SCIENTIFIC REPORT OF EFSA

Tier-1 and Tier-2A Scenario Parameterisation and Example Calculations [1]

In Support of the Revision of the Guidance Document on Persistence in Soil under Council Directive 91/414/EEC and Parliament and Council Regulation (EC) 1107/2009 (SANCO/9188/VI/97 rev. 8, 12.07.2000)

European Food Safety Authority[2, 3]

European Food Safety Authority (EFSA), Parma, Italy

1 On request of EFSA, Question No EFSA-Q-2011-00113, issued on 16/12/2011.

2 Correspondence: pesticides.ppr@efsa.europa.eu

3 Acknowledgement: EFSA wishes to thank the experts for the preparation of this EFSA scientific output: Aaldrik Tiktak, Jan Vanderborght, Michael Klein, Jos Boesten, Richard Bromilow and EFSA staff members Mark Egsmose, Maria Sodani and Judith Ricketts for the support provided to this scientific output. EFSA wishes to thank Tony Hardy, Paulo Sousa, Andreas Schäffer and Theo Brock for reviewing this scientific output.

Suggested citation: European Food Safety Authority; Tier-1 and Tier-2A Scenario Parameterisation and Example Calculations. EFSA Journal 2012;10(1):2433 [64 pp.]. doi:10.2903/j.efsa.2012.2433. Available online: www.efsa.europa.eu/efsajournal

ABSTRACT

European scenarios for exposure of soil organisms to Plant Protection Products are currently not available (EFSA Panel on Plant Protection Products and their Residues (PPR), 2010). In this document, the parameterisation of realistic worst-case scenarios for Tier-1 and Tier-2A simulations is described which are part of a tiered approach. The aim of this scheme is to assess such Predicted Environmental Concentrations (PEC), chosen to be the 90th spatial percentile, resulting from the use of the plant protection product. In order to account for the uncertainty in substance and soil properties, the Tier-2A scenarios are combinations of soil and climatic properties within a zone, for which the predicted concentration is equal to the 95th percentile of all concentrations within the area of annual crops. The selected soil profiles are based on digitised information from topsoil (organic matter and texture) combined with calculated average soil profiles available in the SPADE-1 database. The daily weather information for the scenarios is taken from the MARS database using the period 1990-2009. In order to have a sufficient overview on the differences between simulations performed with the analytical Tier-1 model and the numerical Tier-2A models, PEARL and PELMO test runs are performed covering all relevant substance properties and all evaluation depths. For each of the total-soil scenarios, both models simulate nearly the same concentration. Small differences between PEARL and PELMO can be found for the pore-water scenarios due to differences in the calculation of soil moisture contents. The comparison with the analytical model shows that Tier-1 concentrations are usually above the respective Tier-2A concentrations in accordance with the philosophy of the tiered assessment scheme. However, due to the different handling of soil moisture, Tier-1 simulations may occasionally give concentrations below those of Tier 2A, which occurrence necessitates additional calibration using special model-adjustment factors.

KEY WORDS

Exposure assessment, exposure scenarios, scenario development, soil, parameter uncertainty, scenario uncertainty, plant protection product, PEARL, PELMO

SUMMARY

European scenarios for exposure of soil organisms to Plant Protection Products are currently not available (EFSA Panel on Plant Protection Products and their Residues (PPR), 2010). There is, however, a need for such scenarios at the EU level in view of ongoing discussions in PRAPeR experts' groups[4] on PECSOIL. Therefore, the PPR Panel has started a revision of the existing Guidance Document on Persistence in Soil (SANCO/9188/VI/97 rev. 8, 12.07.2000) by developing tiered exposure-assessment approaches for soil organisms in which European exposure scenarios play an important role. The assessment scheme comprises five tiers, each with realistic worst-case scenarios. The tiered scheme applies to spray applications to annual crops under conventional or reduced tillage but may also be useful for other types of application or other tillage systems.

In this document, the parameterisation of realistic worst-case scenarios for Tier-1 and Tier-2A simulations is described. Here, a realistic worst-case scenario is defined as a combination of soil and climate properties within a certain region for which predicted concentrations (PECs) are equal to a certain percentile of the distribution of concentrations for all climate and soil-property combinations within the region.

The scenarios are part of a tiered approach. The aim of this tiered approach is to assess this spatial percentile, chosen to be the 90th, resulting from the use of the plant protection product (assuming a market share of 100%) and considering the population of agricultural fields (in one of the three regulatory zones) where the crop is grown and in which this plant protection product is applied. Tier 1, Tier 2 B and Tier 2C are proposed to be based on a simple analytical mode, whereas Tier 2A, Tier 3 and Tier 4 will utilise numerical fate models.

The scenarios are combinations of soil and climatic properties within a zone, for which the predicted concentration is equal to the 90th percentile of all concentrations within the area of annual crops. The end-point for the exposure assessment is, however, the 90th percentile of the exposure concentration within the intended area of use of a plant protection product. The area of the selected crop (or combination of crops) will have an effect on the 90th percentile exposure concentration, and so the Tier-2A scenarios as such may not be conservative enough; this problem is handled by introducing crop extrapolation factors.

Furthermore, the overall 90th percentile of the substance concentration is shifted towards higher values if uncertainty in substance properties and soil properties is considered. As a consequence the selected scenario may not be sufficiently conservative if scenarios are selected without consideration of uncertainty about substance and soil properties; such uncertainty has therefore explicitly been incorporated in the scenario-selection procedure. It was found that for the soil exposure end-points (peak concentration in total soil and concentration in the liquid phase), the 90th overall percentile corresponds to the 95th percentile of the cumulative probability density function (cpdf) resulting from median substance properties and deterministic soil properties.

The scenario selection was based on properties of the topsoil (organic matter and texture). However, the fate models also need information about subsoil properties. As the spatial coverage of European soil-profile databases is less than 100%, it was not possible to extract this information from the databases. Instead, average soil profiles, based on all arable soil profiles available in the SPADE-1 database, were calculated. The use of average soil profiles was judged to be acceptable because the evaluation depth for the exposure assessment is only the top 20 cm.

The MARS climate database provides daily weather data for the entire EU-27 in a 25x25 km^2 grid. Therefore, daily weather data as needed by the fate models can be directly extracted for the selected scenario locations from the appropriate MARS grid. The MARS database contains all the parameters required for simulation runs with the current fate models, such as minimum and maximum

[4] Now replaced by Pesticides Unit

temperature, rainfall, potential evapotranspiration and global radiation. A quality check was performed to see if the dataset contains unrealistic data (see EFSA, 2010 for details). The MARS weather data for the period 1990-2009 were used, converting these to a 66-year time-series using the rules described in FOCUS (2000).

Tier-2A scenarios have been developed for a range of annual crops. Crop emergence and harvest dates for these crops were taken from FOCUS (2010). The corresponding FOCUS scenario was selected from a map of FOCUS climatic zones. A crop that is irrigated in the corresponding FOCUS scenario in the same climatic zone was assumed also to be irrigated in the EFSA soil scenario. Ploughing was assumed to occur one month before crop emergence for all locations and all crops because all scenario soils have medium to coarse soil texture. Early ploughing in the preceding winter is assumed to occur only for heavy clay soils. The same crop extrapolation factors were considered for Tier 2A as for Tier 1. Different safety factors were made available for major and minor crops.

In order to have a sufficient overview on the differences between Tier-1 and Tier-2A simulations, test runs were performed that covered all relevant substance properties and all evaluation depths. In most of the comparisons, Tier-1 concentrations were found to be above the respective Tier-2A concentrations in accordance with the philosophy of the tiered assessment scheme. However, due to different handling of soil moisture, Tier-1 simulations can occasionally give concentrations below those of Tier 2A, which occurrence necessitates additional calibration using special model adjustment factors which are provided.

TABLE OF CONTENTS

BACKGROUND AS PROVIDED BY EFSA

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

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

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

TERMS OF REFERENCE AS PROVIDED BY EFSA

The intention with this report is to provide the scientific methodology for the parameterisation and calibration of the EU soil scenarios for estimating exposure of pesticides to soil organisms. The report will provide scientific input to address the terms of references tasked by EFSA to the PPR Panel and approved on the 7th February 2011 by the EFSA Executive Director.

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

1. INTRODUCTION

1.1. Aim of the study

European scenarios for exposure of soil organisms to Plant Protection Products are currently not available (EFSA panel on Plant Protection Products and their Residues (PPR), 2010). There is, however, a need for such scenarios at the EU level in view of ongoing discussions in PRAPeR experts' groups on PEC_{SOIL}. Therefore, the PPR Panel has started a revision of the existing Guidance Document on Persistence in Soil (SANCO/9188/VI/97 rev. 8, 12.07.2000) by developing tiered exposure-assessment approaches for soil organisms in which European exposure scenarios play an important role. The assessment scheme comprises five tiers, each with realistic worst-case scenarios. The tiered scheme applies to spray applications to annual crops under conventional or reduced tillage but may also be useful for other types of application or other tillage systems.

In this document, the parameterisation of realistic worst-case scenarios for Tier-1 and Tier-2A simulations is described. Here, a realistic worst-case scenario is defined as a combination of soil and climate properties within a certain region for which predicted environmental concentrations (PECs) are equal to a high percentile (e.g. 90^{th}) to be set in consultation with risk managers of the distribution of concentrations for all climate and soil-property combinations within the region.

The Tier-2A simulations presented in this report used the models PELMO and PEARL, both these being recommended and parameterised by FOCUS (2000). In principle, the FOCUS models PRZM and MACRO could also have been considered for use in this study. However, due to their conceptual similarities, it is expected that the outputs of the capacity models PELMO and PRZM would be very close, as likewise would be those from PEARL and MACRO which both use the Richards equation for soil hydrology. Thus including MACRO and PRZM would be expected to add little value to the exposure assessment.

1.2. Targets for the exposure assessment

FOCUS (2000) defined realistic worst-case conditions as the 90^{th} percentile of PEC values within the agricultural area of use of the plant protection product in each of ten climatic zones across the EU. The PPR-Panel checked with risk managers at Member State level whether a 90^{th} percentile exposure concentration should also be used here, and their response confirmed this (EFSA Panel on Plant Protection Products and their Residues (PPR), 2010). In their reaction, several Member States also indicated that the exposure-assessment procedure should be kept as simple as possible. Therefore, the PPR-Panel proposes to develop guidance for estimating 90^{th} percentile values of PEC_{SOIL} for only the three zones described in Annex 1 of the new Regulation concerning the placing of plant protection products on the market (Figure 1).

The exposure assessment is considered to be part of the terrestrial ecotoxicological-risk assessment. This implies that it has to encompass all types of concentration that are considered relevant for assessing the ecotoxicological effects. These concentrations are called Ecotoxicologically Relevant types of Concentration, abbreviated to ERC (Boesten *et al.*, 2007). Based on EFSA (2009), the following types of concentrations are considered ecotoxicologically relevant:

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

The maximum value in time (resulting from multiyear applications) will be the target for all types of concentration (Figure 2). So the 90^{th} percentile will be based only on spatial aspects. The spatial 90^{th} percentile PEC_{SOIL} within each of the three zones has to be based on a distribution of individual PEC_{SOIL} values, each of which is intended to be a correct estimate of the average value at the scale of individual agricultural fields to which the substance is applied. The assessment procedure will not account for the random spatial variability within such an individual field because the PPR-Panel considers this level of detail currently not sufficiently relevant for the risk-assessment schemes regarding ecotoxicological effects (EFSA Panel on Plant Protection Products and their Residues (PPR), 2010). The assessment procedure will account for systematic spatial variability (e.g. application of herbicides in orchards in strips below the trees, seed treatments).

Another aspect of the definition of the 90th percentile PEC_{SOIL} is the population of agricultural fields on which the percentile is based. The PPR-Panel proposes to base the definition of the population on the intended area of use e.g. for a plant protection product that is applied in winter wheat, the population of fields on which winter wheat are grown in a particular zone.

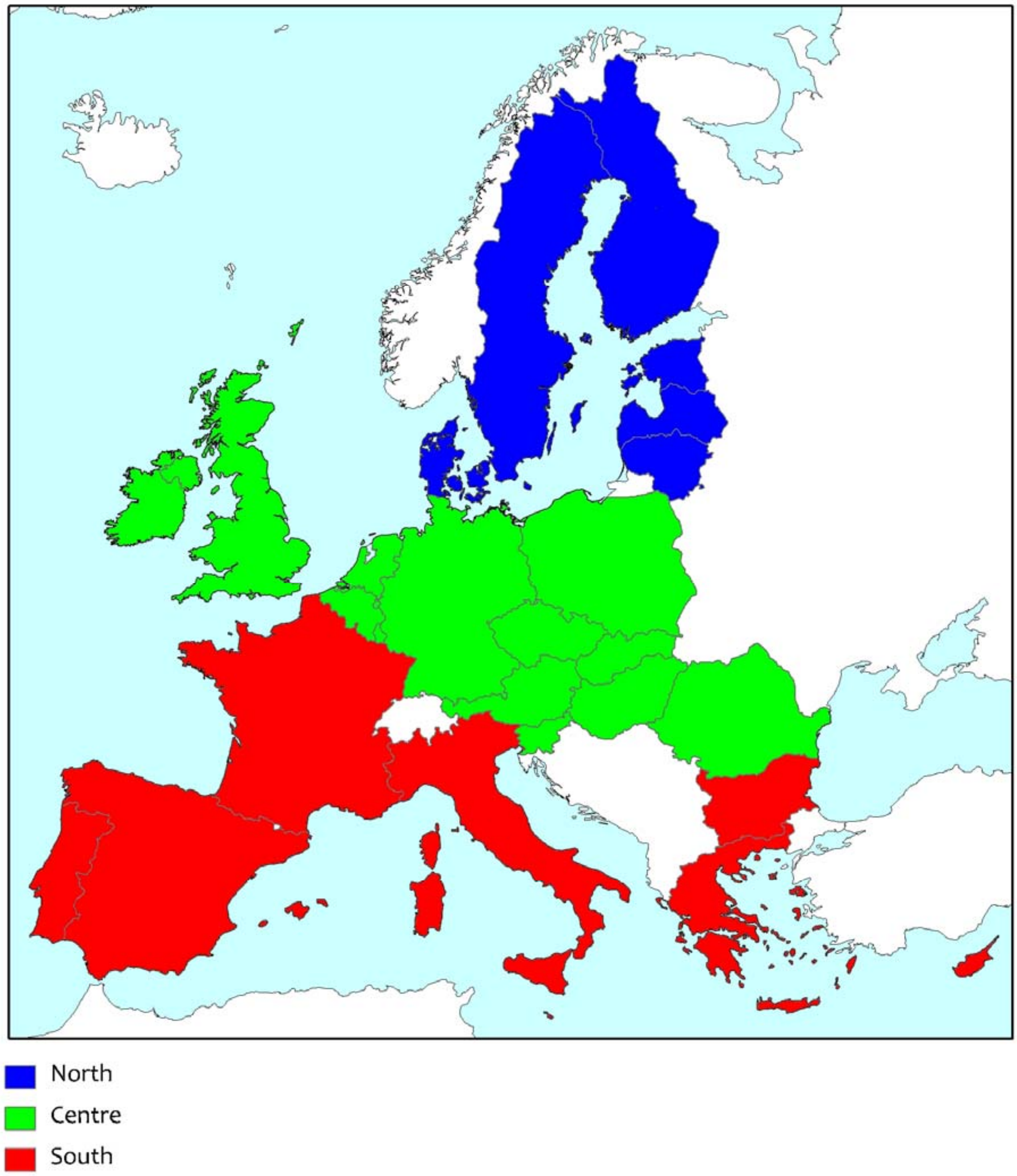

Figure 1: Map with the three regulatory zones described in Annex 1 of the new Regulation concerning the placement of plant protection products on the market (EFSA, 2010).

Different scenarios have to be considered for each combination of crop type, tillage system and application technique, because the exposure assessment for the PEC_{SOIL} depends besides on the pesticide application rate and the kinetics of its dissipation strongly on (i) the type of crop (annual crops, grass, other permanent crops or rice), (ii) the tillage system, and (iii) the application technique of the plant protection product (EFSA Panel on Plant Protection Products and their Residues (PPR), 2010). This report is limited to the calibration of Tier-2A scenarios for annual crops in combination with conventional or reduced tillage and spray applications, because this combination comprises the largest surface area and the largest usage of plant protection products.

The realistic worst-case scenarios parameterised in this report are part of tiered assessment schemes with five tiers (Figure 2). Two schemes were developed, viz. one for the concentration in total soil and one for the pore-water concentration. The schemes for the two types of ERCs are identical but the contents of the tiers differ so there are two parallel tiered assessment schemes. The tiered scheme applies to spray applications to annual crops under conventional or reduced tillage but may also be useful for other types of application or other tillage systems (EFSA, 2011).

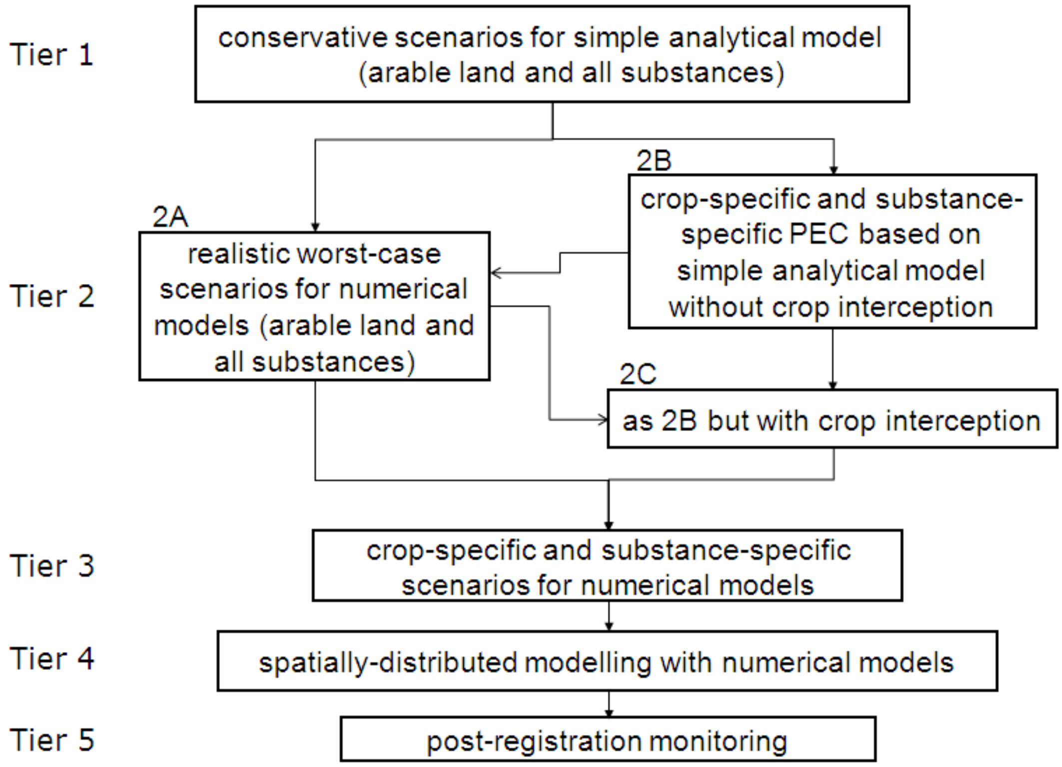

Figure 2: Tiered scheme for the exposure assessment for annual crops with conventional or reduced tillage and spray application. There are two identical assessment schemes, viz. one for the concentration in total soil and one for the concentration in pore water**.**

2. DESCRIPTION OF THE SCENARIOS

2.1. General characterisation of the scenarios

The development of the scenarios has been extensively described in the scientific report of EFSA *Selection of Scenarios for Exposure of Soil Organisms to Plant Protection Products* (see EFSA, 2010). Tier-2A scenarios are combinations of soil and climatic properties within a zone, for which the predicted concentration is equal to the 90^{th} percentile of all concentrations within the area of annual crops. The end-point for the exposure assessment is, however, the 90^{th} percentile of the exposure concentration within the intended area of use of a plant protection product. The area of the selected crop (or combination of crops) will have an effect on the 90^{th} percentile exposure concentration, and so the Tier-2A scenarios as such may not be conservative enough; this problem is handled by introducing safety factors.

The selected scenario may not be sufficiently conservative if scenarios are selected without consideration of uncertainty about substance and soil properties. By explicitly incorporating this uncertainty in the scenario selection procedure, the overall 90^{th} percentile concentration is shifted towards higher values. Such uncertainty has therefore explicitly been incorporated in the scenario-selection procedure. It was found that for the soil exposure end-points (peak concentration in total soil and concentration in the liquid phase), the 90^{th} overall percentile corresponds to the 95^{th} percentile of the cumulative probability density function (cpdf) resulting from median substance properties and deterministic soil properties (*see* Figure 3 taken from EFSA 2010).

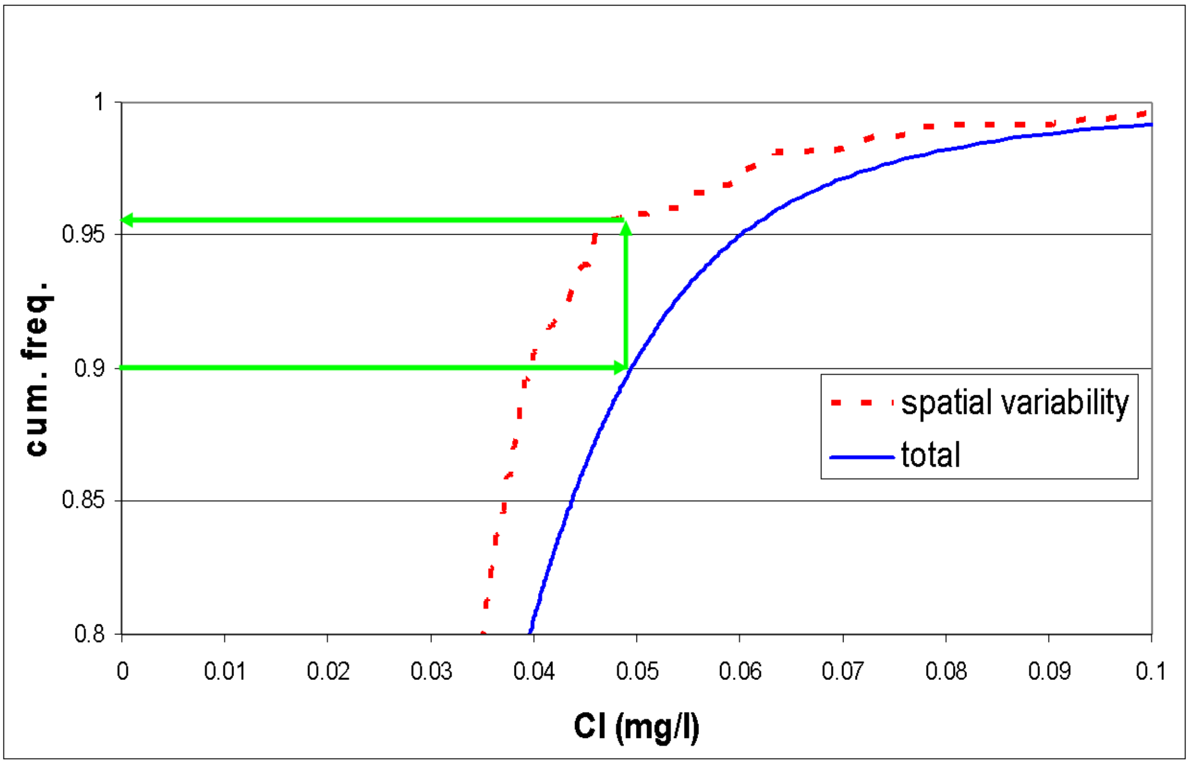

Figure 3: Procedure to derive the spatial percentile of the cpdf that does not consider substance- and soil-property uncertainty (red line) but predicts the same concentration as the 90th percentile of the overall cpdf (cumulative probability density function, blue line). (This example shows the cpdf for the peak pore-water concentrations, Cl, and an ecologically relevant depth of 20 cm for a compound having an ecologically relevant depth zrel = 20 cm, K_{om} = 1000 L kg^{-1} and *DegT50* = 200 d).

2.1.1 Location of the scenarios

The procedure to develop the Tier-1 and Tier-2A scenario locations led to many possible locations that were in the target vulnerability range of 95% to 97% Therefore, the sets of candidate locations were limited to those scenarios that have organic matter contents and temperatures within 1% of the mean value of all candidate locations. This procedure avoided the selection of extreme scenarios. The final locations of the Tier-2A scenarios are presented in Figure 4.

