |
| | 5 | 21 | PEARL | 0.79 | 0.43 | 0.27 | 0.51 | 0.44 | 0.73 |
| | 5 | 21 | PELMO | 0.54 | 0.36 | 0.21 | 0.41 | 0.53 | 1.08 |
| Tier 3B | 5 | 0 | PEARL | 0.90 | 0.55 | 0.30 | 0.58 | 0.51 | 0.97 |
| | 5 | 0 | PELMO | 0.64 | 0.46 | 0.23 | 0.45 | 0.58 | 1.06 |
| | 5 | 21 | PEARL | 0.87 | 0.52 | 0.29 | 0.50 | 0.43 | 0.87 |
| | 5 | 21 | PELMO | 0.61 | 0.42 | 0.23 | 0.41 | 0.51 | 0.93 |

**Table I.16:** Example 4: Final results for metabolite M2, released from pesticide F (via metabolite M1), applied to winter cereals at BBCH 11–19 and BBCH 40–59 at an application rate of 0.5 kg ha$^{-1}$ each

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg kg$^{-1}$) | | | Pore soil water (mg l$^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | 5 | 0 | PERSAM | 5.13 | 2.69 | 2.13 | 1.61 | 1.39 | 1.80 |
| | 5 | 21 | PERSAM | 5.08 | 2.66 | 2.10 | 1.60 | 1.37 | 1.77 |
| Tier 2B | 5 | 0 | PERSAM | 4.35 | 1.97 | 1.21 | 0.80 | 0.93 | 1.31 |
| | 5 | 21 | PERSAM | 4.32 | 1.95 | 1.20 | 0.79 | 0.92 | 1.28 |
| Tier 2C | 5 | 0 | PERSAM | 3.48 | 1.58 | 0.97 | 0.64 | 0.74 | 1.05 |
| | 5 | 21 | PERSAM | 3.46 | 1.56 | 0.96 | 0.63 | 0.73 | 1.02 |
| Tier 2A | 5 | 0 | PEARL | 0.33 | 0.41 | 0.27 | 0.06 | 0.08 | 0.16 |
| | 5 | 0 | PELMO | 0.28 | 0.42 | 0.24 | 0.05 | 0.09 | 0.19 |
| | 5 | 21 | PEARL | 0.33 | 0.41 | 0.27 | 0.06 | 0.07 | 0.14 |
| | 5 | 21 | PELMO | 0.28 | 0.39 | 0.22 | 0.05 | 0.08 | 0.19 |
| Tier 3A | 5 | 0 | PEARL | 0.28 | 0.20 | 0.10 | 0.02 | 0.03 | 0.06 |
| | 5 | 0 | PELMO | 0.24 | 0.21 | 0.09 | 0.02 | 0.03 | 0.07 |
| | 5 | 21 | PEARL | 0.28 | 0.20 | 0.10 | 0.02 | 0.02 | 0.05 |
| | 5 | 21 | PELMO | 0.24 | 0.19 | 0.08 | 0.02 | 0.03 | 0.07 |
| Tier 3B | 5 | 0 | PEARL | 0.41 | 0.26 | 0.12 | 0.02 | 0.03 | 0.06 |
| | 5 | 0 | PELMO | 0.30 | 0.26 | 0.10 | 0.01 | 0.03 | 0.07 |
| | 5 | 21 | PEARL | 0.40 | 0.26 | 0.12 | 0.02 | 0.02 | 0.05 |
| | 5 | 21 | PELMO | 0.30 | 0.25 | 0.10 | 0.01 | 0.03 | 0.07 |

## I.5. Example 5 (accounting for the rapidly dissipation fraction, $F_{field}$)

Example 5 is the same as example 1 (application to winter cereals one day before emergence). However, in this example pesticide A is replaced by pesticide E, 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 G 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 1 and Tier 2B (without accounting for $F_{field}$) are used to select the crop- and substance-specific (refined) scenario adjustment factors for Tier 3A and the crop- and substance-specific scenarios for Tier 3B.

Input into PERSAM at Tier 1 and Tier 2B is exactly the same as in example 1. Consequently, there is no change in the crop- and substance-specific scenario adjustment factors at Tier 3A (Table I.3) and the crop- and substance-specific scenarios at Tier 3B (Table I.4).

As stated in Appendix G, the 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, in order 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 (one day before the crop emergence) is considered, "application to the soil surface" is selected, the application rate is set to 1 kg ha$^{-1}$ (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 in order 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, all results from the numerical models at Tier 2A have to be corrected with the respective default scenario adjustment factors (Table I.2). At Tier 3A crop- and substance-specific (refined) scenario adjustment factors are applied (same as in example 1, Table I.3) and Tier 3B is based on crop- and substance-specific scenarios which are selected using PERSAM (same as in example 1, Table I.4).

Final results for pesticide E at each individual Tier are given in Table I.17.

**Table I.17:** Example 5: Final results for pesticide E (accounting for the rapidly dissipating fraction from field dissipation studies, $F_{field}$), applied to winter cereals one day before emergence at an application rate of 1 kg ha$^{-1}$.