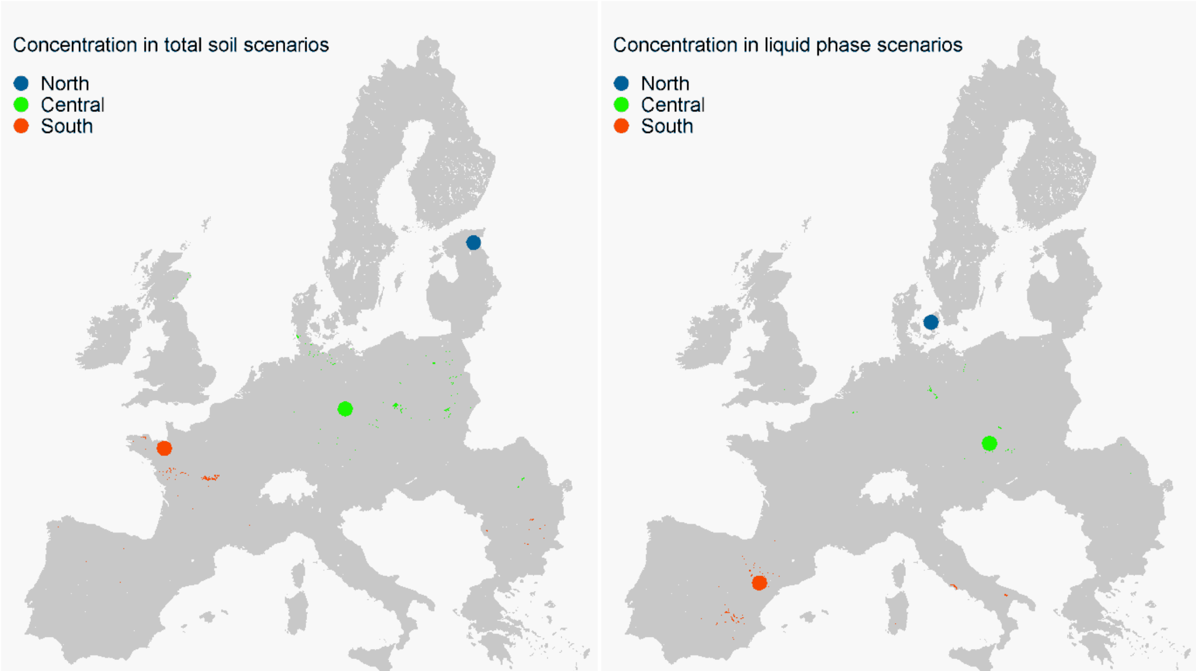

Figure 4: Geographical position of the Tier-2A scenarios that conform to the target vulnerability for all of the 38 substance-depth combinations.

2.1.2 Basic parameters of the scenarios

The scenario selection was based on properties of the topsoil (organic matter and texture). The detailed development of the scenarios has been described previously (EFSA, 2010). The key parameters of the scenarios (Table 1 and 2) are the base for the Tier-1 and Tier-2A simulations. However, when performing Tier-1 simulations, the Arrhenius weighted temperature (*Teff*) has to be used instead of the average temperature.

Table 1: Mean properties of the scenarios for concentration in total soil. T_{MARS} *and* $T_{scenario}$ are yearly average temperatures at the scenario location without and including scaling, T_{eff} is the average Arrhenius weighted temperature over 20 years, f_{om} is the soil organic matter content in mass percent

Zone	T_{MARS} (°C)	$T_{scenario}$ (°C)	T_{eff} (°C)	Texture	Volume fraction of water, θ (m^3 m^{-3})	Dry bulk density, ρ (kg L^{-1})	f_{om} (%)
North	6.15	4.7	7.0	Coarse	0.244	0.95	11.8
Central	9.73	8.0	10.1	Coarse	0.244	1.05	8.6
South	12.35	11.0	12.3	Medium fine	0.385	1.22	4.8

Table 2: Mean properties of the selected scenarios for concentration in the liquid phase. T_{MARS} *and* $T_{scenario}$ are yearly average temperatures at the scenario location without and including scaling, and T_{eff} is the average Arrhenius weighted temperature over 20 years

Zone	T_{MARS} (°C)	$T_{scenario}$ (°C)	T_{eff} (°C)	Texture	Volume fraction of water, θ ($m^3\ m^{-3}$)	Dry bulk density, ρ (kg L^{-1})	f_{om} (%)
North	8.66	8.2	9.8	Medium	0.347	1.39	2.3
Central	9.76	9.1	11.2	Medium	0.347	1.43	1.8
South	13.94	12.8	14.7	Medium	0.347	1.51	1.1

Different scenarios are selected for the concentration in total soil and for the concentration in the liquid phase: the scenarios for the concentration in total soil generally have high organic-matter contents whereas the scenarios for the concentration in the liquid phase generally have low organic-matter contents. The organic matter content generally decreases in the order North > Central > South.

2.2. Description and parameterisation of Tier-1 scenarios

Tier-1 calculation procedures were developed based on the basic scenario parameters (Table 1 and 2) using the single rule that the Tier-1 scenarios have to be more simple and conservative than the corresponding Tier-2A scenarios. As a consequence, Tier 2A will act as the yardstick for Tier 1.

Tier-1 consists of a simple analytical model ('back-of-an-envelope') that was parameterised for the three zones (North/Central/South). A tier can only be simple in practice if the input data are limited. Therefore the input to be provided by the user was restricted to:

i. half-life for degradation in topsoil at 20°C and a moisture content corresponding to field capacity,
ii. the organic-matter/water distribution coefficient (K_{om}),
iii. the annual rate of application for one application per year and in case of more than one application per year additionally the number of applications and the average time interval between applications,
iv. whether application takes place every year, every second year or every third year.

Tier-1 calculations are based on the following conceptual model:

i. no crop interception is assumed,
ii. the substance is applied to the soil surface,
iii. the only loss process from the soil is degradation,
iv. soil properties such as moisture content and temperature are constant in time,
v. the effect of tillage is accounted for by assuming complete mixing over the tillage depth at the moment of tillage (each year in autumn or winter),
vi. adsorption is described by a linear isotherm,
vii. the average exposure concentration over a certain depth is calculated from the sum of the concentration just before the last application and the dose divided by this depth.

The Tier-1 calculations include calculation of concentration in total soil and in pore water. Both peak values and TWA-values for windows up to 56 days are calculated. Tier 1 includes calculation of concentrations of metabolites based on the conservative assumption that each metabolite is applied at the application time of the parent at a dose that is corrected for the kinetic formation fraction (using procedures in FOCUS, 2006) and the molar mass of the metabolite.

The scenario-selection procedures are based on the total surface area of annual crops (see EFSA 2011 for more information). The end-point for the exposure assessment is, however, the 90th percentile of the exposure concentration within the intended area of use of a plant protection product. The area of the selected crop (or combination of crops) will have an effect on the 90th percentile exposure concentration, so the Tier-1 and Tier-2A scenarios may not as such be conservative enough; this problem is handled by introducing safety factors.

The safety factors were derived based on the procedure described in EFSA (2010b). Simulations were performed for 17 annual crops or combinations of crops together covering 100% of the area of annual crops in the EU-27 and for three different substances. For each of these, the 90th percentile concentration (approximated by the 95th spatial percentile) within each regulatory zone was calculated. Crop distributions were based on CAPRI land-use maps (Leip et al., 2008).

The safety factor for each Tier-2A scenario was obtained by comparing the 95th spatial percentile of all 51 Tier-3 simulations with the Tier-2A scenario (which corresponds to the 95th spatial percentile for the entire area of annual crops).

If registration is required for a sub-population, the applicant should derive the safety factor based on the distribution of the sub-population (Table 3). If this information is not available, the safety factor can always be based on the 100th percentile of the entire population of annual crops (Table 4).

Table 3: Crop extrapolation factors for the scenarios based on the 90th percentile of the entire population of annual crops within each zone

Zone	Safety factor for C_T (total-soil concentration)	Safety factor for C_L (pore-water concentration)
North	1.79 (0.64-1.79)	1.02 (0.87-1.02)
Central	1.16 (0.74-1.16)	1.15 (0.93-1.15)
South	1.07 (0.86-1.07)	1.13 (0.86-1.13)

Table 4: Crop extrapolation factors for the scenarios based on the 100th percentile of the entire population of annual crops within each zone

Zone	Safety factor for C_T (total-soil concentration)	Safety factor for C_L (pore-water concentration)
North	3.20 (2.68-3.20)	1.41 (1.22-1.41)[a]
Central	2.13 (1.92-2.13)	1.33 (1.11-1.33)
South	2.60 (1.96-2.60)	1.39 (1.29-1.39)

a) Data points with organic matter content of zero were removed from the dataset

The analytical model (Appendix A) is proposed as the basis for the Tier-1 model, and is also the base for the scenario-selection procedure.

2.3. Parameterisation of Tier-2A scenarios

2.3.1. Soil input data

The scenario selection was based on properties of the topsoil (organic matter and texture) as described in EFSA (2010b). However, the fate models also need information about subsoil properties. If the spatial coverage of European soil-profile databases had been 100%, this information could have been directly extracted from this database. As this is not the case, average soil profiles, based on all arable-soil profiles available in the SPADE-1 database, were calculated for the 0-30, 30-50, 50-100 and 100-

200 cm soil layers (cf. FOCUS, 2000). The use of average soil profiles was judged to be acceptable because the evaluation depth for the exposure assessment is only the top 20 cm.

Soil texture was directly assigned to the scenario, using the soil textural class (Table 1 and 2). The depth-dependent organic-matter content of the scenario was calculated by the equation:

$$f_{om} = f_{z,om} f_{om,0} \tag{1}$$

where f_{om} (kg kg^{-1}) is the mass fraction of organic matter, $f_{z,om}$ is the organic matter content relative to the topsoil organic matter content, and $f_{om,0}$ (kg kg^{-1}) is the organic matter content of the topsoil, which has been derived in the scenario-selection procedure (Table 1 and 2).

Soil bulk density was derived from organic matter using the pedotransfer function (EFSA 2010b, *Appendix D;* Tiktak *et al.*, 2002):

$$\rho = 1800 + 1236 f_{om} - 2910\sqrt{f_{om}} \qquad (r^2 = 0.91) \tag{2}$$

where ρ (kg m^{-3}) is the dry bulk density and f_{om} refers to the organic matter content of the soil layer in the scenario. Soil hydraulic functions as required by PEARL were obtained from the soil textural class using the HYPRES pedotransfer rules (Wösten *et al.*, 1999).

PEARL uses a finite-difference method to solve the Richards equation considering the analytical solutions proposed by van Genuchten (1980) with *K(h)* as the unsaturated conductivity.

$$K(h) = K_s\, S_e^{\lambda} \left[1 - \left(1 - S_e^{\frac{n}{n-1}} \right)^{\frac{n-1}{n}} \right]^2 \tag{3}$$

where K_s (m d^{-1}) is the saturated conductivity, S_e (-) the relative saturation and λ and n empirical parameters. The water content is also calculated based on an analytical equation (van Genuchten, 1980):

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^{\frac{n-1}{n}}} \tag{4}$$

where θ (m^3 m^{-3}) is the volume fraction of water, h (cm) is the soil-water pressure head, θ_s (m^3 m^{-3}) is the volume fraction of water at saturation, θ_r (m^3 m^{-3}) is the residual water content in the extremely dry range and α (cm^{-1}) is an empirical parameter of the function developed by van Genuchten (1980).

The same equation is used to calculate the water content at field capacity and the water content at wilting point for PELMO.

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

In order to describe varying concentrations with soil depth, the soil is divided into compartments in the numerical models.For the topsoil, the thickness of the numerical compartments was set to 2 mm for PEARL for the first cm, and 1 cm for the rest of the first soil horizon. Due to different modelling of the top millimetre in both models, for PELMO two numerical compartments were defined in the first cm (1 mm at the soil surface followed by a compartment of 9 mm) and then, as for PEARL, 1 cm for the rest of the first soil horizon. For the 30-100 cm soil layer, the thickness for both models was set to 2.5 cm and for the 100-200 cm soil layer a thickness of 5 cm was chosen.

The dispersion length was set to 2.5 cm (Vanderborght et al., 2007). This value differs from that used in FOCUS (2010) because the evaluation depth is 1-20 cm, whereas the evaluation depth for the FOCUS scenarios is 100 cm. All other soil parameters, including the depth dependence of transformation, were set to default values (FOCUS, 2010).

All relevant soil profile information for the total-soil and the pore-water scenarios is given in Table 5 to Table 7 and Table 8 to Table 10, respectively.

Table 5: Soil-profile description for the Tier-2A scenario "*Total soil, Northern zone*"

Soil property	Unit	Horizon			
		1	2	3	4
Thickness*,#	(cm)	30	30	40	100
Sand content*,#	(%)	83.2	84.4	85.6	85.8
Silt content*,#	(%)	11.6	10.6	10	9.5
Clay content*,#	(%)	5.2	5	4.4	4.7
Organic carbon content#	(%)	6.84	3.42	2.03	0.70
Organic matter content*	(%)	11.8	5.9	3.5	1.2
pH in water	(-)	6.4	6.7	7.3	7.3
θ_s (saturation)*	(m^3 m^{-3})	0.403	0.366	0.366	0.366
θ_r (residual)*	(m^3 m^{-3})	0.025	0.025	0.025	0.025
θ_{fc} (field capacity) #	(m^3 m^{-3})	0.244	0.179	0.179	0.179
θ_{wp} (wilting point) #	(m^3 m^{-3})	0.0585	0.0364	0.0364	0.0364
α*	(cm^{-1})	0.0383	0.043	0.043	0.043
n*	(-)	1.38	1.52	1.52	1.52
$K_{sa}*_{t*}$	(m d^{-1})	0.6	0.7	0.7	0.7
λ*	(-)	1.25	1.25	1.25	1.25
ρ (dry bulk density) *,#	(kg L^{-1})	0.95	1.17	1.30	1.50
Dispersion length*,#	(cm)	2.5	2.5	5	5
Biodegradation factor*,#	(-)	1	0.5	0.3	0

* PEARL input parameter, # PELMO input parameter

Table 6: Soil profile description for the Tier-2A scenario "*Total soil, Central zone*"

Soil property	Unit	Horizon			
		1	2	3	4
Thickness*,#	(cm)	30	30	40	100
Sand content*,#	(%)	83.2	84.4	85.6	85.8
Silt content*,#	(%)	11.6	10.6	10	9.5
Clay content*,#	(%)	5.2	5	4.4	4.7
OC#	(%)	4.99	2.49	1.68	0.46
OM*	(%)	8.6	4.3	2.9	0.8
pH in water	(-)	6.4	6.7	7.3	7.3
θ_s (saturation)*	(m^3 m^{-3})	0.403	0.366	0.366	0.366
θ_r (residual)*	(m^3 m^{-3})	0.025	0.025	0.025	0.025
θ_{fc} (field capacity) #	(m^3 m^{-3})	0.2438	0.1790	0.1790	0.1790
θ_{wp} (wilting point) #	(m^3 m^{-3})	0.0585	0.0364	0.0364	0.0364
α*	(cm^{-1})	0.0383	0.043	0.043	0.043
n*	(-)	1.3774	1.5206	1.5206	1.5206
K_{sat}*	(m d^{-1})	0.6	0.7	0.7	0.7
λ*	(-)	1.25	1.25	1.25	1.25
ρ (dry bulk density) *,#	(kg L^{-1})	1.05	1.25	1.34	1.55
Dispersion length*,#	(cm)	2.5	2.5	5	5
Biodegradation factor*,#	(-)	1	0.5	0.3	0

* PEARL input parameter, # PELMO input parameter

Table 7: Soil-profile description for the Tier-2A scenario "*Total soil, Southern zone*"

Soil property	Unit	Horizon			
		1	2	3	4
Thickness*,#	(cm)	30	30	40	100
Sand content*,#	(%)	8.7	8.6	7.7	7.5
Silt content*,#	(%)	71	68.8	68.4	69.9
Clay content*,#	(%)	20.3	22.6	23.9	22.6
OC#	(%)	2.78	1.39	0.81	0.29
OM*	(%)	4.8	2.4	1.4	0.5
pH in water	(-)	6.4	6.7	7.3	7.3
θ_s (saturation)*	(m^3 m^{-3})	0.43	0.41	0.41	0.41
θ_r (residual)*	(m^3 m^{-3})	0.01	0.01	0.01	0.01
θ_{fc} (field capacity) #	(m^3 m^{-3})	0.3847	0.3714	0.3714	0.3714
θ_{wp} (wilting point) #	(m^3 m^{-3})	0.1324	0.1488	0.1488	0.1488
α*	(cm^{-1})	0.008	0.008	0.008	0.008
n*	(-)	1.254	1.218	1.218	1.218
K_{sat}*	(m d^{-1})	0.023	0.04	0.04	0.04
λ*	(-)	-0.59	0.5	0.5	0.5
ρ (dry bulk density) *,#	(kg L^{-1})	1.22	1.38	1.47	1.60
Dispersion length*,#	(cm)	2.5	2.5	5	5
Biodegradation factor*,#	(-)	1	0.5	0.3	0

* PEARL input parameter, # PELMO input parameter

Table 8: Soil-profile description for the Tier-2A scenario "*Pore water, Northern zone*"

Soil property	Unit	Horizon			
		1	2	3	4
Thickness*,#	(cm)	30	30	40	100
Sand content*,#	(%)	39.5	38.8	40.3	41
Silt content*,#	(%)	41.5	41.1	38.9	38.3
Clay content*,#	(%)	19	20.1	20.8	20.7
OC#	(%)	1.33	0.64	0.41	0.12
OM*	(%)	2.3	1.1	0.7	0.2
pH in water	(-)	6.8	7.1	7.1	7.1
θ_s (saturation)*	(m^3 m^{-3})	0.439	0.392	0.392	0.392
θ_r (residual)*	(m^3 m^{-3})	0.01	0.01	0.01	0.01
θ_{fc} (field capacity) #	(m^3 m^{-3})	0.3469	0.3237	0.3237	0.3237
θ_{wp} (wilting point) #	(m^3 m^{-3})	0.1497	0.1489	0.1489	0.1489
α*	(cm^{-1})	0.0314	0.0249	0.0249	0.0249
n*	(-)	1.1804	1.1689	1.1689	1.1689
K_{sat}*	(m d^{-1})	0.12061	0.10755	0.10755	0.10755
λ*	(-)	-2.42	-0.7437	-0.7437	-0.7437
ρ (dry bulk density) *,#	(kg L^{-1})	1.39	1.51	1.57	1.67
Dispersion length*,#	(cm)	2.5	2.5	5	5
Biodegradation factor*,#	(-)	1	0.5	0.3	0

* PEARL input parameter, # PELMO input parameter

Table 9: Soil-profile description for the Tier-2A scenario "*Pore water, Central zone*"

Soil property	Unit	Horizon			
		1	2	3	4
Thickness*,#	(cm)	30	30	40	100
Sand content*,#	(%)	39.5	38.8	40.3	41
Silt content*,#	(%)	41.5	41.1	38.9	38.3
Clay content*,#	(%)	19	20.1	20.8	20.7
OC#	(%)	1.04	0.52	0.29	0.12
OM*	(%)	1.8	0.9	0.5	0.2
pH in water	(-)	6.8	7.1	7.1	7.1
θ_s (saturation)*	(m^3 m^{-3})	0.439	0.392	0.392	0.392
θ_r (residual)*	(m^3 m^{-3})	0.01	0.01	0.01	0.01
θ_{fc} (field capacity) #	(m^3 m^{-3})	0.3469	0.3237	0.3237	0.3237
θ_{wp} (wilting point) #	(m^3 m^{-3})	0.1497	0.1489	0.1489	0.1489
α*	(cm^{-1})	0.0314	0.0249	0.0249	0.0249
n*	(-)	1.1804	1.1689	1.1689	1.1689
K_{sat}*	(m d^{-1})	0.12061	0.10755	0.10755	0.10755
λ*	(-)	-2.42	-0.7437	-0.7437	-0.7437
ρ (dry bulk density) *,#	(kg L^{-1})	1.43	1.54	1.60	1.67
Dispersion length*,#	(cm)	2.5	2.5	5	5
Biodegradation factor*,#	(-)	1	0.5	0.3	0

* PEARL input parameter, # PELMO input parameter

Table 10: Soil-profile description for the Tier-2A scenario "*Pore water, Southern zone*"

Soil property	Unit	Horizon			
		1	2	3	4
Thickness*,#	(cm)	30	30	40	100
Sand content*,#	(%)	39.5	38.8	40.3	41
Silt content*,#	(%)	41.5	41.1	38.9	38.3
Clay content*,#	(%)	19	20.1	20.8	20.7
OC#	(%)	0.64	0.29	0.17	0.06
OM*	(%)	1.1	0.5	0.3	0.1
pH in water	(-)	6.8	7.1	7.1	7.1
θ_s (saturation)*	($m^3 m^{-3}$)	0.439	0.392	0.392	0.392
θ_r (residual)*	($m^3 m^{-3}$)	0.01	0.01	0.01	0.01
θ_{fc} (field capacity) #	($m^3 m^{-3}$)	0.3469	0.3237	0.3237	0.3237
θ_{wp} (wilting point) #	($m^3 m^{-3}$)	0.1497	0.1489	0.1489	0.1489
α*	(cm^{-1})	0.0314	0.0249	0.0249	0.0249
n*	(-)	1.1804	1.1689	1.1689	1.1689
K_{sat}*	($m\ d^{-1}$)	0.12061	0.10755	0.10755	0.10755
λ*	(-)	-2.42	-0.7437	-0.7437	-0.7437
ρ (dry bulk density) *,#	($kg\ L^{-1}$)	1.51	1.60	1.64	1.71
Dispersion length*,#	(cm)	2.5	2.5	5	5
Biodegradation factor*,#	(-)	1	0.5	0.3	0

* PEARL input parameter, # PELMO input parameter

2.3.2. *Weather input data and irrigation*

The MARS climate database provides daily weather data for the entire EU-27 in a 25x25 km^2 grid. Therefore, daily weather data as needed by the fate models can be directly extracted for the selected scenario locations from the appropriate MARS grid. The MARS database contains all the parameters required for simulation runs with the current fate models, such as minimum and maximum temperature, rainfall, potential evapotranspiration and global radiation. A quality check was performed to check if the dataset contains unrealistic data (see EFSA Panel on Plant Protection Products and their Residues (PPR), 2010 for details). The MARS weather data for the period 1990-2009 were used, converting these to a 66-year time-series using the rules described in FOCUS (2000). However, for the total-soil scenario in the northern zone, the FOCUS weather data "Jokioinen" were used because the respective data set from the MARS database was not complete.

However, the target annual temperatures for the Tier-2A scenarios were based on the WorldClim dataset used because of its higher spatial resolution of 1 km^2. To guarantee consistency between annual and daily temperature data in the Tier-2A scenarios, the daily temperatures of the MARS time series ($T_{day,MARS}$) were scaled such that their mean always meets the annual temperature given in Table 1 and Table 2:

$$T_{day,scenario} = T_{day,MARS} - T_{MARS} + T_{scenario} \quad (5)$$

where $T_{day,scenario}$ is the daily mean temperature in the scenario, $T_{,scenario}$ is the mean annual temperature of the scenarios (Tables 1 and 2), and T_{MARS} is the mean annual temperature of the MARS time series (Table 11).

A crop that is irrigated in the corresponding FOCUS scenario in the same climatic zone is also assumed to be irrigated in the EFSA soil scenario. So, crops are potentially irrigated in the central zone (total-soil and pore-water scenarios) and the southern zone (pore-water scenario only because irrigation is not assumed for the total-soil scenario "Kremsmünster"). That means, for example, that the total-soil scenario in the central zone is potentially irrigated because the respective FOCUS zone is Châteaudun which is a FOCUS scenario where irrigation is included.

Table 11: Overview on climate properties and irrigation handling for the Tier-2A scenarios

Zone	Endpoint	T_{MARS} (°C)	$T_{scenario}$ (°C)	Scaling parameter (°C)	Member state (see Figure 4)	FOCUS climatic zone	Irrigated
North	Total soil	6.15	4.7	-1.45	Estonia	Jokioinen	no
Central	Total soil	9.73	8.0	-1.73	Germany	Chateaudun	yes
South	Total soil	12.35	11.0	-1.34	France	Kremsmünster	no
North	Pore water	8.66	8.2	-0.46	Denmark	Hamburg	no
Central	Pore water	9.76	9.1	-0.66	Czech Rep.	Chateaudun	yes
South	Pore water	13.94	12.8	-1.14	Spain	Sevilla	yes

Climate information for the total-soil and the pore-water scenarios is given in Table 12 to Table 14 and Table 15 to Table 17, respectively.

Table 12: Temperature, seasonal rainfall and potential evapotranspiration (ET pot) for the scenario "*Total soil, Northern zone*""

Year	Temperature (°C)					Rainfall (mm)					ET pot (mm)
	Spring	Summer	Autumn	Winter	Mean	Spring	Summer	Autumn	Winter	Total	Total
1	4.2	14.6	4.7	-5.3	4.6	83.2	330.9	247.4	142.3	803.8	514.4
2	2.0	15.2	6.5	-5.6	4.6	109.7	201.1	107.2	121.0	539.0	548.4
3	2.6	16.1	7.0	-5.2	5.2	104.7	154.5	189.3	109.5	558.0	566.1
4	6.0	15.7	4.7	-4.8	5.4	143.3	171.1	224.8	157.6	696.8	554.2
5	4.8	14.5	5.8	-1.8	5.9	128.6	374.7	217.1	177.4	897.8	533.7
6	4.2	14.4	5.2	-5.7	4.6	58.9	300.1	235.9	154.8	749.7	523.2
7	5.1	13.9	4.3	-2.9	5.1	132.0	235.4	249.4	187.1	803.9	551.0
8	3.4	14.6	5.4	-4.6	4.7	127.1	210.3	172.4	128.6	638.4	533.9
9	4.1	14.9	4.8	-1.2	5.7	119.3	159.5	175.6	173.6	628.0	617.0
10	4.0	12.7	0.3	-5.3	3.0	87.9	244.5	179.8	205.3	717.5	521.9
11	3.6	14.8	4.2	-7.2	3.9	167.5	193.4	198.3	111.6	670.8	539.5
12	4.2	15.5	5.0	-5.1	4.9	196.0	163.3	116.5	184.3	660.1	526.6
13	2.7	14.4	5.3	-9.5	3.3	79.6	106.8	203.9	111.4	501.7	508.0
14	2.4	16.1	3.9	-4.8	4.5	172.6	189.2	257.6	149.3	768.7	537.9
15	3.5	13.9	2.5	-4.0	4.0	164.4	318.2	115.3	149.0	746.9	475.2
16	3.7	16.3	5.7	-5.4	5.1	89.0	198.2	152.4	234.4	674.0	513.1
17	5.0	14.1	6.2	-2.9	5.7	117.4	218.3	171.2	158.4	665.3	508.3
18	3.8	15.9	5.3	-6.5	4.7	180.1	273.4	250.8	138.7	843.0	535.8
19	5.7	16.5	2.5	-5.5	4.9	100.1	192.0	148.9	196.0	637.0	589.7
20	3.5	15.1	5.0	-5.8	4.5	154.9	356.9	116.7	160.9	789.4	528.5
Average	3.9	15.0	4.7	-4.9	4.7	125.8	229.6	186.5	157.6	699.5	536.3

Table 13: Temperature, seasonal rainfall and potential evapotranspiration (ET pot) for the scenario "*Total soil., Central zone*"

Year	Temperature (°C)					Rainfall (mm)					ET pot (mm)
	Spring	Summer	Autumn	Winter	Mean	Spring	Summer	Autumn	Winter	Total	Total
1	6.9	16.0	8.4	-0.6	7.7	154.3	207.1	126.2	132.5	620.1	749.3
2	7.2	15.6	9.2	-1.0	7.8	86.3	157.9	77.8	101.5	423.5	761.3
3	6.3	17.1	11.2	-1.4	8.4	98.9	173.0	103.8	51.2	426.9	809.5
4	9.4	16.7	6.9	2.0	8.8	151.3	263.7	220.2	89.6	724.8	814.7
5	7.5	16.8	8.0	1.6	8.5	126.5	258.8	128.8	102.8	616.9	790.7
6	8.8	16.2	9.0	-2.4	7.9	200.3	182.4	201.4	140.6	724.7	753.9
7	8.5	16.3	7.7	1.1	8.4	114.9	249.1	211.5	81.9	657.4	754.7
8	6.5	15.9	8.6	-1.0	7.5	17.4	112.5	19.8	32.9	182.6	714.5
9	7.6	17.9	7.3	0.2	8.3	123.5	192.5	113.2	97.1	526.3	795.6
10	8.4	14.8	5.8	0.1	7.3	107.3	245.1	136.5	149.9	638.8	765.2
11	7.8	17.4	8.3	0.5	8.6	273.8	201.2	139.7	142.5	757.2	799.2
12	6.6	16.4	8.0	-0.9	7.5	142.8	240.5	120.1	76.4	579.8	749.8
13	5.1	14.8	7.1	-5.0	5.5	91.2	187.1	139.2	49.0	466.5	645.5
14	6.9	16.4	7.2	-0.7	7.5	85.6	194.6	61.5	133.9	475.6	777.5
15	8.2	15.9	6.7	1.3	8.1	129.4	328.2	238.0	72.3	767.9	737.1
16	8.2	16.0	9.0	0.2	8.4	149.3	260.1	131.0	113.6	654.0	670.0
17	9.2	16.3	9.8	1.1	9.1	165.2	149.2	132.3	142.7	589.4	737.5
18	7.2	16.3	8.6	-0.7	7.9	194.5	190.6	197.7	102.1	684.9	723.9
19	7.9	17.5	7.8	0.2	8.4	104.1	217.0	250.4	121.9	693.4	735.4
20	8.2	18.7	7.9	-1.7	8.3	83.7	167.2	99.9	104.4	455.2	867.6
Average	7.6	16.4	8.1	-0.4	8.0	130.0	208.9	142.5	101.9	583.3	757.6

Table 14: Temperature, seasonal rainfall and potential evapotranspiration (ET pot) for the scenario "*Total soil, Southern zone*"

Year	Temperature (°C)					Rainfall (mm)					ET pot (mm)
	Spring	Summer	Autumn	Winter	Mean	Spring	Summer	Autumn	Winter	Total	Total
1	9.1	17.0	11.9	5.1	10.8	131.5	143.4	146.8	159.1	580.8	803.8
2	9.6	17.6	12.2	4.3	11.0	147.4	83.6	208.5	95.1	534.6	813.8
3	9.5	18.4	13.5	3.9	11.4	148.0	69.1	246.1	184.6	647.8	819.8
4	10.8	15.9	10.3	6.4	10.8	211.7	196.8	106.4	187.7	702.6	725.7
5	9.9	16.2	10.3	5.1	10.4	288.1	98.9	202.1	174.3	763.4	755.4
6	9.8	16.5	12.3	3.3	10.5	162.9	151.0	195.4	218.8	728.1	770.4
7	10.7	17.5	11.7	6.1	11.5	109.0	82.3	163.3	226.1	580.7	755.7
8	9.5	16.7	11.5	2.9	10.1	163.3	94.4	219.5	113.0	590.2	626.2
9	10.1	17.1	11.1	4.2	10.7	123.2	118.1	161.3	73.1	475.7	677.1
10	10.0	16.1	9.1	5.8	10.3	124.7	175.3	272.0	112.2	684.2	723.9
11	9.8	17.8	12.0	6.7	11.6	172.3	101.0	233.4	268.0	774.7	744.7
12	9.5	18.2	11.8	5.7	11.3	126.5	70.3	198.6	315.8	711.2	833.4
13	8.7	17.1	10.9	3.7	10.1	129.1	54.7	190.1	150.6	524.5	797.8
14	10.8	17.5	12.3	4.9	11.4	91.5	282.6	123.1	132.3	629.5	800.2
15	10.2	16.0	11.1	5.4	10.7	198.8	149.7	279.2	184.1	811.8	727.4
16	10.9	17.5	11.9	6.0	11.6	193.7	128.1	200.5	302.9	825.2	772.9
17	9.8	17.2	11.8	6.2	11.3	189.7	163.5	302.7	181.9	837.8	740.3
18	10.2	17.5	11.8	4.7	11.1	259.0	143.5	177.9	223.2	803.6	776.7
19	10.3	16.6	12.2	7.2	11.6	174.5	108.8	291.4	196.3	771.0	789.0
20	11.1	19.6	11.9	4.4	11.8	95.2	113.9	222.2	188.5	619.8	889.8
Average	10.0	17.2	11.6	5.1	11.0	162.0	126.5	207.0	184.4	679.9	767.2

Table 15: Temperature, seasonal rainfall and potential evapotranspiration (ET pot) for the scenario "*Pore water, Northern zone*"

Year	Temperature (°C)					Rainfall (mm)					ET pot (mm)
	Spring	Summer	Autumn	Winter	Mean	Spring	Summer	Autumn	Winter	Total	Total
1	7.1	15.1	9.0	0.5	8.0	77.9	204.7	138.2	128.6	549.4	603.4
2	6.1	15.3	9.7	1.0	8.1	96.1	199.0	114.6	117.8	527.5	638.3
3	5.0	17.1	11.5	1.0	8.7	168.5	194.5	203.2	140.1	706.3	634.5
4	8.5	16.1	8.3	2.7	8.9	129.2	343.3	141.8	241.2	855.5	613.3
5	7.4	16.2	9.4	3.0	9.0	149.3	252.0	181.0	138.7	721.0	681.0
6	7.7	16.1	9.4	0.0	8.4	111.6	213.7	196.1	99.1	620.5	688.0
7	8.2	16.1	8.8	3.3	9.1	108.1	110.8	212.5	88.3	519.7	674.0
8	6.2	15.5	9.0	1.0	7.9	95.7	228.6	136.5	89.7	550.5	658.5
9	7.3	17.4	8.1	2.4	8.8	89.6	67.4	173.1	67.5	397.6	776.1
10	7.4	14.3	6.7	1.5	7.5	30.3	198.2	197.8	137.9	564.2	632.6
11	6.5	16.2	8.7	1.4	8.2	131.8	97.1	232.7	186.4	648.0	662.3
12	5.9	16.5	9.1	0.2	8.0	155.5	95.0	151.4	117.6	519.5	669.1
13	4.6	15.2	8.1	-2.8	6.3	104.7	102.9	137.2	27.5	372.3	607.6
14	5.8	17.0	7.9	0.3	7.8	92.5	113.2	155.2	70.9	431.8	665.3
15	7.1	14.3	7.7	1.8	7.7	137.0	158.8	193.1	100.4	589.3	582.2
16	6.9	15.5	9.7	1.0	8.3	95.5	220.3	84.1	144.5	544.4	621.4
17	7.8	14.6	9.9	2.5	8.7	122.9	128.4	166.0	92.8	510.1	601.0
18	5.9	15.7	9.4	0.3	7.9	84.8	189.2	206.8	73.7	554.5	601.1
19	7.7	17.3	7.9	1.5	8.6	91.0	216.4	215.4	145.8	668.6	645.6
20	6.6	16.8	8.3	-0.1	7.9	126.8	147.0	127.5	93.6	494.9	651.0
Average	6.8	15.9	8.8	1.1	8.2	109.9	174.0	168.2	115.1	567.3	645.3

Table 16: Temperature, seasonal rainfall and potential evapotranspiration (ET pot) for the scenario "*Pore water, Central zone*"

Year	Temperature (°C)					Rainfall (mm)					ET pot (mm)
	Spring	Summer	Autumn	Winter	Mean	Spring	Summer	Autumn	Winter	Total	Total
1	8.2	16.8	9.4	1.1	8.9	92.8	181.5	96.6	105.0	475.9	669.6
2	8.2	16.6	10.3	0.8	9.0	112.3	149.9	148.9	125.1	536.2	695.3
3	7.4	18.3	12.6	0.4	9.7	144.4	162.2	90.6	67.2	464.4	756.2
4	10.5	17.7	8.7	3.4	10.1	192.8	251.5	188.5	135.1	767.9	763.1
5	8.7	17.7	9.3	2.9	9.7	135.2	254.7	99.3	113.6	602.8	758.4
6	10.1	17.4	10.2	-0.7	9.3	130.4	156.9	197.2	125.5	610.0	765.3
7	9.8	17.0	9.2	3.1	9.8	65.5	168.5	126.8	116.6	477.4	753.1
8	7.5	15.9	8.6	0.2	8.1	35.4	66.0	42.2	37.9	181.5	650.5
9	9.1	18.9	8.3	1.7	9.6	121.4	191.0	144.0	90.1	546.5	796.0
10	9.7	15.6	6.6	1.2	8.3	132.1	191.7	88.3	142.9	555.0	703.3
11	9.2	18.3	9.3	1.6	9.6	234.6	187.6	127.9	111.4	661.5	693.2
12	7.8	17.7	9.7	0.6	9.0	148.5	118.8	120.1	96.1	483.5	710.2
13	6.6	15.9	8.2	-3.9	6.8	94.0	135.5	137.3	46.0	412.8	631.7
14	8.0	17.9	8.6	0.6	8.8	117.8	172.2	73.7	133.0	496.7	724.2
15	9.3	16.4	7.6	2.6	9.0	136.8	158.0	184.9	57.5	537.2	673.5
16	9.2	16.9	9.9	1.9	9.5	112.6	158.2	55.3	112.9	439.0	642.5
17	10.0	16.4	10.4	2.4	9.8	102.0	172.9	83.1	112.9	470.9	662.8
18	8.1	17.1	9.7	0.3	8.8	119.1	186.7	137.9	135.8	579.5	673.1
19	8.8	17.8	8.5	1.2	9.1	131.6	285.9	168.7	141.1	727.3	669.7
20	8.8	18.9	8.7	-0.4	9.0	63.3	128.8	131.8	83.2	407.1	763.4
Average	8.8	17.3	9.2	1.1	9.1	121.1	173.9	122.2	104.4	521.7	707.8

Table 17: Temperature, seasonal rainfall and potential evapotranspiration (ET pot) for the scenario "*Pore water, Southern zone*"

Year	Temperature (°C)					Rainfall (mm)					ET pot (mm)
	Spring	Summer	Autumn	Winter	Mean	Spring	Summer	Autumn	Winter	Total	Total
1	10.3	22.0	13.9	4.9	12.8	151.1	51.5	110.2	81.0	393.8	1225.1
2	11.1	20.8	11.9	1.2	11.3	83.7	71.6	213.1	48.8	417.2	1290.6
3	12.1	20.8	14.1	2.2	12.3	40.1	67.6	150.4	42.1	300.2	1328.2
4	11.7	20.4	12.0	5.4	12.4	191.3	80.5	25.2	47.9	344.9	1029.0
5	11.0	20.5	11.9	4.9	12.1	204.7	73.1	134.1	107.3	519.2	909.1
6	12.4	23.4	15.0	4.9	14.0	157.4	72.6	141.0	109.9	480.9	1168.7
7	9.8	17.6	11.6	4.6	10.9	98.3	86.8	93.1	38.6	316.8	799.6
8	10.0	20.1	12.8	4.7	11.9	97.6	31.3	184.6	84.0	397.5	1014.8
9	12.3	20.3	13.6	4.5	12.7	39.4	88.7	111.2	28.3	267.6	1134.4
10	11.6	21.2	12.2	5.3	12.6	91.8	21.5	133.1	13.0	259.4	1178.5
11	12.3	21.9	13.8	6.7	13.7	43.6	12.4	138.1	41.1	235.2	1293.1
12	11.9	21.1	14.2	6.8	13.5	64.2	27.7	21.9	60.7	174.5	1360.8
13	11.3	20.3	12.7	6.1	12.6	91.5	71.4	58.1	184.0	405.0	1247.8
14	12.5	20.1	14.6	6.0	13.3	173.8	132.9	60.4	105.1	472.2	1168.6
15	11.8	21.1	13.2	5.4	12.9	66.5	16.8	68.8	35.6	187.7	1270.6
16	12.5	21.5	13.0	5.2	13.1	118.9	74.1	61.6	48.3	302.9	1278.9
17	12.6	21.2	13.7	6.0	13.4	126.8	45.5	168.4	37.8	378.5	1262.7
18	13.4	21.6	13.5	4.8	13.4	144.0	55.8	126.6	67.2	393.6	1290.3
19	11.9	20.5	14.0	6.5	13.2	138.6	94.4	141.8	58.3	433.1	1228.1
20	12.2	23.6	13.6	5.4	13.7	160.4	28.1	221.3	128.4	538.2	1248.8
Average	11.7	21.0	13.3	5.1	12.8	114.2	60.2	118.2	68.4	360.9	1186.4

2.3.3. *Crop data*

Tier-2A scenarios have been developed for a range of annual crops (typically some 15 crops for each scenario). Crop emergence and harvest dates for these crops were taken from FOCUS (2010). Crop development between emergence and harvest is described with phenological crop-development stages having a value of 0 at emergence, 1 at flowering and 2 at maturity, these crop-development stages and crop parameters being available from existing FOCUS scenarios (FOCUS, 2010). The corresponding FOCUS scenario was selected from a map of FOCUS climatic zones (Figure 5). So, with respect to total soil, Jokioinen crop data were used for the northern, Châteaudun crop data for the central and Kremsmünster crop data for the southern scenario. With respect to pore water, Hamburg crop data were used for the northern, Châteaudun crop data for the central and Sevilla crop data for the southern scenario. An overview on the crops considered for the six scenarios is given in Table 19.

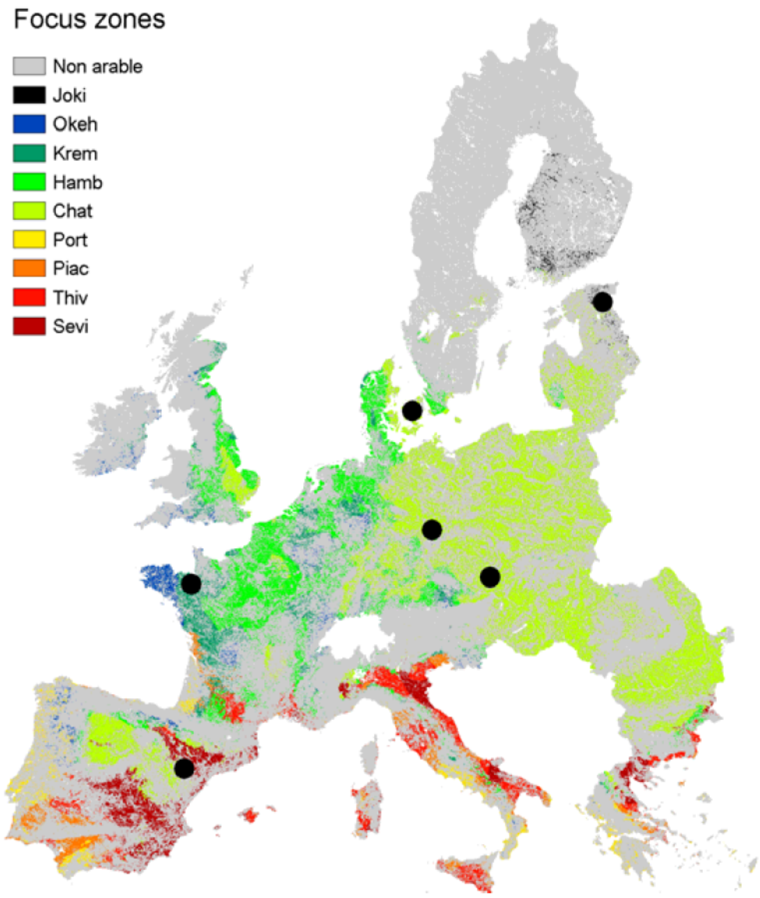

Figure 5: Climatic zones according to the definition given in FOCUS (2000). The dots correspond to the position of the six Tier-2A scenarios.

However, if only the exact FOCUS climatic zone had been used for selecting crops, important crops would have been missing in the soil scenarios. Therefore, an additional crop list was defined based on FOCUS climatic zones that do not meet the climate of the EFSA soil scenario but are representative for the respective political zone (Table 18).

Table 18: Representativeness of the FOCUS climatic zones in the three political zones

Political zone	FOCUS climatic zone	Size (km²)	Fraction of EU (%)	Proportion in zone (%)
North	Chateaudun	40771	4.09	58.85
	Hamburg	17168	1.72	24.75
	Jokioinen	9893	0.99	14.24
	Kremsmünster	1485	0.15	2.16
Central	Chateaudun	367436	36.84	77.17
	Hamburg	80164	8.04	16.84
	Jokioinen	44	0.00	0.00
	Kremsmünster	23463	2.35	4.92
	Okehampton	5057	0.51	1.07
South	Chateaudun	79918	8.01	17.68
	Hamburg	92715	9.30	20.53
	Jokioinen	2	0.00	0.00
	Kremsmünster	43631	4.37	9.64
	Okehampton	16444	1.65	3.64
	Piacenza	42355	4.25	9.38
	Porto	29867	2.99	6.60
	Sevilla	75529	7.57	16.71
	Thiva	71521	7.17	15.82
Total		997463	100.00	

Based on the information in Table 18, further crops are listed in Table 19 and in the column "additional crops" for the total-soil and the pore-water scenarios, respectively; the warm FOCUS climatic scenarios (Piacenza, Porto, Sevilla and Thiva) are not representative for the central political zone. As sunflower and soybean scenarios were not defined by the FOCUS group for the moderate FOCUS climatic zones (Hamburg, Chateaudun, Kremsmünster, Okehampton), these scenarios could not be included in the crop list for the central political zone. However, the CAPRI project (Leip et al., 2008) showed that these crops have at least some importance in the central zone (see also Figure 6 and Figure 7).