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg kg$^{-1}$) | | | Pore soil water (mg l$^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 [(a)] | 5 | 0 | PERSAM | 22.0 | 11.5 | 9.1 | 0.76 | 0.67 | 0.91 |
| | 5 | 21 | PERSAM | 21.8 | 11.4 | 9.0 | 0.75 | 0.66 | 0.90 |
| Tier 2B [(a)] | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 0.37 | 0.45 | 0.68 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 0.37 | 0.44 | 0.67 |
| Tier 2C [(a)] | 5 | 0 | PERSAM | 18.6 | 8.4 | 5.2 | 0.37 | 0.45 | 0.68 |
| | 5 | 21 | PERSAM | 18.5 | 8.4 | 5.1 | 0.37 | 0.44 | 0.67 |
| Tier 2A | 5 | 0 | PEARL | 10.0 | 8.2 | 6.5 | 0.25 | 0.31 | 0.49 |
| | 5 | 0 | PELMO | 10.5 | 8.8 | 6.6 | 0.27 | 0.23 | 0.35 |
| | 5 | 21 | PEARL | 9.9 | 8.1 | 6.5 | 0.22 | 0.29 | 0.43 |
| | 5 | 21 | PELMO | 10.5 | 8.8 | 6.5 | 0.22 | 0.21 | 0.33 |
| Tier 3A | 5 | 0 | PEARL | 8.4 | 4.0 | 2.5 | 0.08 | 0.10 | 0.18 |
| | 5 | 0 | PELMO | 8.9 | 4.3 | 2.5 | 0.09 | 0.08 | 0.13 |
| | 5 | 21 | PEARL | 8.4 | 4.0 | 2.5 | 0.07 | 0.10 | 0.16 |
| | 5 | 21 | PELMO | 8.9 | 4.3 | 2.5 | 0.07 | 0.07 | 0.12 |
| Tier 3B | 5 | 0 | PEARL | 7.5 | 4.1 | 2.5 | 0.08 | 0.11 | 0.18 |
| | 5 | 0 | PELMO | 9.4 | 4.4 | 2.5 | 0.06 | 0.08 | 0.13 |
| | 5 | 21 | PEARL | 7.5 | 4.1 | 2.4 | 0.08 | 0.10 | 0.15 |
| | 5 | 21 | PELMO | 9.3 | 4.4 | 2.5 | 0.06 | 0.07 | 0.12 |

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

## I.6. Example 6 (exposure assessment based on the total amount in soil)

Example 6 is the same as example 1. However, in this case the endpoint concentration in the ecotoxicology study is expressed in terms of the applied rate (kg ha$^{-1}$) only. Therefore, the soil exposure assessment has to be performed on the basis of the concentration in the top 20 cm of soil. Thus, $z_{eco}$ has to be set to 20 cm. As stated in Section 2.7 of this guidance, the procedure in this example may not be applied to tiers that use predefined scenarios (Tiers 1, 2A and 3A) because an inappropriate value of the bulk density would be applied in those tiers. Thus, in order to apply Equation 2 of this guidance (Section 2.7) scenario-specific soil density ($\rho$) values at Tiers 2B, 2C and 3B are obtained from PERSAMs "Tier 3" output (Table I.18).

**Table I.18:** Example 6: Crop- and substance-specific scenarios (X(km)/Y(km)-coordinates) obtained from PERSAMs "Tier 3" for pesticide A to be used for numerical models at Tier 3B

| $z_{eco}$ (cm) | $t_{avg}$ (days) | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|---|
| | | North | Central | South | North | Central | South |
| 20 | 0 | 4989/4377 | 5034/3454 | 3815/3046 | Not applicable | | |

**Table I.19:** Example 6: Scenario-specific $\rho$ (kg $l^{-1}$) values needed to convert the final PEC given in mg $kg^{-1}$ into kg $ha^{-1}$

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Total soil | | | Pore soil water | | |
|---|---|---|---|---|---|---|---|---|
| | | | North | Central | South | North | Central | South |
| Tier 1 | | | Not applicable | | | Not applicable | | |
| Tier 2A | | | Not applicable | | | | | |
| Tier 2B | 20 | 0 | 0.42 | 0.74 | 1.12 | | | |
| Tier 2C | 20 | 0 | 0.42 | 0.74 | 1.12 | | | |
| Tier 3A | | | Not applicable | | | | | |
| Tier 3B | 20 | 0 | 0.42 | 0.74 | 1.12 | | | |

Final results for pesticide A expressed in terms of the total concentration in soil (mg $kg^{-1}$), as well as the applied rate (kg $ha^{-1}$), are given in Table I.20.