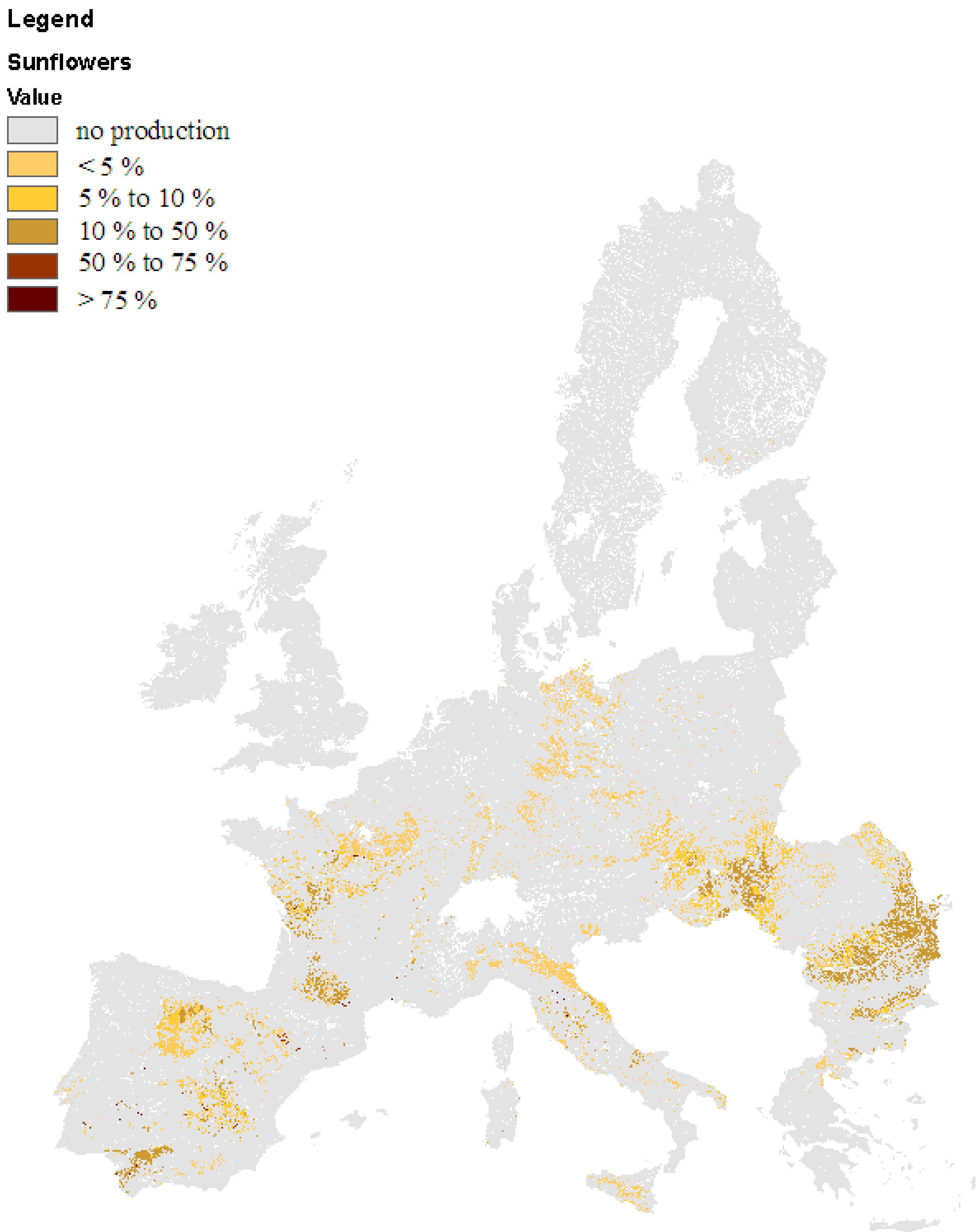

Figure 6: Distribution of sunflower production in the EU (Leip et al., 2008)

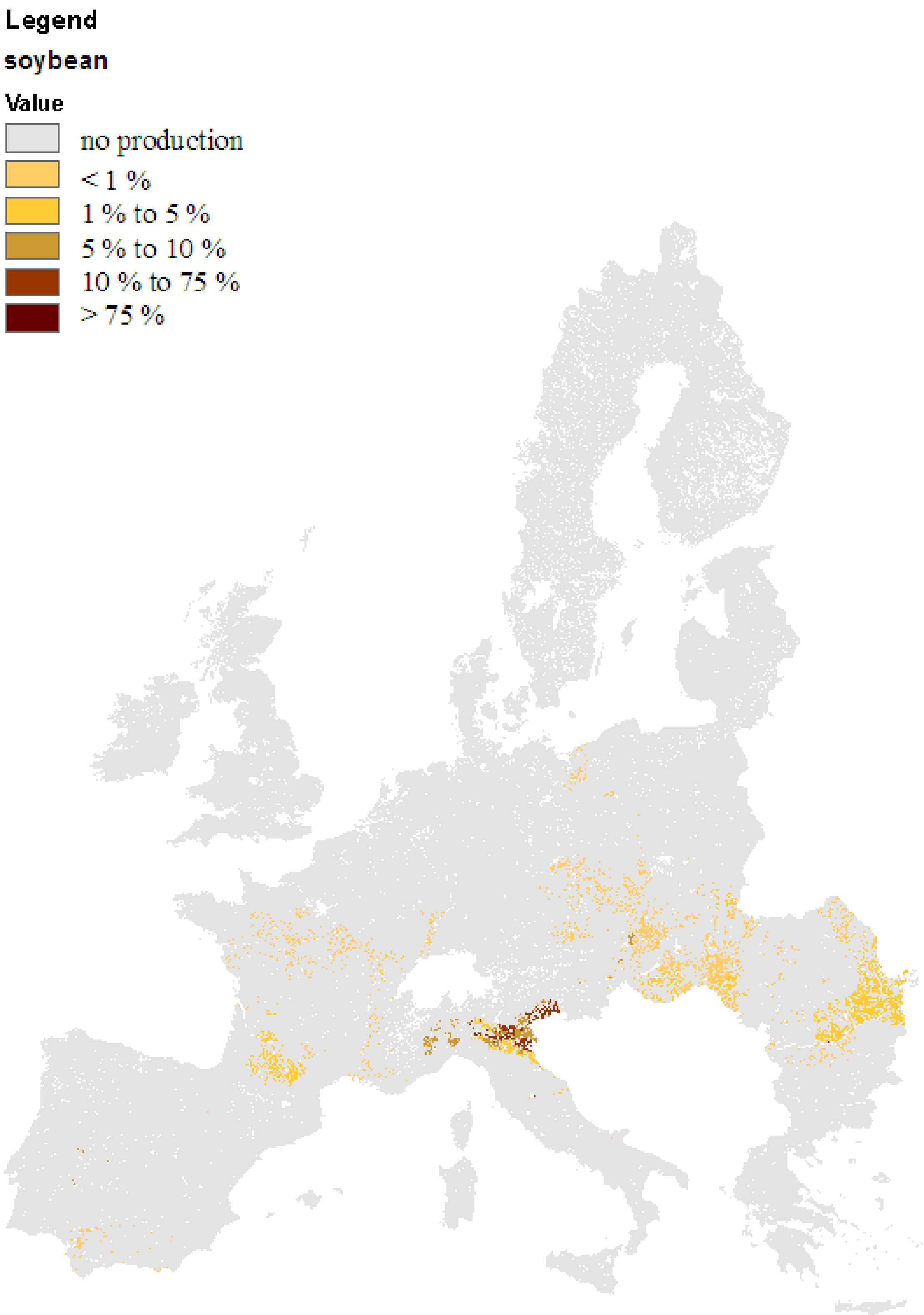

Figure 7: Distribution of soybean production in the EU (Leip et al., 2008)

Therefore these crops were finally added to the crop list for the central zone using the Piacenza crop data as the source (see Table 19).

Table 19: FOCUS crops available for the scenarios

Scenario	FOCUS climatic zone	Primary FOCUS crops	Source of additional FOCUS crops	Additional crops
Total soil Zone North	Jokioinen	sugar beet winter cereals cabbage oilseed rape (summer) onion peas (animal feed) spring cereals	Hamburg	beans (field) maize oilseed rape (winter)
Total soil Zone Central	Chateaudun	sugar beet winter cereals cabbage carrots maize oilseed rape (winter) onion peas (animal feed) spring cereals tomatoes	Piacenza	sunflower soybean
Total soil Zone South	Kremsmünster	sugar beet winter cereals cabbage carrots maize oilseed rape (winter) onion spring cereals	Piacenza	tomato sunflower soybean tobacco
Pore water Zone North	Hamburg	sugar beet winter cereals beans (field) cabbage carrots maize oilseed rape (winter) onion peas (animal feed) spring cereals	Jokioinen	oilseed rape (summer)
Pore water Zone Central	Chateaudun	sugar beet winter cereals cabbage carrots maize oilseed rape (winter) onion peas (animal feed) spring cereals tomato	Piacenza	sunflower soybean
Pore water Zone South	Sevilla	sugar beet winter cereals cabbage cotton maize sunflower tomato	Piacenza Thiva	oilseed rape (winter) soybean tobacco beans (vegetables) onions

As already mentioned, a crop that is irrigated in the corresponding FOCUS scenario in the same climatic zone is assumed also to be irrigated in the EFSA soil scenario. So, crops are potentially irrigated in the CTC, CLC and CLS scenarios. If there is a choice between irrigated and non-irrigated, then take the decision made in Table 11.

Ploughing is assumed to occur one month before crop emergence for all locations and all crops because all scenario soils have medium to coarse soil texture. Early ploughing in the preceding winter is assumed to occur only for heavy clay soils.

PELMO and PEARL need to correct standard data on potential evapotranspiration for individual crop stages; the required Kc factors (Table 20) are calculated for the differing growth stages and Leaf Area Index (LAI) by the procedure described in FOCUS (2009).

Table 20: Correction factors (Kc) for potential transpiration used by PEARL and PELMO for the different crop stages

Crop	Harvest to emergence	Emergence to max LAI	Max LAI to senescence	Senescence to harvest
Beans (field)	1	1.05	1.1	0.7
Beans (vegetables)	1	1.05	1.1	0.7
Cabbage	1	1.05	1.1	0.93
Cotton	1	1.08	1.15	0.9
Maize	1	1.05	1.1	0.83
Rape	1	1.00	1.0	0.93
Peas (animals)	1	1.05	1.1	1.05
Cereals	1	1.05	1.1	0.7
Sugar beet	1	1.05	1.1	0.85
Sunflower	1	1.05	1.1	0.75
Tobacco	1	1.00	1.0	0.93

2.3.4. *Runoff and soil erosion*

As a conservative approach, runoff and soil erosion of substance are not considered as additional processes which may reduce pesticide concentration in soil.

2.3.5. *Crop extrapolation factors*

The same crop extrapolation factors were considered for Tier 2A as has already been explained for Tier 1. Safety factors are available for major and minor crops as shown in Table 3 and Table 4, respectively. The major crops are listed in Table 21.

Table 21: CAPRI crops available for the scenarios

Crop
Barley
Durum wheat
Common wheat
Oats
Rye
Other cereals
Maize
Dry pulses
Rape and turnip rape
Sunflower
Soybean
Other oilseed crops and fibre
Sugar beet
Other fodder on arable land
Other root crops
Tomatoes and other fresh vegetables
Floriculture
Tobacco
Other non-permanent industrial crops
Other crops

3. Results of test runs using the scenarios to compare PELMO and PEARL

3.1. Pesticide input data and application pattern

In order to have a sufficient overview of the Tier-2A simulations and to calibrate the Tier-1 scenarios, the test runs covered all relevant substance properties and all evaluation depths. This is especially important because of the non-linearity of the relation between soil parameters, substance fate parameters and predicted environmental concentrations, as shown in EFSA (2010b).

Therefore, the following general principles were considered for the test simulations:

- Test runs were performed for a set of 19 substances with different properties (Figure 8) with respect to the key parameters sorption (K_{om}) and degradation (*DegT50*). The compounds that belong to the red area in the figure were considered not relevant because due to their properties it is expected that they would exceed the trigger of 0.1 µg L^{-1} in groundwater. Although K_{om} is known to increase as the soil becomes air dry, this was not considered in the present calculations with the numerical models in which K_{om} was taken to be constant. This is expected to lead to a conservative estimate of the PEC in the soil pore water. Therefore the calibration factor for Tier 1 that will be derived from these calculations is expected to be also on the conservative side.
- In order to check the Tier-2A simulations also for transformation products, all example pesticides formed the same single metabolite (molecular mass 250 g mol^{-1}, formation fraction 25%, *DegT50* of 100 d and K_{om} of 50 L kg^{-1}). Only a single metabolite was considered given the limited time available. It is expected that the behaviour of metabolites is already covered by the range of parent compounds considered.
- Two crops were considered, winter cereals (not irrigated) and sugar beet (irrigated)
- A single application of 1 kg ha^{-1} every year for 26 years on 1 day before emergence of the crop.

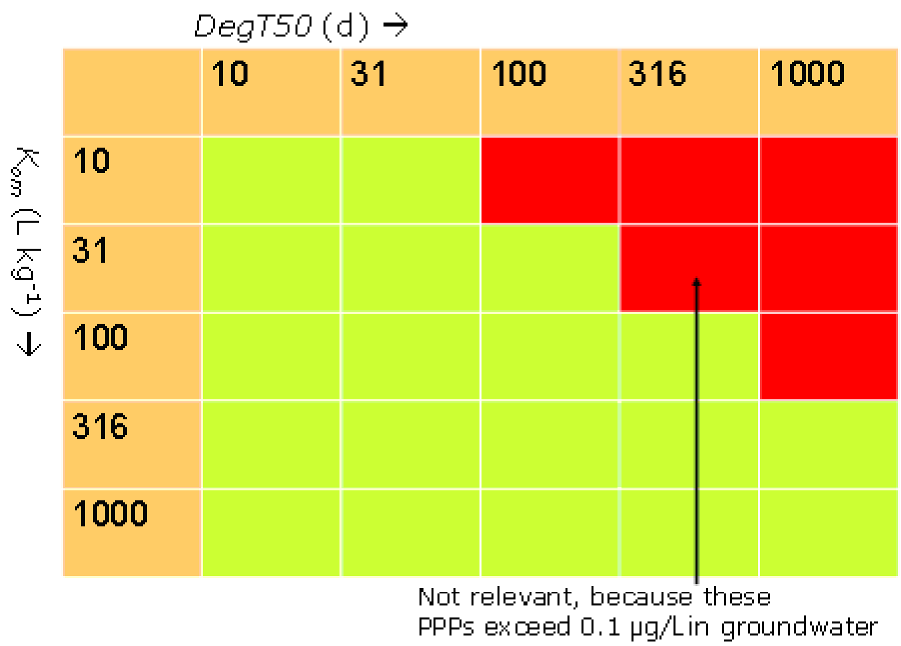

Figure 8: Sorption and degradation data of the 25 substances, of which 19 substances (those in the green area) were used for testing the scenarios.

The remaining pesticide input parameters are summarised (Table 22):

Table 22: Pesticide input parameters used for the test simulations

Parameter	Unit	Value
Molar mass	(g mol^{-1})	300
Solubility in water	(mg L^{-1})	90
Molar enthalpy of dissolution	(kJ mol^{-1})	27
Vapour pressure at 20°C	(mPa)	0.1
Molar enthalpy of vaporisation	(kJ mol^{-1})	95
pKa (if acid or base)	(-)	not considered
Diffusion coefficient in water	(m^2 d^{-1})	4.3 * 10^{-5}
Gas diffusion coefficient	(m^2 d^{-1})	0.43
Reference temperature for degradation, vaporisation and dissolution	(°C)	20
Reference soil moisture for degradation	(-)	at 10 kPa (field capacity)
Factor for the adjustment of degradation rate at different depths	(-)	standard*
Q10-factor (increase of degradation rate with an increase of temperature of 10°C)	(-)	2.58
Arrhenius activation energy	(kJ mol^{-1})	65.4
B (exponent of degradation - moisture relationship according to Walker)	(-)	0.7
Sorption to soil organic carbon (K_{oc})	(dm^3 kg^{-1})	K_{oc} = 1.724 * K_{om}
Exponent of the Freundlich isotherm	(-)	0.9
Non-equilibrium sorption	(-)	not considered
TSCF = transpiration stream concentration factor	(-)	0.5
Number of applications per year	(-)	1
Applied dose	(kg ha^{-1})	1
Incorporation depth	(cm)	0.2

* as given in the scenario

3.2. Endpoints considered in the comparison

For the reason mentioned previously (Chapter 3.1), the test runs also included multiple evaluation depths according to the following scheme:

– All test runs were performed for both endpoints (the concentration in total soil and the concentration in the pore water) including all political zones both for the peak values and TWA-values for windows of 14 and 56 d and considering two evaluation depths (1 cm and 20 cm).

3.3. Results of Tier-2A simulations calculated with PEARL and PELMO

In the following tables, the presented concentrations are calculated by PEARL and PELMO to analyse what differences between the models are to be expected when performing Tier-2A simulations. The simulations cover ecologically relevant depths of 1 cm and 20 cm and include the global maximum concentrations as well as time-weighted average concentrations over 14 d and 56 d.

The results for the total-soil scenarios and the pore-water scenarios in winter cereals for a depth of 1 cm are presented in Table 23 to Table 25 and Table 26 to Table 28, respectively.

For the total-soil scenarios, both models simulated nearly the same concentration independent of the political zone. Similar agreement was found for the pore-water scenarios with respect to the global maximum concentrations (TWA 0). However, the TWA values over 14 d and 56 d for the southern European scenario differed between the two models by up to a factor of two in some exceptional cases. These differences were found especially for rapidly degrading and weakly sorbing compounds. The background to these differences is explained in more detail later (Figure 12 to Figure 15); the differences were considered acceptable in view of the high number of simulation results that were similar for both models.

Table 23: Comparison of PEC_{soil} simulated by PEARL and PELMO for total soil, northern zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 1 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	10.58	10.40	1.02	7.48	9.12	0.82	2.83	3.77	0.75
2	31	10	10.64	10.50	1.01	8.00	9.73	0.82	3.28	4.24	0.77
3	10	31	10.58	10.40	1.02	8.99	9.40	0.96	3.88	4.33	0.90
4	31	31	10.67	10.50	1.02	9.72	10.10	0.96	4.69	5.03	0.93
5	100	31	11.01	10.70	1.03	10.21	10.44	0.98	5.18	5.38	0.96
6	10	100	10.58	10.40	1.02	9.53	9.50	1.00	5.06	5.17	0.98
7	31	100	10.68	10.60	1.01	10.22	10.21	1.00	6.35	6.25	1.02
8	100	100	11.15	11.00	1.01	10.89	10.79	1.01	7.37	7.17	1.03
9	316	100	12.07	11.60	1.04	11.83	11.45	1.03	8.36	7.84	1.07
10	10	316	10.58	10.40	1.02	9.70	9.54	1.02	6.94	6.22	1.12
11	31	316	10.68	10.60	1.01	10.36	10.26	1.01	8.20	7.76	1.06
12	100	316	11.20	11.20	1.00	11.08	10.96	1.01	9.52	9.10	1.05
13	316	316	12.49	12.40	1.01	12.44	12.30	1.01	11.11	10.52	1.06
14	1000	316	14.63	14.10	1.04	14.58	13.90	1.05	13.26	12.20	1.09
15	10	1000	10.58	10.40	1.02	9.83	9.60	1.02	8.08	7.09	1.14
16	31	1000	10.68	10.60	1.01	10.39	10.28	1.01	9.64	8.79	1.10
17	100	1000	11.22	11.20	1.00	11.13	11.08	1.00	10.62	10.08	1.05
18	316	1000	12.70	12.80	0.99	12.66	12.71	1.00	12.30	11.98	1.03
19	1000	1000	15.82	15.90	1.00	15.75	15.50	1.02	15.35	14.92	1.03

Table 24: Comparison of PEC_{soil} simulated by PEARL and PELMO for total soil, central zone ($1\ kg\ ha^{-1}$ the day before emergence of winter cereals, every year), ecologically relevant depth 1 cm

Substance	*DegT50*	*Kom*	TWA 0 d ($\mu g\ kg^{-1}$)			TWA 14 d ($\mu g\ kg^{-1}$)			TWA 56 d ($\mu g\ kg^{-1}$)		
	(d)	($L\ kg^{-1}$)	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	9.51	9.47	1.00	8.85	8.30	1.07	3.84	3.24	1.18
2	31	10	9.55	9.52	1.00	9.10	8.75	1.04	4.19	3.67	1.14
3	10	31	9.51	9.50	1.00	9.14	8.57	1.07	5.24	4.43	1.18
4	31	31	9.56	9.55	1.00	9.40	9.07	1.04	5.81	5.20	1.12
5	100	31	9.82	9.80	1.00	9.74	9.43	1.03	6.22	5.63	1.10
6	10	100	9.51	9.52	1.00	9.18	8.74	1.05	7.02	5.79	1.21
7	31	100	9.56	9.56	1.00	9.45	9.25	1.02	7.92	6.98	1.14
8	100	100	9.88	9.91	1.00	9.83	9.73	1.01	8.52	7.70	1.11
9	316	100	10.67	10.50	1.02	10.58	10.37	1.02	9.24	8.35	1.11
10	10	316	9.51	9.52	1.00	9.19	8.81	1.04	7.83	6.61	1.18
11	31	316	9.56	9.56	1.00	9.46	9.32	1.01	8.91	8.08	1.10
12	100	316	9.91	9.96	1.00	9.86	9.85	1.00	9.61	8.99	1.07
13	316	316	10.93	10.90	1.00	10.91	10.76	1.01	10.54	9.98	1.06
14	1000	316	12.90	12.60	1.02	12.81	12.29	1.04	12.07	10.79	1.12
15	10	1000	9.51	9.52	1.00	9.20	8.91	1.03	7.89	7.22	1.09
16	31	1000	9.57	9.56	1.00	9.46	9.34	1.01	9.00	8.49	1.06
17	100	1000	9.93	9.99	0.99	9.88	9.89	1.00	9.72	9.47	1.03
18	316	1000	11.04	11.20	0.99	11.03	11.11	0.99	10.85	10.60	1.02
19	1000	1000	13.59	13.90	0.98	13.53	13.72	0.99	13.44	13.13	1.02

Table 25: Comparison of PEC_{soil} simulated by PEARL and PELMO for total soil, southern zone ($1\ kg\ ha^{-1}$ the day before emergence of winter cereals, every year), ecologically relevant depth 1 cm

Substance	*DegT50*	*Kom*	TWA 0 d ($\mu g\ kg^{-1}$)			TWA 14 d ($\mu g\ kg^{-1}$)			TWA 56 d ($\mu g\ kg^{-1}$)		
	(d)	($L\ kg^{-1}$)	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	8.19	7.96	1.03	4.73	5.52	0.86	1.68	1.51	1.11
2	31	10	8.20	8.08	1.02	5.06	6.10	0.83	2.01	1.70	1.18
3	10	31	8.19	8.01	1.02	5.91	6.14	0.96	2.33	1.99	1.17
4	31	31	8.21	8.12	1.01	6.37	6.84	0.93	2.84	2.48	1.15
5	100	31	8.36	8.21	1.02	6.62	7.12	0.93	3.15	2.69	1.17
6	10	100	8.19	8.03	1.02	6.98	6.59	1.06	3.39	2.97	1.14
7	31	100	8.22	8.14	1.01	7.59	7.39	1.03	4.25	3.88	1.10
8	100	100	8.42	8.31	1.01	7.96	7.79	1.02	4.76	4.33	1.10
9	316	100	8.91	8.59	1.04	8.48	8.13	1.04	5.26	4.59	1.15
10	10	316	8.19	8.04	1.02	7.22	6.85	1.05	4.54	4.15	1.09
11	31	316	8.22	8.15	1.01	7.86	7.64	1.03	5.91	5.36	1.10
12	100	316	8.45	8.36	1.01	8.30	8.10	1.02	6.66	6.12	1.09
13	316	316	9.11	8.93	1.02	9.05	8.73	1.04	7.43	6.71	1.11
14	1000	316	10.40	9.84	1.06	10.36	9.68	1.07	8.62	7.40	1.17
15	10	1000	8.19	8.07	1.01	7.32	6.99	1.05	5.21	4.93	1.06
16	31	1000	8.22	8.15	1.01	7.88	7.73	1.02	6.92	6.43	1.08
17	100	1000	8.46	8.39	1.01	8.33	8.20	1.02	7.85	7.27	1.08
18	316	1000	9.22	9.11	1.01	9.18	9.00	1.02	8.81	8.15	1.08
19	1000	1000	11.06	10.80	1.02	11.04	10.76	1.03	10.60	9.67	1.10

Table 26: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, northern zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 1 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 14 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 56 d (µg kg^{-1}) PEARL	PELMO	Ratio
1	10	10	19.76	20.60	0.96	8.62	11.29	0.76	2.89	3.08	0.94
2	31	10	19.77	20.90	0.95	9.02	11.83	0.76	3.38	3.28	1.03
3	10	31	10.30	9.24	1.11	5.36	5.80	0.92	1.90	1.75	1.08
4	31	31	10.31	9.36	1.10	5.65	6.12	0.92	2.27	2.11	1.07
5	100	31	10.43	9.43	1.11	5.83	6.24	0.93	2.47	2.27	1.09
6	10	100	3.72	3.12	1.19	2.44	2.30	1.06	1.04	0.98	1.06
7	31	100	3.73	3.16	1.18	2.61	2.45	1.06	1.26	1.23	1.03
8	100	100	3.81	3.21	1.19	2.74	2.54	1.08	1.41	1.35	1.04
9	316	100	3.98	3.28	1.21	2.90	2.61	1.11	1.57	1.43	1.10
10	10	316	1.14	0.93	1.23	0.88	0.77	1.15	0.47	0.42	1.13
11	31	316	1.14	0.94	1.22	0.95	0.83	1.15	0.59	0.54	1.09
12	100	316	1.17	0.96	1.21	1.00	0.87	1.15	0.66	0.61	1.09
13	316	316	1.25	1.02	1.23	1.09	0.93	1.17	0.76	0.67	1.12
14	1000	316	1.36	1.11	1.23	1.20	0.99	1.20	0.87	0.74	1.18
15	10	1000	0.33	0.26	1.24	0.27	0.23	1.17	0.19	0.16	1.18
16	31	1000	0.33	0.27	1.23	0.29	0.25	1.17	0.22	0.19	1.16
17	100	1000	0.34	0.28	1.22	0.31	0.26	1.16	0.25	0.22	1.13
18	316	1000	0.36	0.30	1.20	0.34	0.29	1.15	0.29	0.25	1.14
19	1000	1000	0.42	0.36	1.18	0.39	0.34	1.15	0.35	0.30	1.15

Table 27: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, central zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 1 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 14 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 56 d (µg kg^{-1}) PEARL	PELMO	Ratio
1	10	10	27.35	28.50	0.96	15.65	15.98	0.98	4.82	4.86	0.99
2	31	10	27.36	28.70	0.95	16.24	17.10	0.95	5.24	5.33	0.98
3	10	31	13.67	12.50	1.09	8.80	8.73	1.01	2.95	2.98	0.99
4	31	31	13.68	12.60	1.09	9.18	9.39	0.98	3.28	3.34	0.98
5	100	31	13.83	12.70	1.09	9.50	9.65	0.98	3.52	3.48	1.01
6	10	100	4.80	4.14	1.16	3.59	3.39	1.06	1.50	1.44	1.04
7	31	100	4.81	4.18	1.15	3.76	3.65	1.03	1.71	1.66	1.03
8	100	100	4.90	4.25	1.15	3.93	3.79	1.03	1.85	1.78	1.04
9	316	100	5.07	4.34	1.17	4.13	3.90	1.06	2.01	1.86	1.08
10	10	316	1.45	1.22	1.19	1.22	1.07	1.14	0.67	0.60	1.11
11	31	316	1.46	1.23	1.18	1.28	1.15	1.11	0.78	0.72	1.08
12	100	316	1.49	1.26	1.18	1.34	1.21	1.10	0.85	0.78	1.08
13	316	316	1.57	1.33	1.18	1.43	1.29	1.11	0.94	0.85	1.11
14	1000	316	1.71	1.41	1.21	1.56	1.37	1.14	1.05	0.92	1.14
15	10	1000	0.41	0.35	1.20	0.37	0.31	1.18	0.25	0.21	1.16
16	31	1000	0.42	0.35	1.19	0.38	0.33	1.15	0.30	0.26	1.14
17	100	1000	0.42	0.36	1.18	0.40	0.35	1.14	0.33	0.29	1.14
18	316	1000	0.45	0.39	1.16	0.43	0.39	1.12	0.37	0.33	1.13
19	1000	1000	0.53	0.46	1.15	0.50	0.45	1.11	0.43	0.37	1.16

Table 28: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, southern zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 1 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	33.25	37.40	0.89	19.89	31.27	0.64	6.76	12.06	0.56
2	31	10	33.28	37.80	0.88	20.86	33.14	0.63	7.65	14.25	0.54
3	10	31	18.96	18.80	1.01	12.48	16.42	0.76	4.62	7.47	0.62
4	31	31	18.98	19.00	1.00	13.15	17.45	0.75	5.28	9.31	0.57
5	100	31	19.17	19.10	1.00	13.50	17.81	0.76	5.65	10.05	0.56
6	10	100	7.37	6.78	1.09	5.62	6.14	0.91	2.49	3.49	0.71
7	31	100	7.37	6.85	1.08	5.95	6.53	0.91	2.89	4.43	0.65
8	100	100	7.48	6.93	1.08	6.18	6.70	0.92	3.14	4.85	0.65
9	316	100	7.77	7.06	1.10	6.45	6.82	0.95	3.43	5.07	0.68
10	10	316	2.32	2.06	1.13	1.93	1.89	1.02	1.13	1.29	0.88
11	31	316	2.33	2.08	1.12	2.05	2.02	1.02	1.35	1.62	0.83
12	100	316	2.37	2.12	1.12	2.13	2.08	1.02	1.47	1.79	0.82
13	316	316	2.50	2.22	1.13	2.28	2.17	1.05	1.64	1.93	0.85
14	1000	316	2.71	2.35	1.15	2.51	2.30	1.09	1.86	2.05	0.91
15	10	1000	0.67	0.59	1.14	0.58	0.54	1.08	0.42	0.43	0.97
16	31	1000	0.67	0.60	1.13	0.62	0.58	1.08	0.50	0.50	1.00
17	100	1000	0.69	0.61	1.12	0.65	0.60	1.08	0.55	0.56	0.98
18	316	1000	0.73	0.66	1.12	0.70	0.65	1.08	0.61	0.62	0.99
19	1000	1000	0.84	0.76	1.11	0.81	0.75	1.08	0.72	0.69	1.04

The results for the total-soil scenarios and the pore-water scenarios in winter cereals for a depth of 20 cm are presented in Table 29 to Table 31 and Table 32 to Table 34, respectively.

Looking at Tables 23 to 28, it can be concluded that both models simulated nearly the same concentration independent of both the political zone and the endpoint (total soil/pore water and TWA0/TWA14/TWA56).

Table 29: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, northern zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	0.53	0.52	1.01	0.48	0.47	1.03	0.40	0.35	1.14
2	31	10	0.58	0.60	0.97	0.56	0.57	0.98	0.49	0.48	1.02
3	10	31	0.53	0.52	1.01	0.49	0.48	1.02	0.41	0.37	1.09
4	31	31	0.62	0.64	0.96	0.60	0.62	0.96	0.53	0.54	0.98
5	100	31	0.95	0.95	1.00	0.94	0.93	1.00	0.88	0.87	1.01
6	10	100	0.53	0.52	1.01	0.49	0.48	1.02	0.41	0.38	1.07
7	31	100	0.63	0.64	0.98	0.61	0.62	0.97	0.55	0.55	0.99
8	100	100	1.09	1.14	0.96	1.08	1.13	0.96	1.03	1.08	0.96
9	316	100	2.00	1.93	1.04	1.99	1.92	1.04	1.95	1.88	1.04
10	10	316	0.53	0.52	1.01	0.49	0.48	1.02	0.41	0.38	1.07
11	31	316	0.63	0.64	0.98	0.61	0.62	0.98	0.55	0.56	0.99
12	100	316	1.15	1.23	0.93	1.14	1.22	0.93	1.09	1.18	0.93
13	316	316	2.44	2.55	0.96	2.43	2.54	0.96	2.39	2.50	0.96
14	1000	316	4.57	4.50	1.02	4.56	4.49	1.02	4.52	4.44	1.02
15	10	1000	0.53	0.52	1.02	0.49	0.48	1.02	0.41	0.38	1.07
16	31	1000	0.63	0.64	0.99	0.61	0.62	0.99	0.56	0.56	1.00
17	100	1000	1.17	1.26	0.93	1.16	1.26	0.93	1.12	1.21	0.92
1			2.64	2.83	0.94	2.64	2.81	0.94	2.60	2.78	0.94
8	316	1000									
19	1000	1000	5.77	6.03	0.96	5.76	6.01	0.96	5.72	5.98	0.96

Table 30: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, central zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	0.48	0.48	1.00	0.45	0.43	1.04	0.38	0.35	1.09
2	31	10	0.52	0.53	0.97	0.50	0.51	0.98	0.47	0.46	1.03
3	10	31	0.48	0.48	1.00	0.46	0.44	1.03	0.39	0.37	1.06
4	31	31	0.53	0.55	0.96	0.52	0.54	0.97	0.49	0.49	0.99
5	100	31	0.79	0.79	0.99	0.78	0.78	1.00	0.76	0.76	1.01
6	10	100	0.48	0.48	1.00	0.46	0.45	1.03	0.39	0.37	1.05
7	31	100	0.53	0.55	0.97	0.52	0.54	0.97	0.50	0.50	1.00
8	100	100	0.85	0.89	0.95	0.84	0.89	0.95	0.82	0.87	0.95
9	316	100	1.64	1.58	1.03	1.64	1.58	1.03	1.62	1.56	1.04
10	10	316	0.48	0.48	1.00	0.46	0.45	1.03	0.39	0.38	1.05
11	31	316	0.53	0.54	0.98	0.53	0.53	0.99	0.50	0.50	1.01
12	100	316	0.88	0.96	0.92	0.87	0.95	0.92	0.85	0.93	0.91
13	316	316	1.90	2.05	0.93	1.89	2.05	0.92	1.88	2.03	0.92
14	1000	316	3.86	3.91	0.99	3.85	3.90	0.99	3.84	3.88	0.99
15	10	1000	0.48	0.48	1.00	0.46	0.45	1.03	0.40	0.38	1.05
16	31	1000	0.54	0.54	0.99	0.53	0.53	1.00	0.50	0.49	1.02
17	100	1000	0.89	0.97	0.92	0.89	0.97	0.91	0.87	0.95	0.91
18	316	1000	2.01	2.24	0.90	2.01	2.23	0.90	1.99	2.22	0.90
19	1000	1000	4.56	5.03	0.91	4.55	5.02	0.91	4.53	5.00	0.91

Table 31: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, southern zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	0.41	0.41	1.00	0.37	0.34	1.08	0.26	0.24	1.11
2	31	10	0.42	0.42	1.01	0.40	0.38	1.05	0.35	0.33	1.08
3	10	31	0.41	0.41	1.00	0.37	0.35	1.05	0.27	0.25	1.04
4	31	31	0.43	0.43	1.00	0.41	0.40	1.02	0.37	0.35	1.05
5	100	31	0.59	0.55	1.07	0.58	0.53	1.09	0.53	0.49	1.09
6	10	100	0.41	0.41	1.00	0.37	0.35	1.04	0.27	0.26	1.01
7	31	100	0.44	0.43	1.00	0.41	0.40	1.02	0.37	0.36	1.03
8	100	100	0.65	0.63	1.03	0.63	0.61	1.04	0.60	0.58	1.05
9	316	100	1.12	1.00	1.12	1.12	0.99	1.12	1.07	0.95	1.13
10	10	316	0.41	0.41	1.00	0.37	0.36	1.03	0.27	0.27	1.00
11	31	316	0.44	0.43	1.01	0.41	0.40	1.02	0.37	0.37	1.02
12	100	316	0.67	0.65	1.03	0.65	0.64	1.03	0.63	0.61	1.04
13	316	316	1.34	1.28	1.05	1.33	1.27	1.05	1.30	1.24	1.05
14	1000	316	2.61	2.26	1.16	2.61	2.26	1.16	2.57	2.22	1.16
15	10	1000	0.41	0.41	1.00	0.37	0.36	1.03	0.27	0.27	1.00
16	31	1000	0.44	0.43	1.02	0.41	0.40	1.03	0.37	0.37	1.02
17	100	1000	0.68	0.66	1.03	0.67	0.64	1.04	0.64	0.62	1.04
18	316	1000	1.45	1.41	1.02	1.44	1.40	1.02	1.42	1.38	1.03
19	1000	1000	3.30	3.19	1.03	3.29	3.18	1.04	3.26	3.15	1.04

Table 32: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, northern zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	0.99	1.03	0.96	0.74	0.76	0.97	0.57	0.53	1.06
2	31	10	1.00	1.05	0.96	0.82	0.82	1.00	0.70	0.64	1.10
3	10	31	0.51	0.46	1.11	0.37	0.37	1.01	0.29	0.26	1.09
4	31	31	0.53	0.47	1.12	0.41	0.40	1.02	0.35	0.32	1.08
5	100	31	0.66	0.53	1.26	0.56	0.46	1.22	0.50	0.41	1.23
6	10	100	0.19	0.16	1.19	0.14	0.13	1.05	0.10	0.10	1.07
7	31	100	0.19	0.16	1.19	0.16	0.15	1.05	0.13	0.12	1.05
8	100	100	0.27	0.22	1.23	0.23	0.20	1.14	0.21	0.18	1.14
9	316	100	0.41	0.31	1.33	0.37	0.29	1.28	0.36	0.28	1.28
10	10	316	0.06	0.05	1.23	0.04	0.04	1.10	0.03	0.03	1.08
11	31	316	0.06	0.05	1.24	0.05	0.05	1.09	0.04	0.04	1.06
12	100	316	0.09	0.07	1.19	0.08	0.07	1.11	0.07	0.06	1.09
13	316	316	0.16	0.13	1.20	0.15	0.13	1.15	0.14	0.13	1.15
14	1000	316	0.26	0.21	1.27	0.25	0.20	1.25	0.25	0.20	1.24
15	10	1000	0.02	0.01	1.24	0.01	0.01	1.15	0.01	0.01	1.10
16	31	1000	0.02	0.01	1.24	0.02	0.01	1.14	0.01	0.01	1.08
17	100	1000	0.03	0.02	1.17	0.02	0.02	1.11	0.02	0.02	1.08
18	316	1000	0.05	0.04	1.12	0.05	0.04	1.09	0.05	0.04	1.08
19	1000	1000	0.10	0.09	1.09	0.10	0.09	1.08	0.10	0.09	1.07

Table 33: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, central zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	1.37	1.43	0.96	1.10	0.84	1.31	0.74	0.58	1.27
2	31	10	1.40	1.44	0.97	1.19	0.92	1.30	0.93	0.72	1.30
3	10	31	0.68	0.63	1.09	0.53	0.45	1.19	0.36	0.32	1.14
4	31	31	0.71	0.64	1.11	0.59	0.51	1.16	0.47	0.40	1.17
5	100	31	0.87	0.69	1.26	0.76	0.65	1.16	0.66	0.57	1.16
6	10	100	0.24	0.21	1.16	0.19	0.17	1.12	0.13	0.12	1.07
7	31	100	0.25	0.21	1.18	0.21	0.19	1.11	0.17	0.16	1.08
8	100	100	0.33	0.28	1.20	0.30	0.27	1.10	0.26	0.24	1.08
9	316	100	0.49	0.39	1.24	0.45	0.39	1.18	0.42	0.36	1.17
10	10	316	0.07	0.06	1.19	0.06	0.05	1.14	0.04	0.04	1.07
11	31	316	0.08	0.06	1.21	0.07	0.06	1.13	0.06	0.05	1.07
12	100	316	0.10	0.09	1.15	0.10	0.09	1.09	0.09	0.08	1.06
13	316	316	0.18	0.16	1.15	0.17	0.15	1.10	0.16	0.15	1.08
14	1000	316	0.31	0.25	1.24	0.30	0.24	1.22	0.29	0.24	1.22
15	10	1000	0.02	0.02	1.20	0.02	0.02	1.18	0.01	0.01	1.10
16	31	1000	0.02	0.02	1.20	0.02	0.02	1.16	0.02	0.02	1.09
17	100	1000	0.03	0.03	1.14	0.03	0.03	1.10	0.03	0.02	1.06
18	316	1000	0.06	0.05	1.07	0.06	0.05	1.04	0.05	0.05	1.02
19	1000	1000	0.12	0.12	1.07	0.12	0.11	1.06	0.12	0.11	1.05

Table 34: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, southern zone (1 kg ha^{-1} the day before emergence of winter cereals, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	1.66	1.87	0.89	1.40	1.56	0.90	0.90	0.94	0.96
2	31	10	1.69	1.90	0.88	1.49	1.66	0.90	1.10	1.10	1.00
3	10	31	0.95	0.94	1.01	0.76	0.82	0.92	0.51	0.54	0.94
4	31	31	0.96	0.96	1.01	0.81	0.88	0.93	0.63	0.63	0.99
5	100	31	1.14	1.06	1.08	0.92	0.94	0.98	0.78	0.75	1.04
6	10	100	0.37	0.34	1.09	0.29	0.31	0.96	0.21	0.23	0.92
7	31	100	0.38	0.35	1.09	0.32	0.33	0.96	0.25	0.26	0.96
8	100	100	0.47	0.41	1.16	0.40	0.38	1.05	0.35	0.34	1.02
9	316	100	0.73	0.55	1.32	0.65	0.53	1.24	0.59	0.49	1.20
10	10	316	0.12	0.10	1.13	0.10	0.09	1.02	0.07	0.07	0.95
11	31	316	0.12	0.11	1.13	0.10	0.10	1.03	0.09	0.09	0.96
12	100	316	0.16	0.13	1.18	0.14	0.13	1.07	0.12	0.12	1.01
13	316	316	0.28	0.23	1.20	0.26	0.22	1.15	0.24	0.21	1.13
14	1000	316	0.47	0.38	1.22	0.45	0.38	1.19	0.44	0.37	1.19
15	10	1000	0.03	0.03	1.14	0.03	0.03	1.07	0.02	0.02	0.99
16	31	1000	0.03	0.03	1.14	0.03	0.03	1.08	0.03	0.03	0.98
17	100	1000	0.05	0.04	1.16	0.04	0.04	1.09	0.04	0.04	1.02
18	316	1000	0.09	0.08	1.13	0.08	0.08	1.10	0.08	0.07	1.08
19	1000	1000	0.18	0.16	1.12	0.18	0.16	1.12	0.18	0.16	1.10

The results for the total-soil scenarios and the pore-water scenarios in sugar beet for a depth of 1 cm are presented in Table 35 to Table 37 and Table 38 to Table 40, respectively.

The comparison for sugar beet leads to nearly the same conclusions as for winter cereals: for the total-soil scenarios, both models simulated nearly the same concentration independent of the political zone. Similar agreement was found for the pore-water scenarios with respect to the global maximum concentrations (TWA 0). However, in contrast to winter cereals there is better agreement for the porewater TWA values over 14 d and 56 d in the southern European scenario whereas less agreement was found for the TWA over 14 and 56 d in the respective northern and central European scenarios.

Table 35: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, northern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 1 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	10.58	10.40	1.02	8.11	9.32	0.87	2.94	3.13	0.94
2	31	10	10.62	10.50	1.01	8.70	9.99	0.87	3.43	3.54	0.97
3	10	31	10.58	10.40	1.02	9.33	9.44	0.99	3.74	3.53	1.06
4	31	31	10.67	10.60	1.01	10.07	10.15	0.99	4.52	4.18	1.08
5	100	31	10.99	10.80	1.02	10.56	10.47	1.01	5.03	4.49	1.12
6	10	100	10.58	10.40	1.02	9.54	9.48	1.01	4.85	4.15	1.17
7	31	100	10.69	10.60	1.01	10.29	10.21	1.01	6.19	5.20	1.19
8	100	100	11.17	11.00	1.02	10.95	10.75	1.02	7.26	5.91	1.23
9	316	100	12.10	11.70	1.03	11.82	11.41	1.04	8.09	6.49	1.25
10	10	316	10.58	10.40	1.02	9.57	9.50	1.01	5.92	5.19	1.14
11	31	316	10.70	10.60	1.01	10.31	10.25	1.01	8.02	6.98	1.15
12	100	316	11.24	11.10	1.01	11.07	10.93	1.01	9.54	8.21	1.16
13	316	316	12.58	12.50	1.01	12.51	12.23	1.02	10.83	9.60	1.13
14	1000	316	14.66	14.30	1.03	14.65	14.15	1.04	13.02	11.26	1.16
15	10	1000	10.58	10.50	1.01	9.58	9.50	1.01	6.45	5.87	1.10
16	31	1000	10.70	10.60	1.01	10.32	10.25	1.01	8.88	8.16	1.09
17	100	1000	11.27	11.20	1.01	11.12	11.01	1.01	10.45	9.72	1.07
18	316	1000	12.81	12.90	0.99	12.76	12.66	1.01	12.34	11.63	1.06
19	1000	1000	15.91	16.00	0.99	15.86	15.90	1.00	15.52	14.65	1.06

Table 36: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, central zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 1 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (μg kg^{-1})			TWA 14 d (μg kg^{-1})			TWA 56 d (μg kg^{-1})		
			PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	9.51	9.39	1.01	8.42	8.47	0.99	2.97	2.44	1.22
2	31	10	9.51	9.46	1.01	8.61	8.93	0.96	3.18	2.59	1.23
3	10	31	9.51	9.42	1.01	9.11	8.68	1.05	3.78	2.98	1.27
4	31	31	9.53	9.49	1.00	9.34	9.18	1.02	4.16	3.28	1.27
5	100	31	9.69	9.58	1.01	9.53	9.41	1.01	4.38	3.43	1.28
6	10	100	9.51	9.44	1.01	9.18	8.76	1.05	4.86	3.94	1.23
7	31	100	9.54	9.52	1.00	9.42	9.27	1.02	5.54	4.55	1.22
8	100	100	9.81	9.75	1.01	9.72	9.64	1.01	5.99	4.94	1.21
9	316	100	10.39	10.10	1.03	10.30	10.06	1.02	6.51	5.30	1.23
10	10	316	9.51	9.44	1.01	9.19	8.90	1.03	6.14	5.17	1.19
11	31	316	9.54	9.53	1.00	9.43	9.30	1.01	7.26	6.23	1.17
12	100	316	9.85	9.83	1.00	9.77	9.75	1.00	7.94	6.88	1.15
13	316	316	10.69	10.60	1.01	10.66	10.56	1.01	8.75	7.61	1.15
14	1000	316	12.18	11.80	1.03	12.18	11.80	1.03	9.85	8.30	1.19
15	10	1000	9.51	9.46	1.00	9.20	8.98	1.02	6.85	6.10	1.12
16	31	1000	9.54	9.53	1.00	9.43	9.34	1.01	8.34	7.56	1.10
17	100	1000	9.86	9.87	1.00	9.79	9.78	1.00	9.20	8.42	1.09
18	316	1000	10.84	10.80	1.00	10.81	10.80	1.00	10.24	9.37	1.09
19	1000	1000	13.09	13.10	1.00	13.05	13.00	1.00	12.41	11.25	1.10

Table 37: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, southern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 1 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (μg kg^{-1})			TWA 14 d (μg kg^{-1})			TWA 56 d (μg kg^{-1})		
			PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	8.19	8.06	1.02	4.28	6.61	0.65	1.47	1.93	0.76
2	31	10	8.20	8.13	1.01	4.58	7.01	0.65	1.95	2.13	0.92
3	10	31	8.19	8.08	1.01	5.52	6.87	0.80	2.01	2.30	0.87
4	31	31	8.21	8.16	1.01	5.95	7.32	0.81	2.74	2.85	0.96
5	100	31	8.37	8.27	1.01	6.24	7.54	0.83	3.15	3.10	1.01
6	10	100	8.19	8.09	1.01	6.84	7.15	0.96	2.88	2.98	0.97
7	31	100	8.22	8.17	1.01	7.42	7.64	0.97	4.09	4.02	1.02
8	100	100	8.44	8.37	1.01	7.84	7.96	0.98	4.82	4.57	1.05
9	316	100	8.93	8.71	1.02	8.39	8.33	1.01	5.38	4.90	1.10
10	10	316	8.19	8.09	1.01	7.22	7.33	0.99	3.95	3.64	1.08
11	31	316	8.22	8.18	1.00	7.86	7.84	1.00	5.47	5.16	1.06
12	100	316	8.46	8.41	1.01	8.32	8.22	1.01	6.46	6.06	1.07
13	316	316	9.16	9.05	1.01	9.09	8.89	1.02	7.37	6.78	1.09
14	1000	316	10.40	9.96	1.04	10.29	9.81	1.05	8.59	7.60	1.13
15	10	1000	8.19	8.09	1.01	7.27	7.40	0.98	4.51	4.17	1.08
16	31	1000	8.22	8.18	1.00	7.90	7.92	1.00	6.49	5.93	1.10
17	100	1000	8.48	8.43	1.01	8.37	8.32	1.01	7.66	7.11	1.08
18	316	1000	9.28	9.22	1.01	9.24	9.16	1.01	8.70	8.13	1.07
19	1000	1000	11.13	10.80	1.03	11.08	10.71	1.03	10.47	9.79	1.07

Table 38: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, northern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 1 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
			PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	23.71	23.90	0.99	10.61	20.62	0.51	4.69	7.06	0.66
2	31	10	23.73	24.30	0.98	11.12	22.18	0.50	6.27	7.91	0.79
3	10	31	11.31	9.91	1.14	6.02	8.73	0.69	2.71	3.63	0.74
4	31	31	11.33	10.00	1.13	6.39	9.43	0.68	3.63	4.70	0.77
5	100	31	11.45	10.10	1.13	6.62	9.67	0.68	4.20	5.18	0.81
6	10	100	3.85	3.20	1.20	2.67	2.86	0.93	1.27	1.54	0.82
7	31	100	3.86	3.24	1.19	2.83	3.09	0.92	1.73	2.09	0.83
8	100	100	3.94	3.31	1.19	2.97	3.20	0.93	2.04	2.38	0.85
9	316	100	4.07	3.40	1.20	3.16	3.26	0.97	2.29	2.53	0.91
10	10	316	1.15	0.94	1.23	0.94	0.84	1.12	0.51	0.52	0.99
11	31	316	1.16	0.95	1.22	1.00	0.91	1.10	0.72	0.72	1.00
12	100	316	1.18	0.98	1.21	1.05	0.95	1.11	0.85	0.84	1.02
13	316	316	1.27	1.05	1.21	1.15	1.01	1.14	0.97	0.93	1.05
14	1000	316	1.37	1.13	1.21	1.26	1.09	1.16	1.08	0.99	1.08
15	10	1000	0.33	0.26	1.24	0.28	0.24	1.19	0.17	0.15	1.10
16	31	1000	0.33	0.27	1.23	0.30	0.26	1.18	0.24	0.21	1.12
17	100	1000	0.34	0.28	1.21	0.32	0.27	1.17	0.28	0.25	1.12
18	316	1000	0.37	0.31	1.19	0.35	0.30	1.16	0.32	0.29	1.12
19	1000	1000	0.42	0.36	1.17	0.41	0.36	1.14	0.38	0.32	1.16