**Table I.20:** Example 6: Final results (total soil only) for pesticide A, applied to winter cereals at 1 kg $ha^{-1}$ one day before emergence, expressed in terms of the total concentration in soil (mg $kg^{-1}$) and the applied rate (kg $ha^{-1}$)

| Tier | $z_{eco}$ (cm) | $t_{avg}$ (days) | Model | Total soil (mg $kg^{-1}$) | | | Total soil (kg $ha^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | North | Central | South | North | Central | South |
| Tier 1 | Not applicable | | | | | | | | |
| Tier 2B | 20 | 0 | PERSAM | 11.4 | 4.4 | 2.5 | 9.5 | 6.4 | 5.6 |
| | 20 | 21 | PERSAM | 11.3 | 4.3 | 2.5 | 9.5 | 6.4 | 5.5 |
| Tier 2C | 20 | 0 | PERSAM | 11.4 | 4.4 | 2.5 | 9.5 | 6.4 | 5.6 |
| | 20 | 21 | PERSAM | 11.3 | 4.3 | 2.5 | 9.5 | 6.4 | 5.5 |
| Tier 2A | Not applicable | | | | | | | | |
| Tier 3A | Not applicable | | | | | | | | |
| Tier 3B | 20 | 0 | PEARL | 6.6 | 2.7 | 1.5 | 5.5 | 4.1 | 3.3 |
| | 20 | 0 | PELMO | 7.4 | 3.3 | 1.5 | 6.2 | 4.8 | 3.4 |
| | 20 | 21 | PEARL | 6.5 | 2.7 | 1.5 | 5.5 | 4.1 | 3.3 |
| | 20 | 21 | PELMO | 7.4 | 3.3 | 1.5 | 6.2 | 4.8 | 3.4 |

# Appendix J. Results of simulations for all scenarios and application of one example substance

## J.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 sorbing and persistent example substance "P" using an ecotoxicological averaging depth of 20 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$^{-1}$ one day before emergence of the crop (the substance was applied to the soil surface).

The $K_{om}$ of substance P at reference conditions was 1 000 l kg$^{-1}$ 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$^{-1}$ (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 (2007), the molar activation energy $E_{Act}$ was assumed to be 65.4 kJ mol$^{-1}$ ($Q_{10}$ = 2.58). Other substance properties were set 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 are based on PERSAM version 1.0.2, PEARL kernel version 3.2.2 (25 March 2015) and PELMO version 4.02 (28 March 2015). Note that these models are still under development. Results may change when updated models are released.

## J.2. Results

Tables J.1 and J.2 show that differences between PELMO and PEARL were usually less than 20 %. For peas and winter cereals in the CTC scenario, differences were larger. The reason for this is not clear.

Results in Table J.3 show that differences in canopy drip were very small for the CLN scenario (not irrigated). However, for the irrigated crops of the CLC and CLS scenarios PELMO generated 40–160 mm more irrigation and this sometimes led to a considerably higher canopy drip than PEARL (at most 129 mm for CLS strawberries). Results in Table J.4 again show very small differences in canopy drip for the non-irrigated CTN and CTS scenarios, but for the irrigated CTC scenarios PELMO generated 40 to 90 mm more irrigation, which led to differences in canopy drip of 20 to 50 mm. Results in Tables J.5 and J.6 show that PEARL–PELMO differences in annual potential transpiration were always smaller than about 10 mm, except for oilseed rape and winter cereals: for these crops differences larger than 10 mm (up to 60 mm) were found in all scenarios.

Differences between percolation past 1 m depth between PEARL and PELMO were small for all non-irrigated scenarios (Tables J.7 and J.8). For the irrigated scenarios PELMO generated more percolation caused by the higher simulated irrigation. The percolation of the CLN, CLC, CTC and CTS scenarios usually ranges between 50 and 150 mm. The percolation of the CTN scenario is considerably higher (about 300 mm) and that of the CLS scenario is very low. This very low percolation of the CLS scenario is remarkable because it is an irrigated scenario.

Figure J.1 compares annual average percolation of all crops of the EFSA soil scenarios with the FOCUS groundwater scenarios. The results show that five of the six EFSA soil scenarios generated less percolation than any of the FOCUS groundwater scenarios (only Seville and Thiva have comparable percolations). Only the CTN scenario had a percolation that is comparable to most of the FOCUS groundwater scenarios.

The results of the water balance calculations in Tables J.3 to J.8 do not include runoff. This was switched off in PELMO. In the PEARL simulations runoff did not occur except in the CTN scenario in which the annual average runoff of water ranged from 8 to 9 mm for the different crops. Therefore, runoff of water had little effect on the water balance.

Please note that results for a few crop location combinations are missing. These will be made available before the models are released for regulatory use.