Table 39: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, central zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 1 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
			PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	22.99	29.30	0.78	11.34	19.90	0.57	3.82	5.04	0.76
2	31	10	22.99	29.70	0.77	11.94	21.89	0.55	4.28	5.57	0.77
3	10	31	12.45	12.60	0.99	7.20	9.36	0.77	2.56	2.53	1.01
4	31	31	12.45	12.70	0.98	7.61	10.39	0.73	2.92	2.87	1.02
5	100	31	12.47	12.80	0.97	7.78	10.74	0.72	3.07	3.00	1.03
6	10	100	4.64	4.13	1.12	3.35	3.48	0.96	1.34	1.02	1.32
7	31	100	4.64	4.19	1.11	3.57	3.77	0.95	1.58	1.20	1.31
8	100	100	4.68	4.24	1.10	3.69	3.91	0.94	1.71	1.28	1.33
9	316	100	4.74	4.28	1.11	3.79	3.96	0.96	1.79	1.31	1.36
10	10	316	1.44	1.21	1.19	1.17	1.08	1.08	0.57	0.39	1.47
11	31	316	1.44	1.23	1.17	1.25	1.17	1.07	0.70	0.48	1.47
12	100	316	1.46	1.26	1.16	1.30	1.21	1.07	0.77	0.53	1.46
13	316	316	1.52	1.31	1.16	1.37	1.26	1.09	0.84	0.57	1.48
14	1000	316	1.59	1.36	1.17	1.44	1.30	1.11	0.91	0.60	1.51
15	10	1000	0.41	0.34	1.20	0.35	0.31	1.14	0.20	0.15	1.36
16	31	1000	0.41	0.35	1.19	0.38	0.34	1.13	0.26	0.19	1.33
17	100	1000	0.42	0.36	1.17	0.39	0.35	1.12	0.29	0.22	1.32
18	316	1000	0.45	0.39	1.16	0.42	0.38	1.11	0.32	0.25	1.31
19	1000	1000	0.50	0.43	1.15	0.48	0.42	1.13	0.37	0.27	1.34

Table 40: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, southern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 1 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 14 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 56 d (µg kg^{-1}) PEARL	PELMO	Ratio
1	10	10	51.52	37.80	1.36	28.48	30.94	0.92	9.17	10.60	0.87
2	31	10	51.52	38.10	1.35	29.32	33.10	0.89	9.81	12.41	0.79
3	10	31	23.95	18.90	1.27	15.88	16.21	0.98	5.44	6.04	0.90
4	31	31	23.95	19.00	1.26	16.41	17.40	0.94	5.89	7.36	0.80
5	100	31	23.97	19.10	1.26	16.62	17.79	0.93	6.08	7.86	0.77
6	10	100	8.03	6.79	1.18	6.24	6.04	1.03	2.49	2.68	0.93
7	31	100	8.03	6.86	1.17	6.47	6.49	1.00	2.77	3.32	0.83
8	100	100	8.08	6.93	1.17	6.61	6.66	0.99	2.91	3.59	0.81
9	316	100	8.17	7.01	1.17	6.74	6.73	1.00	3.01	3.70	0.81
10	10	316	2.39	2.06	1.16	2.05	1.86	1.10	1.04	0.98	1.06
11	31	316	2.39	2.08	1.15	2.14	2.01	1.07	1.19	1.26	0.95
12	100	316	2.42	2.13	1.14	2.20	2.07	1.06	1.28	1.39	0.92
13	316	316	2.50	2.22	1.13	2.30	2.12	1.08	1.40	1.47	0.95
14	1000	316	2.60	2.30	1.13	2.41	2.17	1.11	1.53	1.53	1.00
15	10	1000	0.68	0.59	1.15	0.61	0.53	1.14	0.38	0.32	1.18
16	31	1000	0.68	0.60	1.14	0.64	0.57	1.11	0.45	0.43	1.05
17	100	1000	0.69	0.61	1.13	0.66	0.60	1.10	0.50	0.48	1.05
18	316	1000	0.72	0.65	1.11	0.70	0.63	1.10	0.56	0.53	1.06
19	1000	1000	0.80	0.73	1.10	0.78	0.71	1.09	0.63	0.58	1.10

The results for the total-soil scenarios and the pore-water scenarios in winter cereals for a depth of 20 cm are presented in Table 35 to Table 37 and Table 38 to Table 40, respectively.

Looking at the tables, it can be concluded that both models simulated nearly the same concentration independent of both the political zone and the endpoint (total soil/pore water and TWA0/TWA14/TWA56).

Table 41: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, northern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 20 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 14 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 56 d (µg kg^{-1}) PEARL	PELMO	Ratio
1	10	10	0.53	0.52	1.01	0.46	0.47	1.00	0.30	0.30	0.99
2	31	10	0.57	0.55	1.03	0.53	0.51	1.05	0.44	0.42	1.05
3	10	31	0.53	0.52	1.02	0.47	0.47	1.00	0.31	0.31	1.00
4	31	31	0.62	0.62	1.00	0.59	0.58	1.01	0.50	0.48	1.03
5	100	31	0.92	0.85	1.07	0.90	0.83	1.09	0.83	0.76	1.09
6	10	100	0.53	0.53	1.01	0.48	0.47	1.01	0.32	0.31	1.02
7	31	100	0.64	0.63	1.01	0.61	0.60	1.02	0.52	0.51	1.02
8	100	100	1.11	1.09	1.02	1.09	1.06	1.03	1.02	0.99	1.03
9	316	100	2.00	1.84	1.09	1.99	1.82	1.09	1.92	1.75	1.09
10	10	316	0.53	0.52	1.01	0.48	0.48	1.01	0.32	0.31	1.04
11	31	316	0.65	0.64	1.00	0.62	0.62	1.01	0.53	0.52	1.01
12	100	316	1.19	1.21	0.98	1.17	1.20	0.98	1.10	1.12	0.98
13	316	316	2.52	2.55	0.99	2.51	2.53	0.99	2.43	2.46	0.99
14	1000	316	4.60	4.46	1.03	4.59	4.45	1.03	4.54	4.40	1.03
15	10	1000	0.53	0.53	1.01	0.48	0.48	1.01	0.33	0.31	1.04
16	31	1000	0.65	0.65	1.00	0.62	0.62	1.00	0.53	0.52	1.01
17	100	1000	1.22	1.26	0.97	1.21	1.25	0.97	1.13	1.17	0.97
18	316	1000	2.77	2.89	0.96	2.75	2.87	0.96	2.69	2.81	0.96
19	1000	1000	5.86	6.04	0.97	5.85	6.03	0.97	5.80	5.98	0.97

Table 42: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, central zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 20 cm

Substance	*DegT50* (d)	*Kom* (L kg^{-1})	TWA 0 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 14 d (µg kg^{-1}) PEARL	PELMO	Ratio	TWA 56 d (µg kg^{-1}) PEARL	PELMO	Ratio
1	10	10	0.48	0.48	1.00	0.45	0.44	1.02	0.33	0.31	1.08
2	31	10	0.48	0.48	1.01	0.47	0.46	1.01	0.41	0.38	1.08
3	10	31	0.48	0.47	1.00	0.46	0.45	1.02	0.34	0.33	1.05
4	31	31	0.50	0.50	1.00	0.49	0.48	1.01	0.43	0.42	1.03
5	100	31	0.66	0.64	1.03	0.65	0.62	1.05	0.60	0.55	1.09
6	10	100	0.48	0.48	1.00	0.46	0.45	1.02	0.35	0.33	1.04
7	31	100	0.51	0.51	1.00	0.50	0.50	1.01	0.45	0.44	1.01
8	100	100	0.78	0.77	1.02	0.78	0.76	1.02	0.73	0.71	1.04
9	316	100	1.34	1.23	1.09	1.33	1.22	1.10	1.30	1.17	1.11
10	10	316	0.48	0.48	1.00	0.46	0.45	1.02	0.35	0.33	1.04
11	31	316	0.51	0.52	1.00	0.50	0.50	1.00	0.45	0.45	1.01
12	100	316	0.82	0.83	0.99	0.81	0.82	0.99	0.77	0.78	1.00
13	316	316	1.66	1.65	1.00	1.65	1.64	1.01	1.62	1.61	1.01
14	1000	316	3.14	2.94	1.07	3.14	2.94	1.07	3.12	2.90	1.07
15	10	1000	0.48	0.48	1.00	0.46	0.45	1.02	0.35	0.33	1.04
16	31	1000	0.51	0.51	1.00	0.50	0.50	1.00	0.45	0.45	1.01
17	100	1000	0.83	0.85	0.98	0.83	0.84	0.98	0.79	0.80	0.99
18	316	1000	1.81	1.84	0.98	1.80	1.84	0.98	1.77	1.80	0.98
19	1000	1000	4.06	4.09	0.99	4.05	4.08	0.99	4.02	4.05	0.99

Table 43: Comparison of PEC_{soil} simulated by PEARL and PELMO for the total-soil scenario, southern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	0.41	0.41	1.00	0.36	0.36	0.99	0.22	0.20	1.13
2	31	10	0.42	0.41	1.02	0.40	0.39	1.01	0.32	0.28	1.16
3	10	31	0.41	0.41	1.00	0.36	0.37	0.98	0.23	0.21	1.07
4	31	31	0.43	0.42	1.02	0.41	0.41	1.00	0.34	0.31	1.09
5	100	31	0.58	0.52	1.12	0.57	0.51	1.12	0.52	0.44	1.19
6	10	100	0.41	0.41	1.00	0.36	0.37	0.98	0.23	0.22	1.03
7	31	100	0.44	0.43	1.02	0.42	0.41	1.01	0.35	0.33	1.04
8	100	100	0.66	0.60	1.09	0.65	0.59	1.09	0.60	0.54	1.10
9	316	100	1.14	0.96	1.19	1.13	0.95	1.19	1.10	0.91	1.21
10	10	316	0.41	0.41	1.00	0.36	0.37	0.98	0.23	0.23	1.01
11	31	316	0.44	0.43	1.03	0.42	0.42	1.01	0.35	0.34	1.02
12	100	316	0.68	0.64	1.06	0.67	0.64	1.06	0.63	0.60	1.06
13	316	316	1.38	1.28	1.08	1.38	1.27	1.08	1.34	1.24	1.08
14	1000	316	2.62	2.23	1.17	2.61	2.23	1.17	2.59	2.20	1.18
15	10	1000	0.41	0.41	1.00	0.36	0.37	0.98	0.23	0.23	1.01
16	31	1000	0.44	0.43	1.03	0.42	0.41	1.02	0.35	0.35	1.02
17	100	1000	0.69	0.66	1.06	0.69	0.65	1.05	0.65	0.61	1.05
18	316	1000	1.50	1.44	1.04	1.49	1.44	1.04	1.46	1.41	1.04
19	1000	1000	3.35	3.21	1.04	3.34	3.20	1.04	3.32	3.18	1.04

Table 44: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, northern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	1.19	1.20	0.99	0.88	1.03	0.85	0.53	0.51	1.04
2	31	10	1.21	1.23	0.98	0.97	1.11	0.87	0.76	0.66	1.15
3	10	31	0.57	0.50	1.14	0.42	0.44	0.95	0.25	0.24	1.06
4	31	31	0.59	0.52	1.13	0.46	0.47	0.98	0.36	0.33	1.10
5	100	31	0.70	0.59	1.19	0.60	0.53	1.13	0.52	0.42	1.25
6	10	100	0.19	0.16	1.20	0.15	0.14	1.04	0.09	0.09	1.05
7	31	100	0.20	0.17	1.19	0.17	0.16	1.06	0.13	0.12	1.05
8	100	100	0.28	0.22	1.24	0.25	0.21	1.16	0.22	0.19	1.18
9	316	100	0.41	0.31	1.33	0.38	0.30	1.28	0.36	0.27	1.33
10	10	316	0.06	0.05	1.23	0.05	0.04	1.13	0.03	0.03	1.08
11	31	316	0.06	0.05	1.22	0.05	0.05	1.14	0.04	0.04	1.06
12	100	316	0.09	0.07	1.21	0.08	0.07	1.15	0.07	0.06	1.13
13	316	316	0.16	0.13	1.21	0.16	0.13	1.18	0.15	0.13	1.18
14	1000	316	0.26	0.20	1.29	0.26	0.20	1.27	0.25	0.20	1.28
15	10	1000	0.02	0.01	1.24	0.01	0.01	1.17	0.01	0.01	1.10
16	31	1000	0.02	0.01	1.23	0.02	0.01	1.18	0.01	0.01	1.12
17	100	1000	0.03	0.02	1.18	0.02	0.02	1.15	0.02	0.02	1.11
18	316	1000	0.05	0.05	1.13	0.05	0.05	1.12	0.05	0.04	1.10
19	1000	1000	0.11	0.10	1.11	0.11	0.10	1.10	0.10	0.09	1.10

Table 45: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, central zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	0.96	1.15	0.84	0.92	1.02	0.90	0.55	0.45	1.23
2	31	10	0.98	1.15	0.85	0.98	1.13	0.86	0.71	0.58	1.24
3	10	31	0.49	0.62	0.79	0.48	0.48	0.98	0.29	0.24	1.20
4	31	31	0.50	0.62	0.80	0.51	0.54	0.94	0.38	0.32	1.19
5	100	31	0.51	0.64	0.81	0.53	0.56	0.95	0.44	0.36	1.21
6	10	100	0.19	0.23	0.82	0.18	0.17	1.03	0.11	0.10	1.15
7	31	100	0.19	0.23	0.83	0.19	0.19	1.02	0.15	0.13	1.12
8	100	100	0.24	0.27	0.89	0.23	0.22	1.06	0.20	0.17	1.17
9	316	100	0.31	0.34	0.91	0.31	0.26	1.19	0.28	0.22	1.27
10	10	316	0.06	0.07	0.90	0.06	0.05	1.08	0.04	0.03	1.15
11	31	316	0.07	0.07	0.93	0.06	0.06	1.06	0.05	0.04	1.10
12	100	316	0.09	0.09	1.02	0.08	0.08	1.06	0.07	0.07	1.06
13	316	316	0.15	0.15	1.04	0.14	0.12	1.13	0.13	0.11	1.15
14	1000	316	0.22	0.22	1.01	0.21	0.17	1.25	0.20	0.16	1.29
15	10	1000	0.02	0.02	1.02	0.02	0.02	1.14	0.01	0.01	1.17
16	31	1000	0.02	0.02	1.05	0.02	0.02	1.12	0.01	0.01	1.11
17	100	1000	0.03	0.03	1.17	0.03	0.02	1.08	0.02	0.02	1.04
18	316	1000	0.06	0.05	1.21	0.05	0.05	1.08	0.05	0.04	1.06
19	1000	1000	0.11	0.10	1.14	0.10	0.09	1.12	0.09	0.08	1.12

Table 46: Comparison of PEC_{soil} simulated by PEARL and PELMO for pore water, southern zone (1 kg ha^{-1} the day before emergence of sugar beet, every year), ecologically relevant depth 20 cm

Substance	*DegT50*	*Kom*	TWA 0 d (µg kg^{-1})			TWA 14 d (µg kg^{-1})			TWA 56 d (µg kg^{-1})		
	(d)	(L kg^{-1})	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio	PEARL	PELMO	Ratio
1	10	10	2.58	1.89	1.36	1.88	1.55	1.21	1.08	0.84	1.29
2	31	10	2.58	1.91	1.35	1.95	1.66	1.18	1.27	1.01	1.26
3	10	31	1.20	0.95	1.27	0.91	0.81	1.13	0.56	0.47	1.19
4	31	31	1.20	0.95	1.26	0.95	0.87	1.09	0.67	0.58	1.15
5	100	31	1.22	0.96	1.26	0.98	0.90	1.09	0.73	0.63	1.15
6	10	100	0.40	0.34	1.18	0.33	0.30	1.09	0.21	0.19	1.10
7	31	100	0.29	0.35	0.83	0.28	0.33	0.85	0.24	0.24	1.00
8	100	100	0.44	0.38	1.15	0.39	0.36	1.07	0.31	0.30	1.06
9	316	100	0.53	0.44	1.21	0.46	0.42	1.11	0.40	0.36	1.11
10	10	316	0.12	0.10	1.16	0.10	0.09	1.12	0.07	0.06	1.09
11	31	316	0.12	0.11	1.14	0.11	0.10	1.08	0.08	0.08	1.04
12	100	316	0.15	0.13	1.13	0.14	0.13	1.07	0.12	0.11	1.02
13	316	316	0.22	0.20	1.14	0.21	0.19	1.10	0.19	0.18	1.07
14	1000	316	0.32	0.26	1.21	0.30	0.26	1.15	0.29	0.25	1.14
15	10	1000	0.03	0.03	1.15	0.03	0.03	1.14	0.02	0.02	1.11
16	31	1000	0.03	0.03	1.14	0.03	0.03	1.11	0.03	0.02	1.05
17	100	1000	0.04	0.04	1.11	0.04	0.04	1.08	0.04	0.03	1.02
18	316	1000	0.08	0.07	1.09	0.07	0.07	1.06	0.07	0.07	1.03
19	1000	1000	0.14	0.13	1.11	0.14	0.13	1.10	0.14	0.13	1.09

In order to give a deeper view into the simulation results of the two Tier-2A models (PELMO and PEARL), two runs (substances P01: K_{om}: 10 L kg^{-1}, DegT50: 10 d; P02: K_{om}: 10 L kg^{-1}, DegT50: 31 d) with extreme differences are presented in more detail in the following figures.

Example 1: Substance P01, total-soil scenario, southern zone, ERC 1 cm, sugar beet

For the comparison between the two models, the 13th simulation year was selected when PELMO calculated the all-time high for the time-weighted average concentration over 14 days (TWA14) in that specific year (given as 6.61 mg kg^{-1} in Table 37). However, the PEARL calculation resulted in 4.28 mg kg^{-1} for the same situation (see also Table 37). The relevant simulation period is highlighted also in Figure 9.

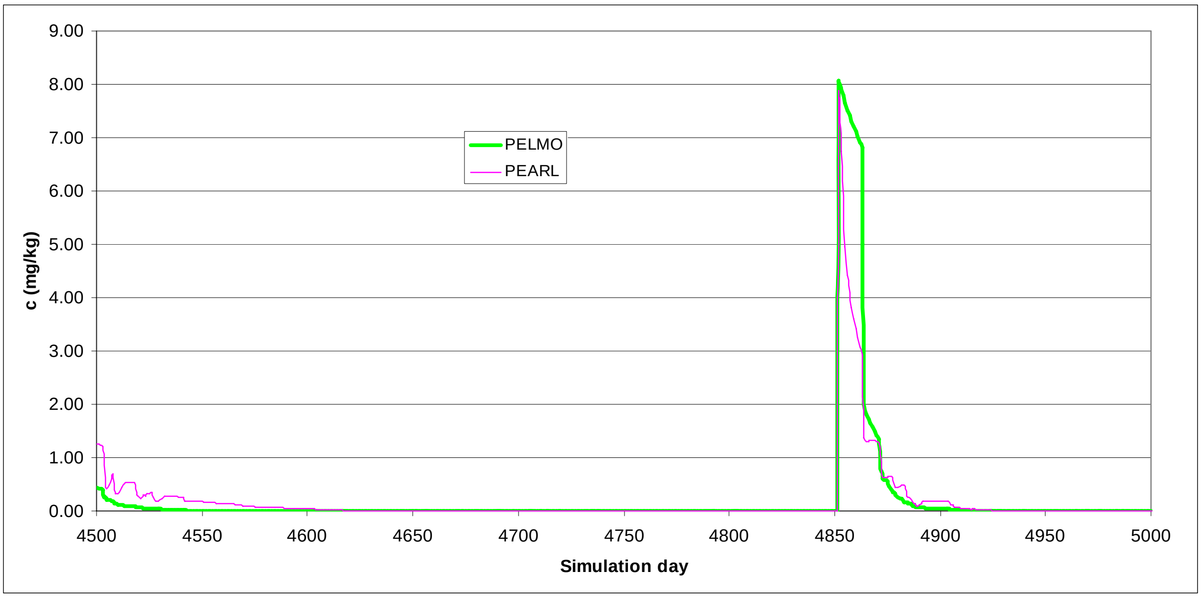

Figure 9: Concentration in total soil of P01 (soil depth: 1 cm) calculated by PELMO and PEARL for the southern zone (application: 1kg ha^{-1} in sugar beet, 1 day before emergence)

The differences in the concentrations could hardly be caused by different calculation of soil temperatures (Figure 10) as these are rather close for the whole simulation period.

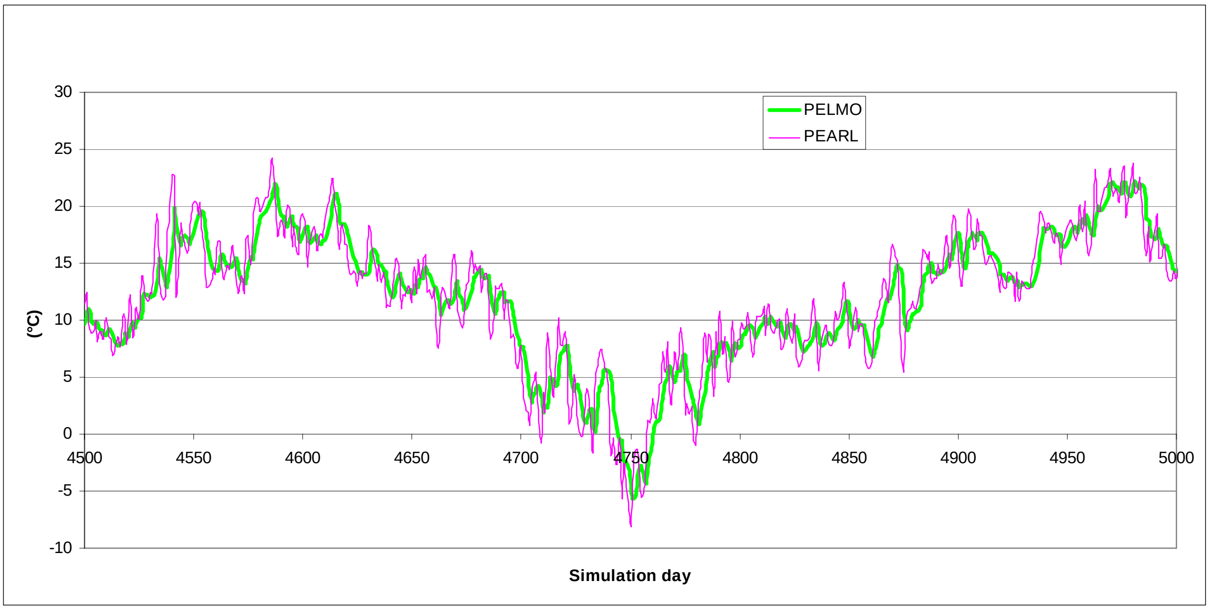

Figure 10: Soil temperatures at 1 cm soil depth calculated by PELMO and PEARL for the southern zone (total-soil scenario)

However, it becomes obvious that differences in the soil moisture calculations between PELMO and PEARL (Figure 11) were the reason for differences in this specific simulation (Figure 9). During the relevant time period that PELMO selected for the calculation of the TWA, significantly lower soil moisture contents were simulated by PELMO than PEARL which led to a reduced degradation rate in the PELMO simulation and finally also to a higher TWA. During other periods, i.e., between 4550 and 4700 days, PEARL simulated significantly lower soil moistures compared to the PELMO model.

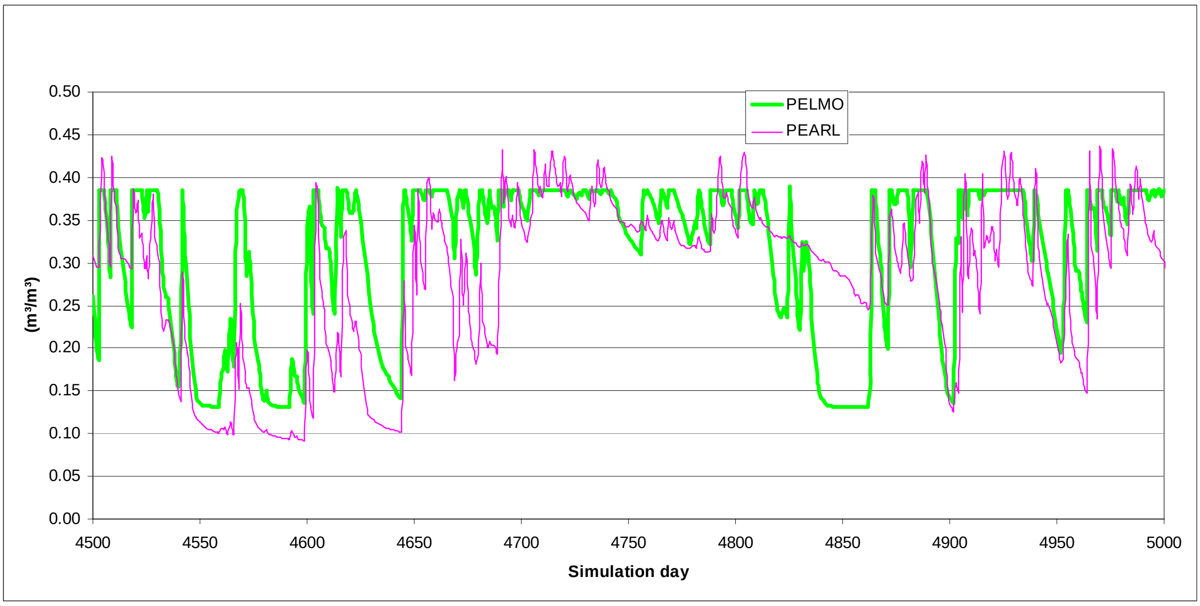

Figure 11: Soil moisture content calculated by PELMO and PEARL for the southern zone (total-soil scenario)

Example 2: Substance P02, pore-water scenario, northern zone, ERC 1 cm, sugar beet

For this run, the final simulation year was selected by PELMO for the calculation of TWA14 in pore water and which gave 22.18 mg L^{-1} (Table 38). However, the PEARL calculation gave 11.12 mg L^{-1} for the same situation (Table 38). The situation is highlighted also in Figure 12.

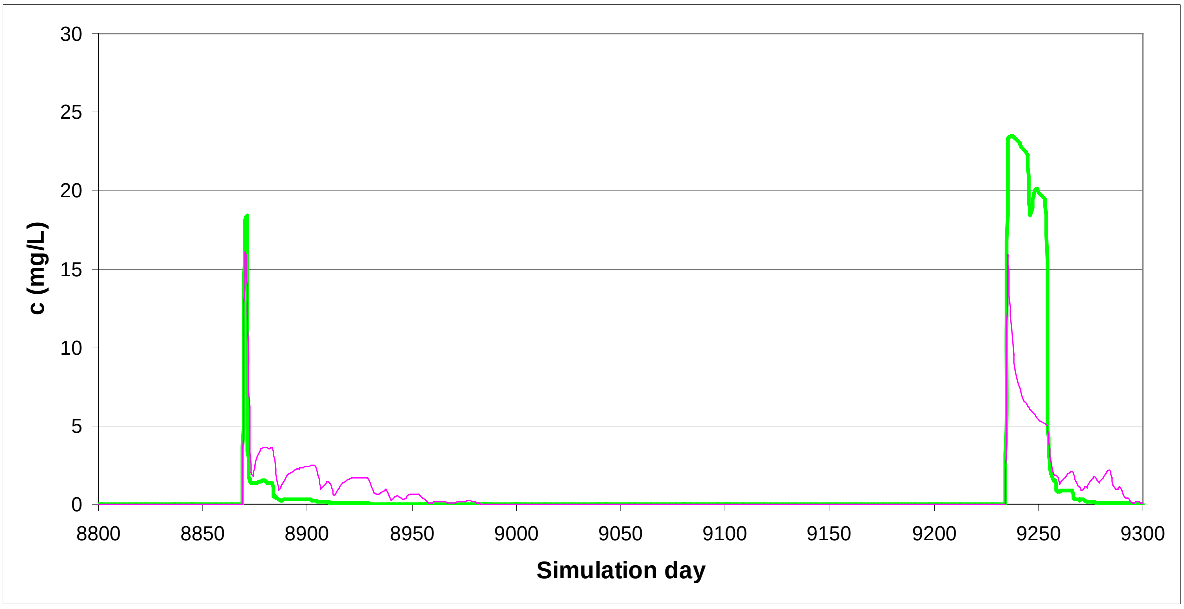

Figure 12: Concentrations of P02 in pore water (soil depth: 1 cm) calculated by PELMO and PEARL for the northern zone (application: 1 kg ha^{-1} in sugar beet, 1 day before emergence)

As before, differences in the pore-water concentrations can hardly be caused by different calculation of soil temperatures as they are very similar for the whole simulation period of more than one year (Figure 13).

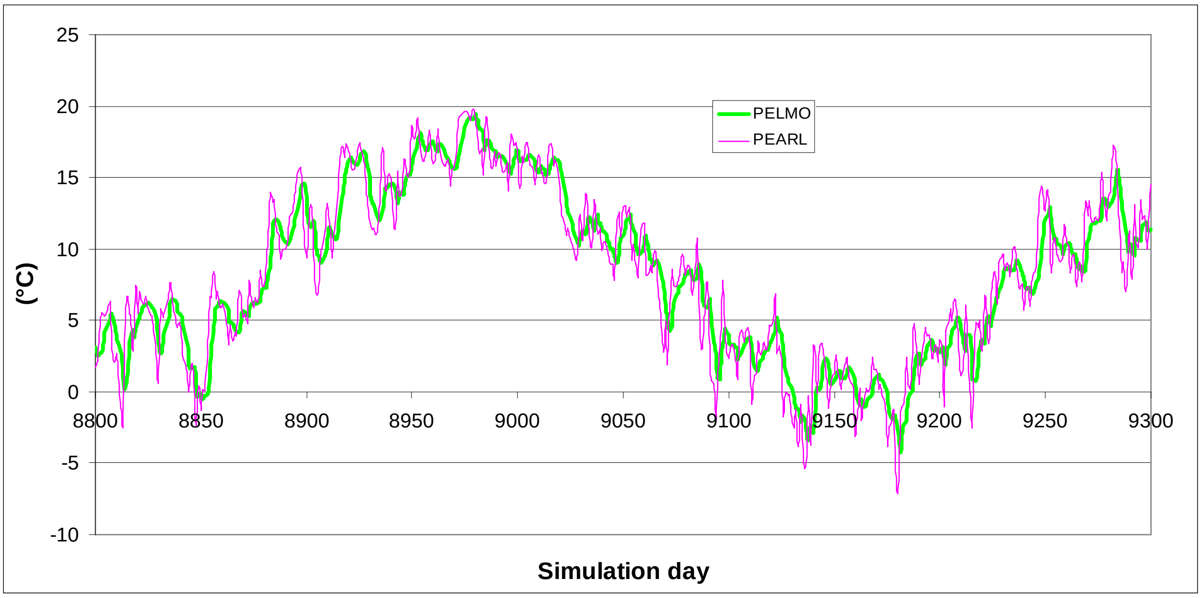

Figure 13: Soil temperatures at 1 cm soil depth calculated by PELMO and PEARL for the southern zone (total-soil scenario)

However, differences in the soil-moisture calculations between PELMO and PEARL (Figure 14) should be again the explanation for different pore-water concentrations. In the decisive simulation period shortly after the application, soil is estimated to be significantly drier in PELMO than in the PEARL simulation with similar consequences as in the previous example. The clear cut-off at 0.35 m^3 m^{-3} in the PELMO simulation (Figure 14) is an effect of the capacity approach which induces fast leaching to deeper soil layers when the soil exceeds field capacity.

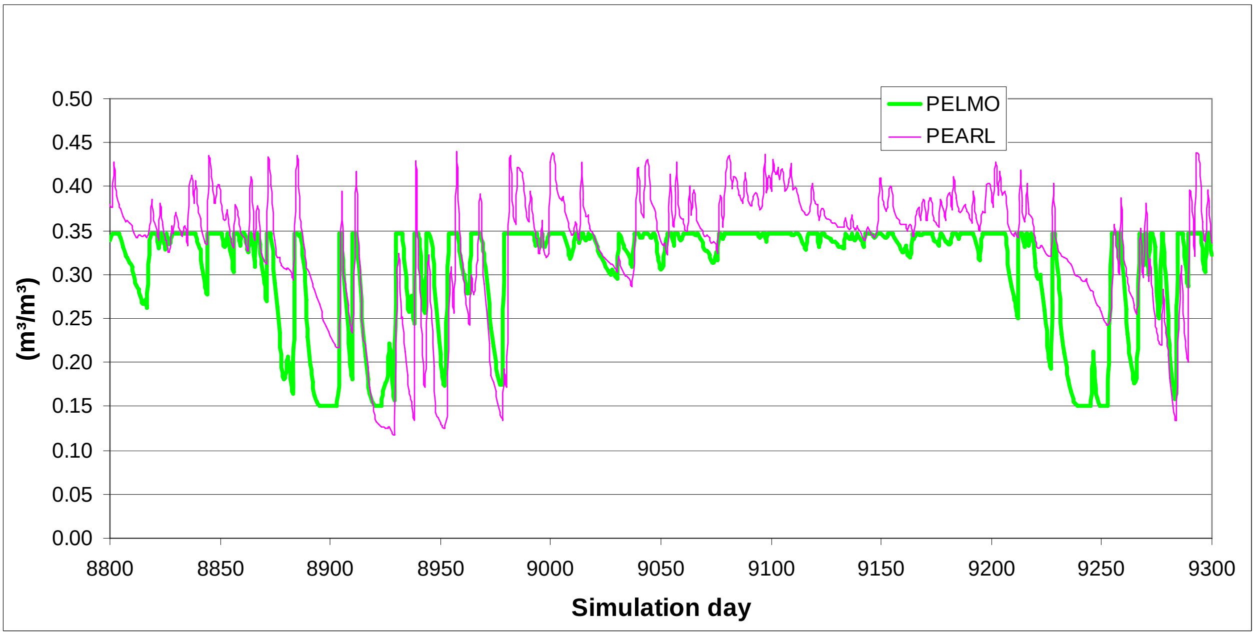

Figure 14: Soil moisture content calculated by PELMO and PEARL for the southern zone (total-soil scenario)

Figure 12 shows a second difference between the two Tier-2A models which becomes even more pronounced in Figure 15 where the concentration in total soil of P02 is shown:

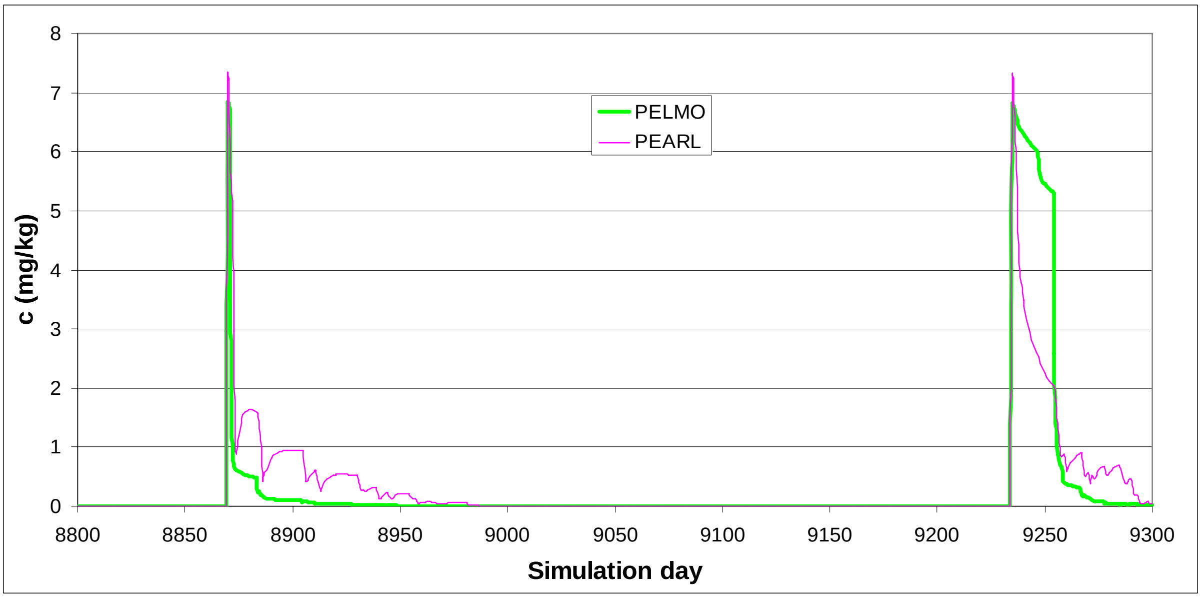

Figure 15: Concentration in total soil of P02 (soil depth: 1 cm) calculated by PELMO and PEARL for the northern zone (application: 1 kg ha^{-1} in sugar beet, 1 day before emergence)

4. TEST CALCULATIONS TO CALIBRATE TIER 1

4.1. Input data and application pattern

Calculations were carried out for all six scenarios both with the Tier-1 and Tier-2A models both for the peak values and TWA values for windows of 14 and 56 d of all parents and metabolites for the three regulatory zones North (N), Central (C), and South (S).

Variation of pesticide properties in two crops (single application)

- 19 pesticides as used in Section 3 with a single metabolite (formation fraction 25%, *DegT50* of 100 d and K_{om} of 50 L kg^{-1})
- One application of 1 kg ha^{-1} every year for 26 years on 1 day before emergence of the crop.
- crops: winter cereals (WC) and sugar beet (SB)

4.2. Calibration procedure

Calculations were done for both PELMO and PEARL. Results were analysed per model but at the end the same adjustment factors were calculated for both models (most conservative choice).

The first step is a graphical comparison between the outcomes from Tier 1 and Tier 2A for the following 12 situations each for 19 parent compounds or their metabolites:

1. Peak concentrations for the parent compounds
2. Peak concentrations for the metabolites
3. 14-d TWA concentrations for the parent compounds
4. 14-d TWA concentrations for the metabolites
5. 56-d TWA concentrations for the parent compounds
6. 56-d TWA concentrations for the metabolites

Concentrations averaged over the top 1 cm and averaged over the top 20 cm were considered.

4.3. Results of the simulations

All results of the comparison are shown in Figure 16 to Figure 27. In the graphs, symbols below the line represent situations where Tier-1 concentrations were above the respective Tier-2A concentrations; this is in accordance with the philosophy of the tiered assessment scheme. However, if symbols are above the one-to-one line, PEARL or PELMO calculated higher concentrations than Tier 1 possibly because the analytical Tier-1 model considers permanently optimal soil moisture conditions whereas the numerical models estimate dynamic soil moisture which may lead to slower degradation in soil.

The results of the total-soil scenarios with an ecologically relevant depth of 1 cm are summarised in Figure 16 to Figure 18.

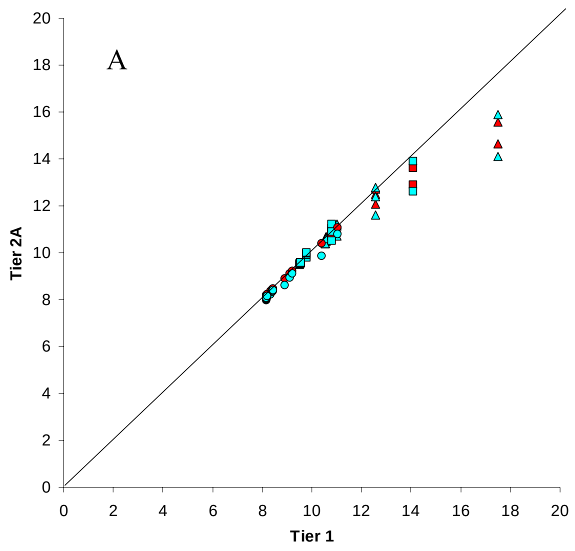

Figure 16: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for total soil and TWA 0 d (1 kg ha^{-1} the day before emergence in winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 1 cm for the northern (N), central (C) and southern (S) regulatory zones

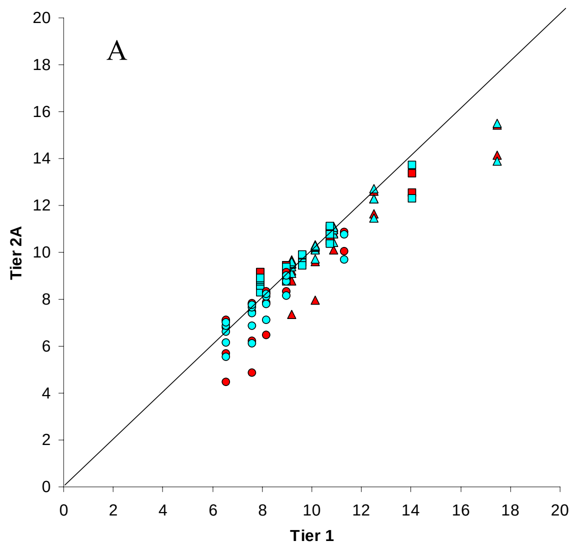

Figure 17: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for total soil and TWA 14 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 1 cm for the northern (N), central (C) and southern (S) regulatory zones

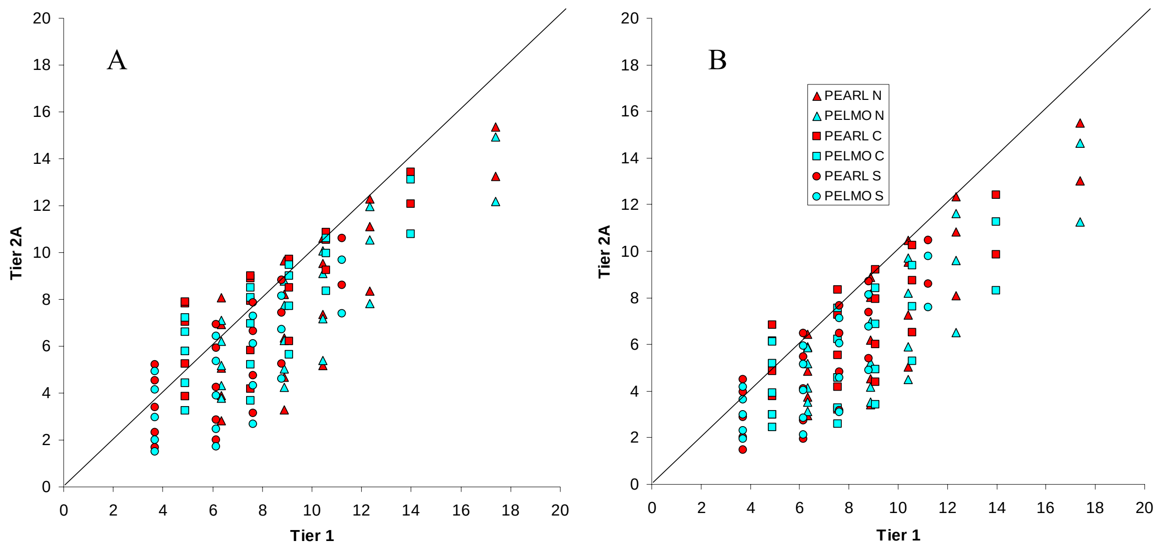

Figure 18: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for total soil and TWA 56 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 1 cm for the northern (N), central (C) and southern (S) regulatory zones

The results of the total-soil scenarios with an ecologically relevant depth of 20 cm are summarised in Figure 19 to Figure 21.

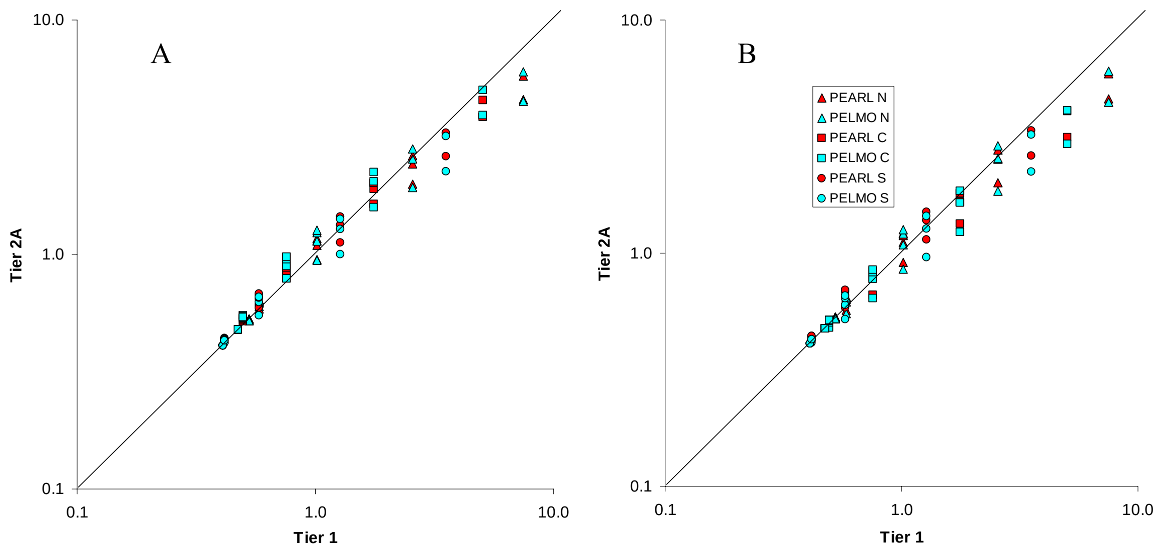

Figure 19: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for total soil and TWA 0 d (1 kg ha^{-1} the day before crop emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 20 cm for the northern (N), central (C) and southern (S) regulatory zones

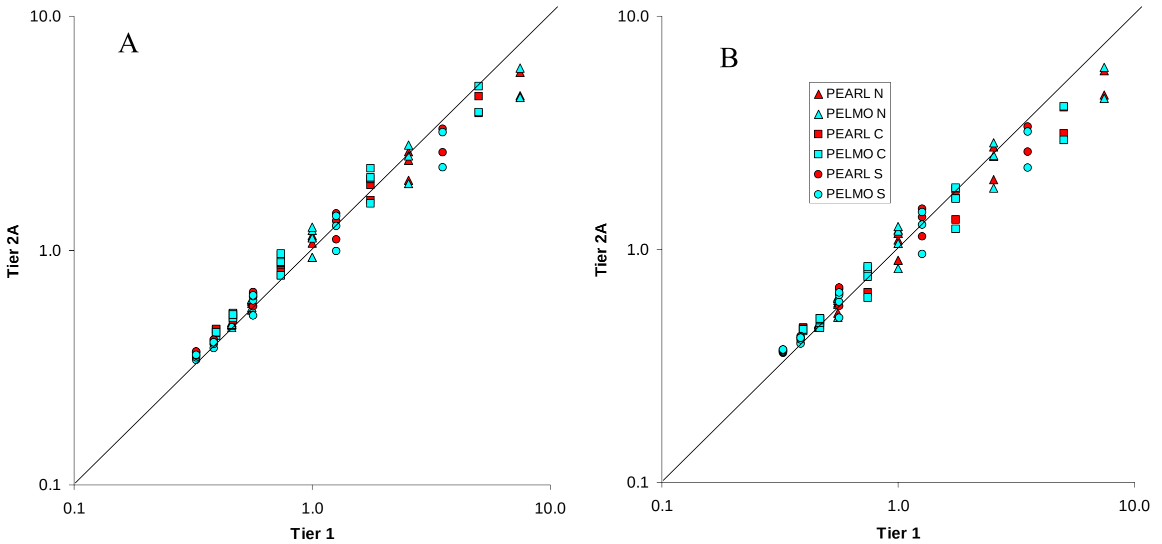

Figure 20: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for total soil and TWA 14 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 20 cm for the northern (N), central (C) and southern (S) regulatory zones

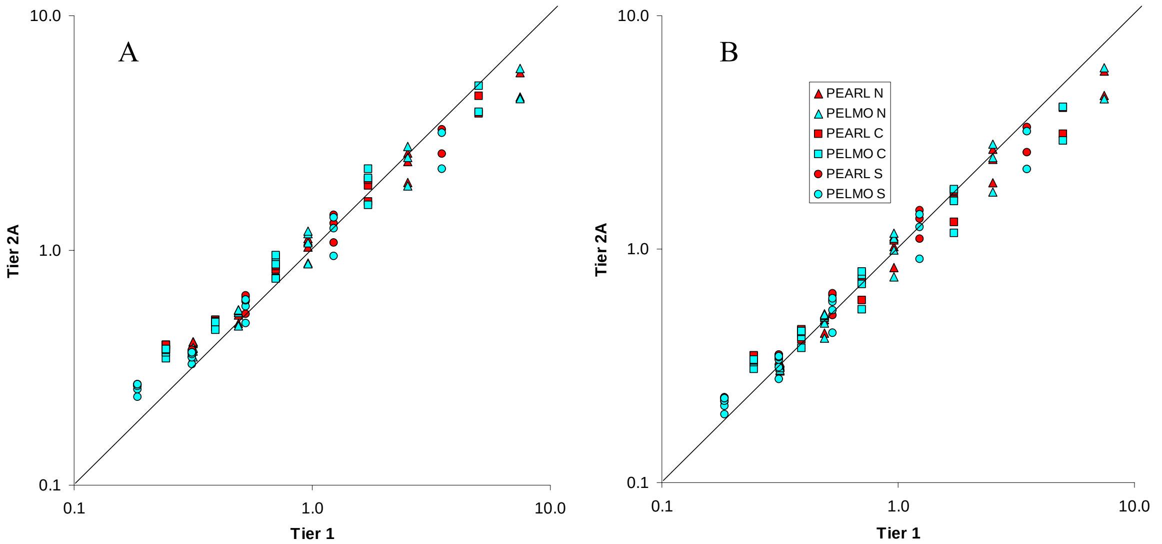

Figure 21: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for total soil and TWA 56 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 20 cm for the northern (N), central (C) and southern (S) regulatory zones

The results of the pore-water scenarios and an ecologically relevant depth of 1 cm are summarised in Figure 22 to Figure 24.