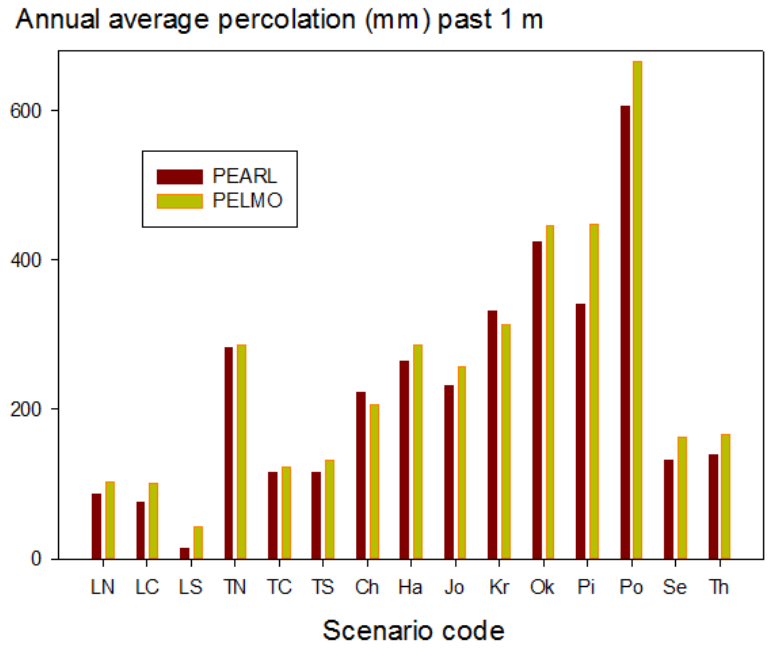


**Figure J.1:** Annual average percolation (mm year$^{-1}$) of the EFSA soil scenarios compared with that of the FOCUS groundwater scenarios. Average values of all crops are shown

**Table J.1:** Concentration in pore water (mg $l^{-1}$) for pesticide P in the top 20 cm of soil. The percentage difference was calculated by dividing the difference by the value of PELMO

| Scenario | Crop | PELMO | PEARL | Difference (%) |
|---|---|---|---|---|
| CLN | Beans | 0.1095 | 0.1082 | –1.15 |
| | Cabbage | 0.1053 | 0.1048 | –0.49 |
| | Carrots | 0.1055 | 0.1033 | –2.09 |
| | Maize | 0.1071 | 0.1029 | –3.90 |
| | Onions | 0.1083 | 0.1062 | –1.95 |
| | Peas | 0.1099 | 0.1085 | –1.32 |
| | Rapeseed summer | 0.1091 | 0.1052 | –3.59 |
| | Rapeseed winter | 0.1096 | 0.0992 | –9.50 |
| | Sugar beets | 0.1078 | 0.1061 | –1.60 |
| | Spring cereals | 0.1087 | 0.1063 | –2.25 |
| | Strawberries | 0.1045 | 0.1036 | –0.83 |
| | Winter cereals | 0.1093 | 0.1014 | –7.23 |
| CLC | Cabbage | 0.1006 | 0.0985 | –2.10 |
| | Carrots | 0.1011 | 0.0977 | –3.38 |
| | Linseed | 0.1223 | 0.1177 | –3.80 |
| | Maize | 0.0984 | 0.0934 | –5.12 |
| | Onions | 0.1092 | 0.1032 | –5.49 |
| | Peas | 0.1274 | 0.1187 | –6.81 |
| | Rapeseed winter | 0.1262 | 0.1073 | –14.94 |
| | Sugar beets | 0.0896 | 0.0877 | –2.08 |
| | Spring cereals | 0.1290 | 0.1164 | –9.78 |
| | Soybeans | 0.0981 | 0.0931 | –5.08 |
| | Strawberries | 0.0944 | 0.0917 | –2.87 |
| | Sunflowers | 0.0916 | 0.0888 | –3.09 |
| | Tomatoes | 0.1044 | 0.0961 | –7.97 |
| | Winter cereals | 0.1283 | 0.1090 | –15.03 |
| CLS | Beans | 0.1149 | 0.1147 | –0.14 |
| | Cabbage | 0.1155 | 0.1258 | 8.89 |
| | Cotton | 0.1435 | 0.1413 | –1.56 |
| | Linseed | 0.1677 | 0.1806 | 7.67 |
| | Maize | 0.1409 | 0.1390 | –1.34 |
| | Onions | 0.1453 | 0.1558 | 7.19 |
| | Rapeseed winter | 0.1726 | 0.1690 | –2.08 |
| | Sugar beets | 0.1642 | 0.1340 | –18.37 |
| | Soybeans | 0.1173 | 0.1115 | –4.97 |
| | Strawberries | 0.1286 | 0.1390 | 8.09 |
| | Sunflowers | 0.1411 | 0.1362 | –3.47 |
| | Tobacco | 0.1161 | 0.1133 | –2.38 |
| | Tomatoes | 0.1526 | 0.1422 | –6.84 |
| | Winter cereals | 0.1802 | 0.1680 | –6.77 |

**Table J.2:** Concentration in total soil (mg $kg^{-1}$) for pesticide P in the top 20 cm of soil. The per cent difference was calculated by dividing the difference by the value for PELMO. The yellow colours indicate differences larger than 20 %

| Scenarios | Crop | PELMO | PEARL | Difference (%) |
|---|---|---|---|---|
| CTN | Beans | 6.44 | 5.73 | –11.06 |
| | Cabbage | 6.37 | 5.81 | –8.77 |
| | Maize | 6.35 | 5.69 | –10.49 |
| | Onions | 6.36 | 6.02 | –5.34 |
| | Peas | 6.37 | 5.68 | –10.90 |
| | Rapeseed summer | 6.38 | 5.63 | –11.64 |
| | Rapeseed winter | 6.11 | 5.42 | –11.28 |
| | Sugar beets | 6.31 | 5.72 | –9.38 |
| | Spring cereals | 6.35 | 5.64 | –11.08 |
| | Strawberries | 6.50 | 6.08 | –6.51 |
| | Winter cereals | 6.34 | 5.51 | –13.14 |
| CTC | Cabbage | 4.20 | 3.92 | –6.66 |
| | Carrots | 4.22 | 3.86 | –8.63 |
| | Linseed | 4.86 | 4.37 | –10.09 |
| | Maize | 4.03 | 4.16 | 3.25 |
| | Onions | 4.35 | 4.54 | 4.44 |
| | Peas | 5.11 | 3.72 | –27.24 |
| | Rapeseed winter | 5.10 | 4.09 | –19.81 |
| | Sugar beets | 3.76 | 3.94 | 4.87 |
| | Spring cereals | 5.15 | 4.56 | –11.62 |
| | Soybeans | 4.08 | 3.72 | –8.79 |
| | Strawberries | 3.99 | 3.68 | –7.80 |
| | Sunflowers | 3.79 | 3.55 | –6.29 |
| | Tomatoes | 4.32 | 3.57 | –17.27 |
| | Winter cereals | 5.16 | 3.76 | –27.07 |
| CTS | Cabbage | 2.99 | 2.93 | –1.79 |
| | Carrots | 3.00 | 2.87 | –4.40 |
| | Linseed | 3.02 | 3.00 | –0.44 |
| | Maize | 3.06 | 2.89 | –5.50 |
| | Onions | 3.05 | 2.96 | –3.07 |
| | Rapeseed winter | 2.98 | 2.76 | –7.37 |
| | Sugar beets | 3.02 | 2.95 | –2.22 |
| | Spring cereals | 3.04 | 2.95 | –2.93 |
| | Soybeans | 3.04 | 2.96 | –2.60 |
| | Strawberries | 2.96 | 2.90 | –2.18 |
| | Sunflowers | 3.01 | 2.87 | –4.71 |
| | Tobacco | 3.01 | 2.85 | –5.47 |
| | Tomatoes | 3.05 | 2.88 | –5.50 |
| | Winter cereals | 3.02 | 2.82 | –6.50 |

**Table J.3:** Annual averages of rainfall, irrigation and wash-off (pore water scenarios)

| Location | Crop | Rainfall (mm) | Irrigation (mm) | | Canopy drip (mm) | | Throughfall (mm) | |
|---|---|---|---|---|---|---|---|---|
| | | Both models | PELMO | PEARL | PELMO | PEARL | PELMO | PEARL |
| CLN | Beans | 567 | 0 | 0 | 148 | 148 | 419 | 419 |
| | Cabbage | 567 | 0 | 0 | 167 | 167 | 400 | 400 |
| | carrots | 567 | 0 | 0 | 140 | 140 | 427 | 427 |
| | Maize | 567 | 0 | 0 | 166 | 166 | 401 | 402 |
| | Onions | 567 | 0 | 0 | 131 | 131 | 436 | 436 |
| | Peas | 567 | 0 | 0 | 148 | 148 | 419 | 419 |
| | RapeseedS | 567 | 0 | 0 | 126 | 126 | 442 | 442 |
| | RapeseedW | 567 | 0 | 0 | 127 | 133 | 440 | 435 |
| | Sugar beets | 567 | 0 | 0 | 191 | 191 | 376 | 377 |
| | CerealsS | 567 | 0 | 0 | 159 | 159 | 409 | 409 |
| | Strawberries | 567 | 0 | 0 | 155 | 154 | 413 | 413 |
| | CerealsW | 567 | 0 | 0 | 122 | 127 | 445 | 441 |
| CLC | Cabbage | 522 | 231 | 145 | 279 | 237 | 474 | 429 |
| | Carrots | 522 | 189 | 117 | 234 | 201 | 477 | 438 |
| | Linseed | 522 | 0 | 0 | 169 | 169 | 356 | 353 |
| | Maize | 522 | 264 | 183 | 334 | 292 | 451 | 413 |
| | Onions | 522 | 160 | 88 | 217 | 182 | 465 | 427 |
| | Peas | 522 | 0 | 0 | 153 | 153 | 369 | 368 |
| | RapeseedW | 522 | 0 | 0 | 122 | 141 | 400 | 381 |
| | Sugar beets | 522 | 325 | 222 | 455 | 388 | 392 | 356 |
| | CerealsS | 522 | 0 | 0 | 147 | 147 | 375 | 375 |
| | Soybeans | 522 | 255 | 180 | 406 | 348 | 370 | 354 |
| | Strawberries | 522 | 263 | 163 | 309 | 254 | 476 | 430 |
| | Sunflowers | 522 | 318 | 205 | 402 | 331 | 438 | 395 |
| | Tomatoes | 522 | 182 | 121 | 293 | 251 | 411 | 392 |
| | CerealsW | 522 | 0 | 0 | 133 | 137 | 389 | 385 |
| CLS | Beans | 361 | 484 | 424 | 456 | 423 | 386 | 361 |
| | Cabbage | 361 | 565 | 402 | 427 | 324 | 499 | 439 |
| | Cotton | 361 | 238 | 199 | 292 | 260 | 307 | 300 |
| | Linseed | 361 | 0 | 0 | 94 | 94 | 267 | 267 |
| | Maize | 361 | 345 | 291 | 386 | 342 | 320 | 310 |
| | Onions | 361 | 195 | 79 | 176 | 109 | 380 | 331 |
| | RapeseedW | 361 | 0 | 0 | 87 | 89 | 274 | 272 |
| | Sugar beets | 361 | 299 | 263 | 378 | 351 | 282 | 273 |
| | Soybeans | 361 | 519 | 477 | 525 | 488 | 354 | 349 |
| | Strawberries | 361 | 596 | 481 | 579 | 450 | 378 | 392 |
| | Sunflowers | 361 | 305 | 246 | 266 | 234 | 399 | 373 |
| | Tobacco | 361 | 561 | 482 | 448 | 442 | 474 | 401 |
| | Tomatoes | 361 | 160 | 138 | 178 | 168 | 342 | 331 |
| | CerealsW | 361 | 0 | 0 | 151 | 150 | 210 | 211 |