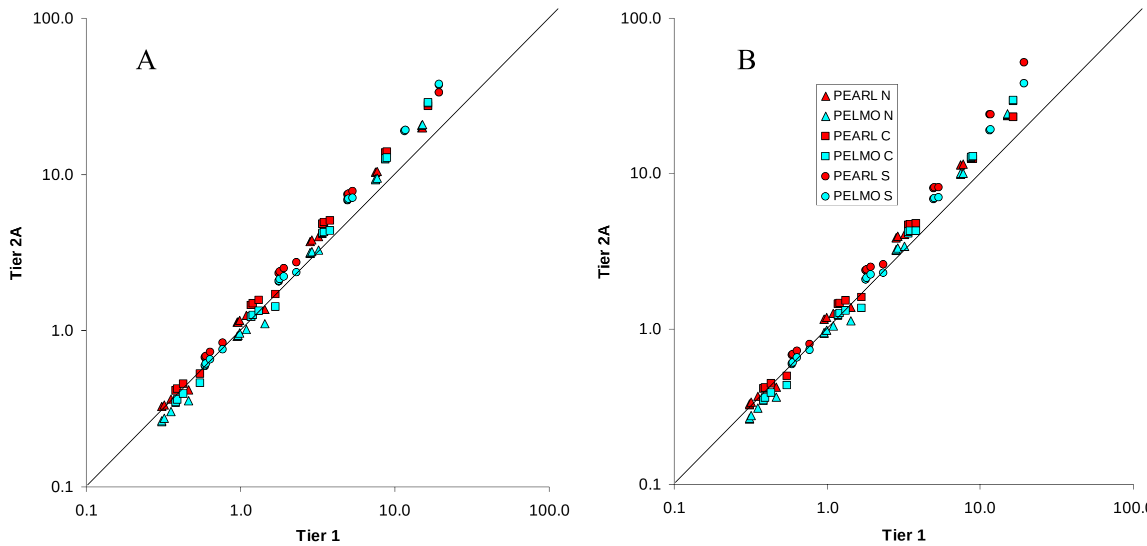

Figure 22: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for pore water and TWA 0 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 1 cm for the northern (N), central (C) and southern (S) regulatory zones

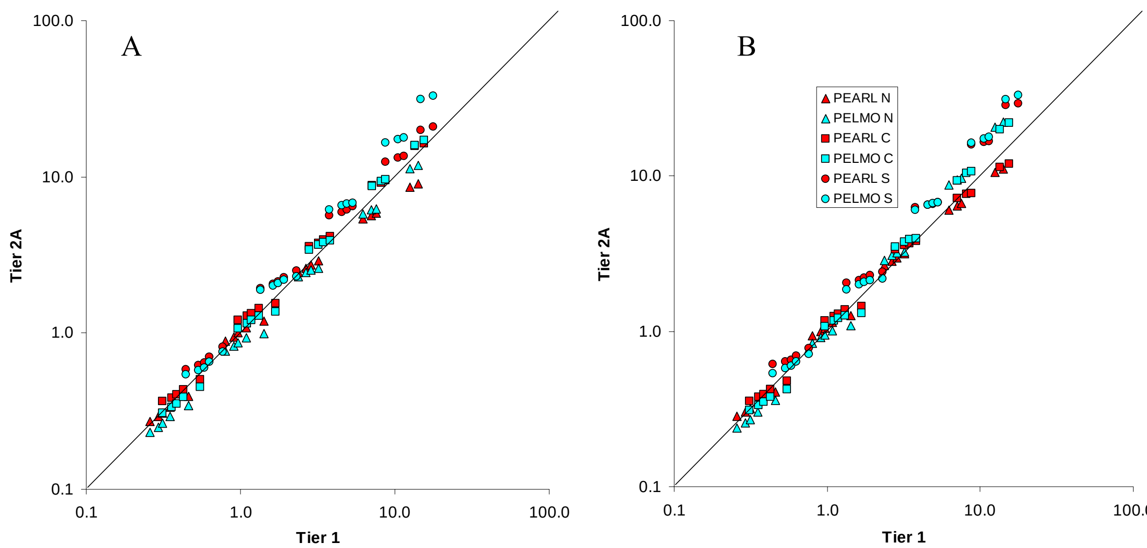

Figure 23: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for pore water and TWA 14 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 1 cm for the northern (N), central (C) and southern (S) regulatory zones

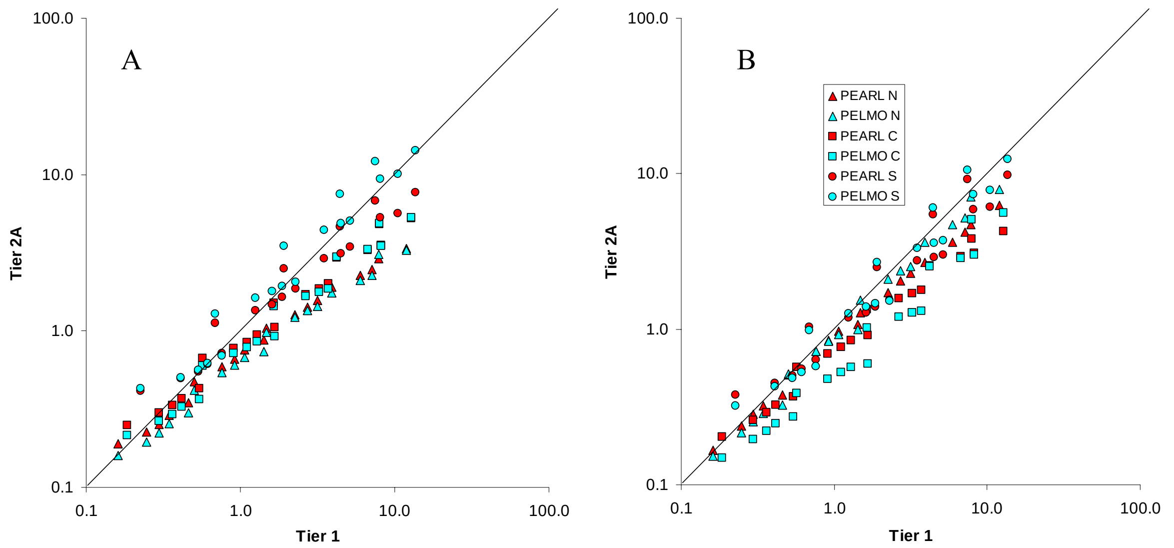

Figure 24: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for pore water and TWA 56 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 1 cm for the northern (N), central (C) and southern (S) regulatory zones

The results of the pore-water scenarios and an ecologically relevant depth of 1 cm are summarised in Figure 25 to Figure 27.

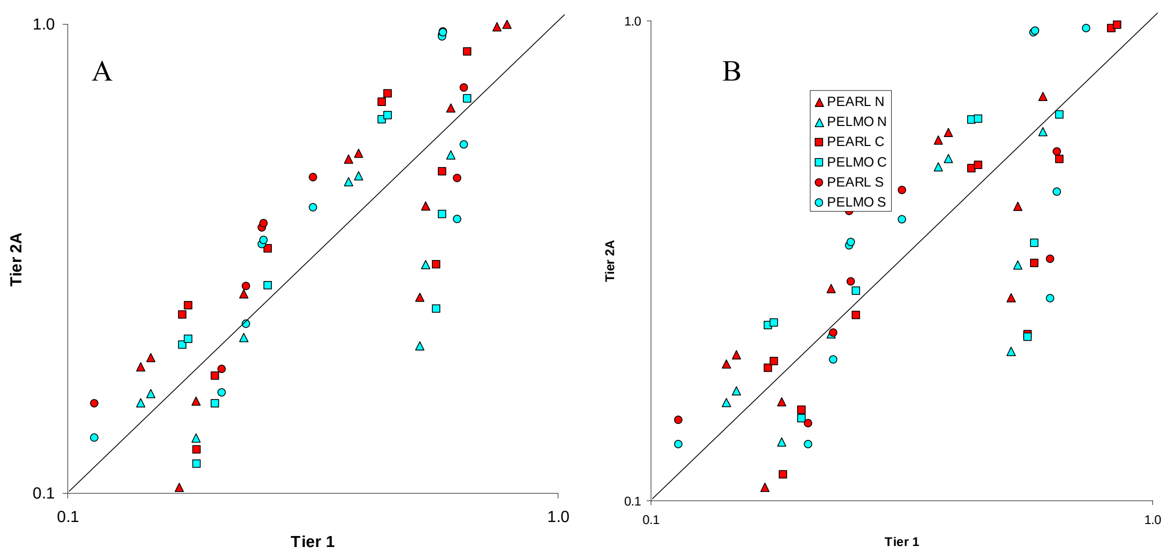

Figure 25: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for pore water and TWA 0 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 20 cm for the northern (N), central (C) and southern (S) regulatory zones

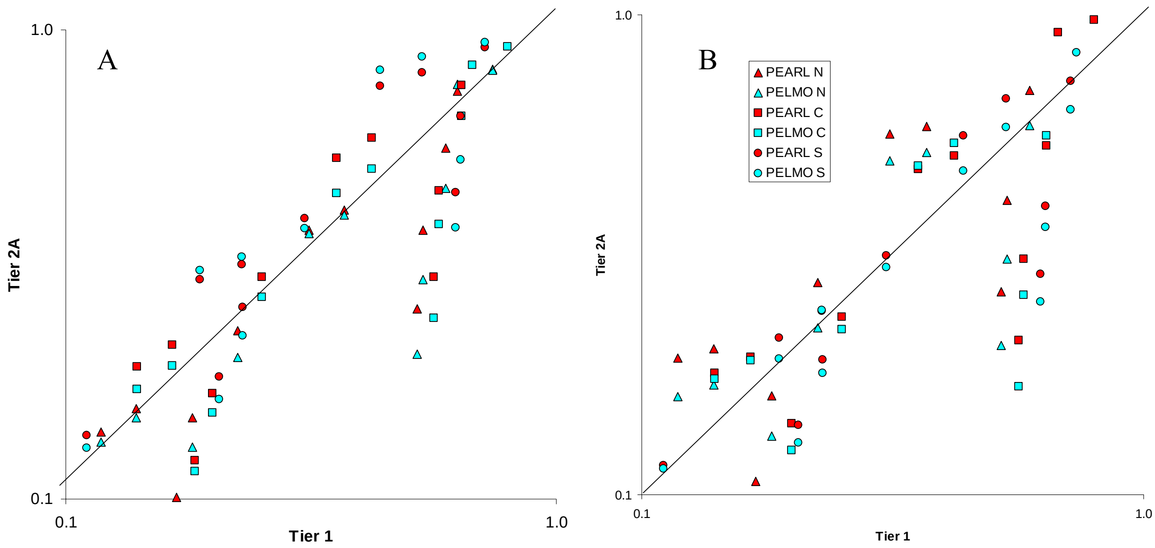

Figure 26: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for pore water and TWA 14 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 20 cm for the northern (N), central (C) and southern (S) regulatory zones

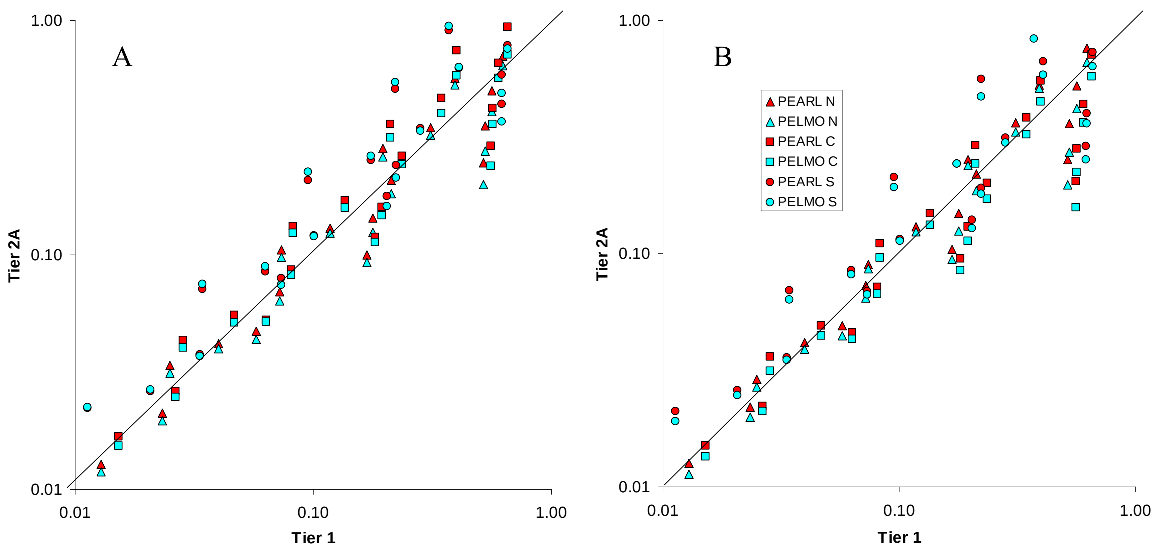

Figure 27: Comparison of PEC_{soil} simulated by PEARL and PELMO (Tier 2A) with those from Tier 1 for pore water and TWA 56 d (1 kg ha^{-1} the day before emergence of winter cereals (A) and sugar beet (B), every year), ecologically relevant depth 20 cm for the northern (N), central (C) and southern (S) regulatory zones

4.4. Possible model adjustment factors

The differences between Tier 1 and Tier 2A (Table 47), based on the results above, demonstrate that additional model adjustment is necessary to guarantee that Tier-1 results will be above respective Tier-2A simulations independent of the substance, political zone and crop.

Table 47: Calculated adjustment factors between Tier 1 and Tier 2A ($PEC_{Tier\ 2A}$/ $PEC_{Tier\ 1}$)

Endpoint	Relevant soil depth (cm)	Zone	TWA 0 d	up to TWA 14 d	up to TWA 56d
Total soil	1	Northern zone	1.03	1.07	1.27
Total soil	1	Central zone	1.04	1.16	1.61
Total soil	1	Southern zone	1.02	1.13	1.41
Total soil	20	Northern zone	1.24	1.25	1.29
Total soil	20	Central zone	1.29	1.30	1.61
Total soil	20	Southern zone	1.20	1.21	1.45
Total soil	all ERD	Northern zone	1.24	1.25	1.28
Total soil	all ERD	Central zone	1.29	1.30	1.61
Total soil	all ERD	Southern zone	1.20	1.21	1.45
Total soil	all ERD	all Zones	1.29	1.30	1.61
Pore water	1	Northern zone	1.62	1.64	1.17
Pore water	1	Central zone	1.79	1.47	1.35
Pore water	1	Southern zone	2.64	2.13	1.90
Pore water	20	Northern zone	1.59	1.64	1.46
Pore water	20	Central zone	1.72	1.63	1.86
Pore water	20	Southern zone	2.64	2.55	2.89
Pore water	all ERD	Northern zone	1.62	1.64	1.46
Pore water	all ERD	Central zone	1.79	1.63	1.86
Pore water	all ERD	Southern zone	2.64	2.55	2.89
Pore water	all ERD	all Zones	2.64	2.55	2.89
Total soil and Pore water	1	Northern zone	1.62	1.64	1.27
Total soil and Pore water	1	Central zone	1.79	1.47	1.61
Total soil and Pore water	1	Southern zone	2.64	2.13	1.90
Total soil and Pore water	20	Northern zone	1.59	1.64	1.46
Total soil and Pore water	20	Central zone	1.72	1.63	1.86
Total soil and Pore water	20	Southern zone	2.64	2.55	2.89
Total soil and Pore water	all ERD	Northern zone	1.62	1.64	1.46
Total soil and Pore water	all ERD	Central zone	1.79	1.63	1.86
Total soil and Pore water	all ERD	Southern zone	2.64	2.55	2.89
Total soil and Pore water	all ERD	all Zones	2.64	2.55	2.89

REFERENCES

Boesten JJTI, Köpp H, Adriaanse PI, Brock TCM, and Forbes VE, 2007. Conceptual model for improving the link between exposure and effects in the aquatic risk assessment of pesticides. Ecotoxicology and Environmental Safety (66), 291–308.

EFSA Panel on Plant Protection Products and their Residues (PPR), 2010, Scientific Opinion on outline proposals for assessment of exposure of organisms to substances in soil. The EFSA Journal 2010; 8(1):1442 [38 pp].

EFSA (European Food Safety Authority), 2010, Selection of Scenarios for Exposure of Soil Organisms to Plant Protection Products. EFSA Journal 2010;8(6):1642 [82pp.]. doi:10.2903/j.efsa.2010.1642. Available online: www.efsa.europa.eu

EFSA (European Food Safety Authority), 2012. Scientific Opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations in soil. In preparation.

FOCUS, 1997. Soil persistence models and EU registration. Report of the FOCUS modelling Work group. EC Document SANCO/9188/VI/97.

FOCUS, 2000. FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup. EC Document Reference Sanco/321/2000 rev.2, 202 pp.

FOCUS, 2006. Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration. Report of the FOCUS Work Group on Degradation Kinetics. EC Document Reference Sanco/10058/2005 version 2.0, 434 pp.

FOCUS, 2010. Assessing potential movement of active substances and their metabolites to ground water in the EU. EC Document reference Sanco/xxx/2010. Available at FOCUS website http://viso.ei.jrc.it/focus.

Leip A, Marchi G, Koeble R, Kempen M, Britz W, and Li C, 2008. Linking an economic model for European agriculture with a mechanistic model to estimate nitrogen and carbon losses from arable soils in Europe. Biogeosciences (5):73-94.

Tiktak A, de Nie DS, van der Linden AMA and Kruijne R, 2002. Modelling the leaching and drainage of pesticides in the Netherlands: the GeoPEARL model. Agronomie (22):373-387.

Van Genuchten M, 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Science Society of America Journal (44):892-898.

Vanderborght J and Vereecken H, 2007. Review of dispersivities for transport modelling in soils. Vadose Zone Journal (6):1-28.

Wösten JHM, Nemes A, Lilly A and Le Bas C, 1999. Development and use of a database of hydraulic properties of European soils. Geoderma (90):169–185.

APPENDICES

A. DESCRIPTION OF THE TIER-1 MODEL

In PERSAM, firstly the initial concentration in total soil directly after application is calculated:

$$C_{T,ini} = \frac{DOSE}{\rho z_{rel}} \tag{1}$$

where $C_{T,ini}$ (mg kg^{-1}) is the initial concentration in total soil, *DOSE* is the annual application rate (kg ha^{-1} or mg dm^{-2}), z_{rel} (dm) is the ecologically relevant depth, and ρ is the dry-soil bulk density (kg dm^{-3}). In the second step, the background concentration, $C_{T,plateau}$ (mg kg^{-1}), just before the next application after an infinite number of annual applications, is calculated:

$$C_{T,plateau} = \frac{z_{rel}}{z_{til}} C_{T,ini} \frac{e^{-365 f_T k_{ref}}}{1 - e^{-365 f_T k_{ref}}} \tag{2}$$

where z_{til} (dm) is the plough depth (fixed at 20 cm), and k_{ref} (d^{-1}) is the reference first-order rate coefficient at a reference temperature T_{ref} (ie 20^{o}C) and reference soil moisture content θ_{ref}. The dimensionless factor f_T accounts for the effect of temperature on degradation, and is given by:

$$\mathrm{f_T} = \exp\left(\frac{-E}{R}\left[\frac{1}{T} - \frac{1}{T_{ref}}\right]\right) \tag{3}$$

where E is the Arrhenius activation energy, (kJ mol^{-1}), R is the gas constant (0.008314 kJ mol^{-1} K^{-1}), T (K) is the temperature, and T_{ref} (K) is the temperature at reference conditions (20^{o}C). The first-order rate coefficient is calculated from the degradation half-life

$$k_{ref} = \frac{\ln(2)}{DegT_{50}} \tag{4}$$

where *DegT50* (d) is the degradation half-life in soil at the reference temperature.

The background concentration corresponds to the residue remaining immediately before the next application. The maximum concentration directly after application is calculated by:

$$C_{T,peak} = C_{T,ini} + C_{T,plateau} \tag{5}$$

where $C_{T,peak}$ (mg kg^{-1}) is the maximum concentration in total soil. The concentration in the liquid phase is calculated from the total concentration in the soil assuming a linear sorption isotherm:

$$C_L = \frac{C_T}{\theta / \rho + f_{om} K_{om}} \tag{6}$$

where C_L (mg L^{-1}) is the concentration in the liquid phase, C_T (mg kg^{-1}) is the concentration in total soil, θ (m^3 m^{-3}) is the volume fraction of liquid in soil, f_{om} (kg kg^{-1}) is the mass fraction of organic matter, and K_{om} (dm^3 kg^{-1}) is the coefficient for sorption on organic matter. The concentration in the liquid phase can be calculated for the initial concentration ($C_{L,ini}$), the background concentration ($C_{L,plateau}$) and for the maximum concentration ($C_{L,peak}$).

PERSAM can also be used to calculate TWA concentrations, these being defined as the concentration that is averaged over a certain time period after the application:

$$C_{TWA}\left(t_{avg}\right) = \frac{1}{t_{avg}} \int_{0}^{t_{avg}} C(t')dt' \tag{7}$$

where t_{avg} (d) is the time period after application and over which concentrations are averaged and t' is a dummy time integration variable. For a substance undergoing first-order decay, the TWA total-soil concentration, $C_{T,TWA}$ for a certain period after the application, t_{avg}, is calculated from:

$$C_{T,TWA}\left(t_{avg}\right) = \frac{1}{t_{avg}} \int_{0}^{t_{avg}} C_{T,peak} \exp\left(-f_T k_{ref} t'\right)dt' \tag{8}$$

or:

$$C_{T,TWA}\left(t_{avg}\right) = \frac{C_{T,peak}}{t_{avg} f_T\ k_{ref}} \left[1 - \exp\left(-f_T k_{ref} t_{avg}\right)\right] \tag{9}$$

It should be noted that $C_{T,TWA}$ also depends on the decay rate. This is in contrast to $C_{T,peak}$, in which only the first term $C_{T,plateau}$, depends on the decay rate. The TWA concentration calculated using Eq. (9) only applies for one application of a substance per year. For multiple applications, the TWA concentration after the i[th] application during a year $C_{T,TWA,i}(t_{avg})$ can be calculated by summing up individual doses and applying the total annual dose on one day.

B. PEARL DOCUMENTATION

Input and output files

C. PELMO DOCUMENTATION

Input and output files

GLOSSARY AND ABBREVIATIONS

CAPRI:	Common Agricultural Policy Regionalised Impact modelling system (an economic model developed to support EU policy)
CL	Concentration in the liquid phase (pore-water concentration, mass/volume)
Corine	Coordinate Information on the Environment
CT	Concentration in total soil (mass/mass)
DegT50	Half-life resulting from transformation of substance in the soil matrix
EFSA	European Food Safety Authority
ERC	Ecotoxicologically Relevant Concentration
ERD	Ecotoxicologically Relevant soil depth
ETpot	Potential evapotranspiration
FOCUS	FOrum for Co-ordination of pesticide fate models and their Use
K_{oc}	Organic carbon/water partition coefficient
K_{om}	Organic matter/water partition coefficient
MARS	Monitoring Agricultural ResourceS
OCTOP:	European map of organic carbon content in topsoil provided by JRC-Ispra (Italy)
PEARL	Pesticide Emission At Regional and Local scales (one of the FOCUS fate models)
PEC	Predicted Environmental Concentration
PELMO	Pesticide Leaching Model (one of the FOCUS fate models)
PPP	Plant Protection Product
PPR	Plant Protection Products and their Residues
SPADE	Soil Profile Analytical Database
TWA	Time-Weighted Average
WorldClim:	Global Climate Data. WorldClim is a set of global climate layers (climate grids) with a spatial resolution of a square kilometre. They can be used for mapping and spatial modelling in a GIS or other computer programs (http://www.worldclim.org/)
z_{rel}	Ecotoxicologically Relevant Soil Depth