CerealsS, cereals summer; CerealsW, cereals winter; RapeseedS, rapeseed summer; RapeseedW, rapeseed winter.

**Table J.4:** Annual averages of rainfall, irrigation and wash-off (total content scenarios)

| Location | Crop | Rainfall (mm) | Irrigation (mm) | | Canopy drip (mm) | | Throughfall (mm) | |
|---|---|---|---|---|---|---|---|---|
| | | Both models | PELMO | PEARL | PELMO | PEARL | PELMO | PEARL |
| CTN | Beans | 699 | 0 | 0 | 188 | 187 | 512 | 513 |
| | Cabbage | 699 | 0 | 0 | 168 | 167 | 532 | 533 |
| | Maize | 699 | 0 | 0 | 196 | 196 | 503 | 504 |
| | Onions | 699 | 0 | 0 | 147 | 147 | 553 | 553 |
| | Peas | 699 | 0 | 0 | 156 | 156 | 543 | 543 |
| | RapeseedS | 699 | 0 | 0 | 164 | 165 | 535 | 535 |
| | RapeseedW | 699 | 0 | 0 | 164 | 171 | 535 | 528 |
| | Sugar beets | 699 | 0 | 0 | 231 | 231 | 469 | 469 |
| | CerealsS | 699 | 0 | 0 | 172 | 172 | 527 | 527 |
| | Strawberries | 699 | 0 | 0 | 156 | 155 | 543 | 545 |
| | CerealsW | 699 | 0 | 0 | 165 | 173 | 534 | 527 |
| CTC | Cabbage | 583 | 216 | 142 | 299 | 267 | 499 | 462 |
| | Carrots | 583 | 182 | 118 | 256 | 231 | 509 | 475 |
| | Linseed | 583 | 0 | 0 | 206 | 209 | 377 | 379 |
| | Maize | 583 | 255 | 190 | 372 | 339 | 466 | 439 |
| | Onions | 583 | 149 | 96 | 236 | 218 | 496 | 466 |
| | Peas | 583 | 0 | 0 | 182 | 185 | 402 | 403 |
| | RapeseedW | 583 | 0 | 0 | 135 | 155 | 449 | 434 |
| | Sugar beets | 583 | 323 | 242 | 498 | 447 | 409 | 383 |
| | CerealsS | 583 | 0 | 0 | 163 | 164 | 420 | 425 |
| | Soybeans | 583 | 244 | 188 | 445 | 404 | 382 | 372 |
| | Strawberries | 583 | 260 | 182 | 331 | 291 | 513 | 479 |
| | Sunflowers | 583 | 313 | 222 | 440 | 386 | 457 | 424 |
| | Tomatoes | 583 | 166 | 126 | 316 | 293 | 433 | 421 |
| | CerealsW | 583 | 0 | 0 | 151 | 155 | 433 | 433 |
| CTS | Cabbage | 680 | 0 | 0 | 161 | 161 | 519 | 519 |
| | Carrots | 680 | 0 | 0 | 146 | 147 | 534 | 533 |
| | Linseed | 680 | 0 | 0 | 157 | 158 | 523 | 522 |
| | Maize | 680 | 0 | 0 | 129 | 129 | 551 | 551 |
| | Onions | 680 | 0 | 0 | 104 | 104 | 576 | 576 |
| | RapeseedW | 680 | 0 | 0 | 132 | 141 | 548 | 539 |
| | Sugar beets | 680 | 0 | 0 | 172 | 171 | 508 | 509 |
| | CerealsS | 680 | 0 | 0 | 148 | 148 | 532 | 532 |
| | Soybeans | 680 | 0 | 0 | 182 | 182 | 498 | 498 |
| | Strawberries | 680 | 0 | 0 | 149 | 149 | 531 | 531 |
| | Sunflowers | 680 | 0 | 0 | 160 | 160 | 520 | 520 |
| | Tobacco | 680 | 0 | 0 | 145 | 145 | 535 | 535 |
| | Tomatoes | 680 | 0 | 0 | 124 | 124 | 556 | 556 |
| | CerealsW | 680 | 0 | 0 | 119 | 125 | 561 | 555 |

CerealsS, cereals summer; CerealsW, cereals winter; RapeseedS, rapeseed summer; RapeseedW, rapeseed winter.

**Table J.5:** Annual averages of potential and actual evaporation (pore water scenarios)

| Location | Crop | Potential evapotranspiration (mm) | | Actual evapotranspiration (mm) | |
|---|---|---|---|---|---|
| | | PELMO | PEARL | PELMO | PEARL |
| CLN | Beans | 649 | 651 | 465 | 479 |
| | Cabbage | 640 | 640 | 450 | 474 |
| | Carrots | 637 | 638 | 460 | 473 |
| | Maize | 657 | 656 | 472 | 473 |
| | Onions | 614 | 616 | 442 | 452 |
| | Peas | 673 | 673 | 473 | 487 |
| | RapeseedS | 661 | 639 | 456 | 460 |
| | RapeseedW | 663 | 638 | 482 | 482 |
| | Sugar beets | 662 | 663 | 467 | 484 |
| | CerealsS | 653 | 655 | 472 | 489 |
| | Strawberries | 645 | 645 | 457 | 486 |
| | CerealsW | 638 | 647 | 472 | 482 |
| CLC | Cabbage | 700 | 700 | 606 | 559 |
| | Carrots | 699 | 700 | 604 | 554 |
| | Linseed | 691 | 693 | 460 | 485 |
| | Maize | 721 | 722 | 645 | 592 |
| | Onions | 675 | 676 | 572 | 525 |
| | Peas | 740 | 740 | 468 | 488 |
| | RapeseedW | 719 | 700 | 493 | 498 |
| | Sugar beets | 730 | 731 | 695 | 645 |
| | CerealsS | 704 | 705 | 461 | 472 |
| | Soybeans | 710 | 712 | 620 | 590 |
| | Strawberries | 708 | 708 | 663 | 611 |
| | Sunflowers | 727 | 728 | 687 | 621 |
| | Tomatoes | 710 | 711 | 598 | 559 |
| | CerealsW | 693 | 702 | 472 | 478 |
| CLS | Beans | 1 176 | 1 179 | 783 | 758 |
| | Cabbage | 1 186 | 1 178 | 850 | 746 |
| | Cotton | 1 186 | 1 187 | 568 | 558 |
| | Linseed | 1 155 | 1 158 | 353 | 360 |
| | Maize | 1 184 | 1 186 | 662 | 638 |
| | Onions | 1 159 | 1 162 | 503 | 431 |
| | RapeseedW | 1 203 | 1 176 | 357 | 360 |
| | Sugar beets | 1 172 | 1 173 | 618 | 617 |
| | Soybeans | 1 186 | 1 190 | 834 | 812 |
| | Strawberries | 1 186 | 1 187 | 866 | 826 |
| | Sunflowers | 1 171 | 1 173 | 632 | 596 |
| | Tobacco | 1 186 | 1 185 | 849 | 803 |
| | Tomatoes | 1 172 | 1 173 | 502 | 496 |
| | CerealsW | 1 237 | 1 173 | 347 | 357 |

CerealsS, cereals summer; CerealsW, cereals winter; RapeseedS, rapeseed summer; RapeseedW, rapeseed winter.

**Table J.6:** Annual averages of potential and actual evaporation (pore water scenarios)

| Location | Crop | Potential evapotranspiration (mm) | | Actual evapotranspiration (mm) | |
|---|---|---|---|---|---|
| | | PELMO | PEARL | PELMO | PEARL |
| CTN | Beans | 542 | 544 | 432 | 436 |
| | Cabbage | 535 | 535 | 400 | 405 |
| | Maize | 547 | 548 | 433 | 432 |
| | Onions | 511 | 511 | 357 | 375 |
| | Peas | 558 | 558 | 422 | 425 |
| | RapeseedS | 551 | 531 | 421 | 412 |
| | RapeseedW | 553 | 529 | 443 | 432 |
| | Sugar beets | 549 | 549 | 411 | 418 |
| | CerealsS | 539 | 541 | 415 | 418 |
| | Strawberries | 536 | 536 | 383 | 394 |
| | CerealsS | 529 | 539 | 409 | 425 |
| CTC | Cabbage | 749 | 749 | 641 | 591 |
| | Carrots | 748 | 750 | 644 | 587 |
| | Linseed | 739 | 741 | 503 | 502 |
| | Maize | 772 | 773 | 677 | 633 |
| | Onions | 723 | 724 | 605 | 559 |
| | Peas | 791 | 792 | 514 | 504 |
| | RapeseedW | 769 | 750 | 527 | 505 |
| | Sugar beets | 781 | 782 | 734 | 696 |
| | CerealsS | 754 | 755 | 496 | 475 |
| | Soybeans | 760 | 762 | 651 | 629 |
| | Strawberries | 758 | 758 | 703 | 656 |
| | Sunflowers | 778 | 779 | 725 | 672 |
| | Tomatoes | 759 | 760 | 628 | 596 |
| | CerealsW | 743 | 752 | 505 | 481 |
| CTS | Cabbage | 762 | 763 | 511 | 535 |
| | Carrots | 757 | 760 | 531 | 541 |
| | Linseed | 745 | 748 | 514 | 544 |
| | Maize | 776 | 778 | 567 | 558 |
| | Onions | 733 | 736 | 514 | 521 |
| | RapeseedW | 794 | 760 | 569 | 553 |
| | Sugar beets | 777 | 779 | 578 | 566 |
| | CerealsS | 775 | 778 | 565 | 576 |
| | Soybeans | 768 | 772 | 508 | 532 |
| | Strawberries | 767 | 768 | 544 | 564 |
| | Sunflowers | 784 | 786 | 578 | 578 |
| | Tobacco | 767 | 767 | 566 | 566 |
| | Tomatoes | 770 | 772 | 567 | 568 |
| | CerealsW | 759 | 771 | 564 | 566 |

CerealsS, cereals summer; CerealsW, cereals winter; RapeseedS, rapeseed summer; RapeseedW, rapeseed winter.

**Table J.7:** Annual averages of percolation past 1 m (pore water scenarios)

| Location | Crop | Percolation past 1 m (mm) | |
|---|---|---|---|
| | | PELMO | PEARL |
| CLN | Beans | 100 | 84 |
| | Cabbage | 117 | 90 |
| | Carrots | 106 | 90 |
| | Maize | 93 | 91 |
| | Onions | 125 | 112 |
| | Peas | 92 | 76 |
| | RapeseedS | 110 | 104 |
| | RapeseedW | 84 | 82 |
| | Sugar beets | 99 | 80 |
| | CerealsS | 93 | 74 |
| | Strawberries | 110 | 77 |
| | CerealsW | 94 | 81 |
| CLC | Cabbage | 145 | 108 |
| | Carrots | 105 | 85 |
| | Linseed | 59 | 37 |
| | Maize | 139 | 113 |
| | Onions | 106 | 85 |
| | Peas | 49 | 34 |
| | RapeseedW | 24 | 24 |
| | Sugar beets | 150 | 99 |
| | CerealsS | 58 | 49 |
| | Soybeans | 155 | 112 |
| | Strawberries | 118 | 73 |
| | Sunflowers | 151 | 106 |
| | Tomatoes | 102 | 84 |
| | CerealsW | 45 | 44 |
| CLS | Beans | 61 | 27 |
| | Cabbage | 76 | 17 |
| | Cotton | 31 | 2 |
| | Linseed | 7 | 1 |
| | Maize | 44 | 14 |
| | Onions | 52 | 9 |
| | RapeseedW | 4 | 1 |
| | Sugar beets | 43 | 7 |
| | Soybeans | 46 | 25 |
| | Strawberries | 91 | 16 |
| | Sunflowers | 34 | 11 |
| | Tobacco | 73 | 40 |
| | Tomatoes | 18 | 4 |
| | CerealsW | 14 | 4 |

CerealsS, cereals summer; CerealsW, cereals winter; RapeseedS, rapeseed summer; RapeseedW, rapeseed winter.

**Table J.8:** Annual averages of percolation past 1 m (total concentration scenarios)

| Location | Crop | Percolation past 1 m (mm) | |
|---|---|---|---|
| | | PELMO | PEARL |
| CTN | Beans | 266 | 263 |
| | Cabbage | 299 | 293 |
| | Maize | 265 | 267 |
| | Onions | 341 | 324 |
| | Peas | 276 | 274 |
| | RapeseedS | 277 | 286 |
| | RapeseedW | 256 | 266 |
| | Sugar beets | 287 | 281 |
| | CerealsS | 283 | 281 |
| | Strawberries | 315 | 305 |
| | CerealsW | 289 | 274 |
| CTC | Cabbage | 158 | 137 |
| | Carrots | 122 | 117 |
| | Linseed | 80 | 84 |
| | Maize | 161 | 144 |
| | Onions | 126 | 124 |
| | Peas | 69 | 82 |
| | RapeseedW | 56 | 81 |
| | Sugar beets | 172 | 132 |
| | CerealsS | 87 | 111 |
| | Soybeans | 176 | 145 |
| | Strawberries | 140 | 113 |
| | Sunflowers | 171 | 136 |
| | Tomatoes | 120 | 117 |
| | CerealsW | 78 | 106 |
| CTS | Cabbage | 169 | 136 |
| | Carrots | 149 | 130 |
| | Linseed | 166 | 128 |
| | Maize | 112 | 113 |
| | Onions | 165 | 150 |
| | RapeseedW | 110 | 117 |
| | Sugar beets | 109 | 105 |
| | CerealsS | 114 | 94 |
| | Soybeans | 172 | 139 |
| | Strawberries | 136 | 106 |
| | Sunflowers | 101 | 93 |
| | Tobacco | 113 | 105 |
| | Tomatoes | 112 | 102 |
| | CerealsW | 115 | 104 |

CerealsS, cereals summer; CerealsW, cereals winter; RapeseedS, rapeseed summer; RapeseedW, rapeseed winter.

## Appendix K. Excel sheet for the fraction of the dose reaching the soil

The Excel sheet, available at the link below, provides background information on how the fraction of applied substance reaching the soil was derived.

http://www.efsa.europa.eu/en/efsajournal/doc/4093ax1.xls