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Generic Guidance for Tier 1 FOCUS Ground Water Assessments

About this document

This document is based on the reports of the FOCUS Groundwater Scenarios workgroup (finalised in 2000), the FOCUS Ground Water Work Group (finalised in 2009), the FOCUS Work Group on Degradation Kinetics (finalised in 2006), the EFSA guidance on $DegT50_{matrix}$ (finalised in 2014) the EFSA PPR scientific opinion on FOCUS, 2009, assessment of lower tiers (finalised in 2013) and European Commission 2014 that updated FOCUS, 2009 considering the EFSA PPR scientific opinions of 2013. This document does not replace the official FOCUS reports or EFSA documents. However, a need was identified to maintain the definition of the FOCUS ground water scenarios and the guidance for their use in an up-to-date version controlled document, as changes become necessary. That is the purpose of this document. The previous versions of this document were entitled Generic Guidance for FOCUS Groundwater Scenarios.

Summary of changes made since the FOCUS Groundwater Scenarios Report (SANCO/321/2000 rev.2).

New in Version 1.0

The only changes in this version compared with the original report are editorial ones.

The original report stands alone and is not replaced by the current document. Therefore, some sections of the original report have not been repeated here, since they do not form part of the definition of the FOCUS scenarios or provide specific guidance for their use.

Appendices B-E of the original report are not included in this document. They have been separated to form four model parameterisation documents, which complement the present document. The present document describes the underlying scenario definitions and their use, whilst the model parameterisation documents describe how the scenarios have been implemented in each of the simulation models.

New in Version 1.1

Several values in the crop interception table (Table 1.6) have been changed and some footnotes to this table have been added. As a result, the page numbering in the report and Table of Contents was changed.

New in Version 2.0

The content was changed to include the guidance pertinent to Tier 1 assessments in the documents prepared by FOCUS Ground Water Work Group (SANCO/13144/2010) and the FOCUS Work Group on Degradation Kinetics (SANCO/10058/2005, version 2.0). A change was made to achieve consistency with the FOCUS Surface Water Scenarios workgroup (SANCO/4802/2001/2001-rev 2) guidance. Via footnotes, information on evaluation practice agreed between Member State competent authority experts, that attend EFSA PRAPeR meetings has been added.

The title of this document was changed to indicate that this guidance applied only to Tier 1 scenarios.

New in Version 2.1

Wording on selecting pesticide input parameters has been updated to reflect the exponent for moisture response that has to be used with FOCUS_MACROv5.5.3 and above. For transparency changes from Version 2.0 are highlighted in yellow.

New in Version 2.2

Wording on selecting pesticide input parameters has been updated to reflect the EFSA guidance (2014) and implementable recommendations of the EFSA PPR scientific opinion (2013a) on FOCUS, 2009, assessment of lower tiers which were included in European Commission, 2014. For transparency changes from Version 2.0 are highlighted in yellow.

New in Version 2.3

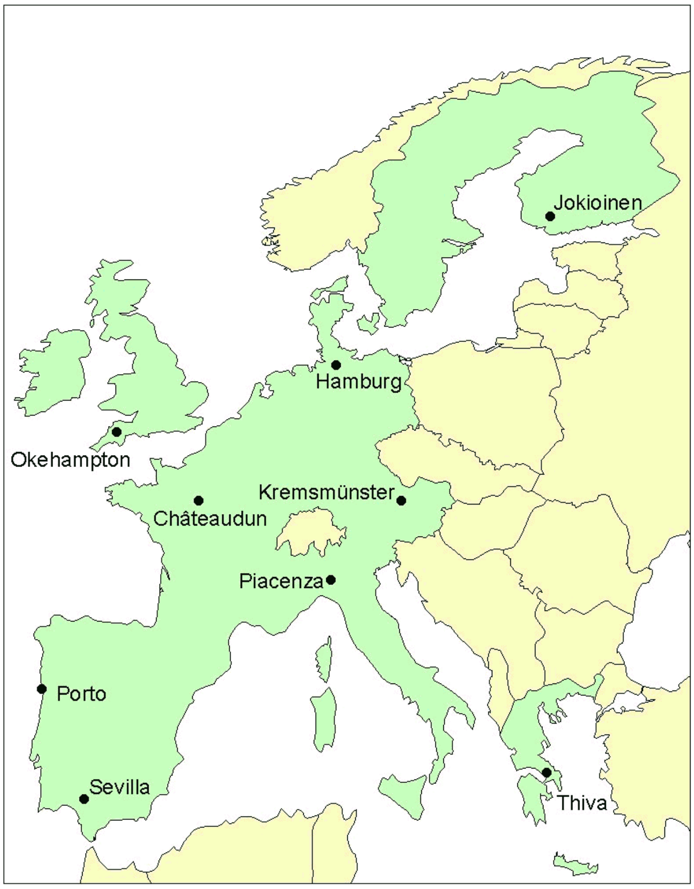
Equations for converting pH measured in $CaCl_2$ and KCl to pH measured in H_2O have been updated and irrigation water in PEARL and PELMO is now applied at the soil surface for the crops apples, citrus and vines. Both these updates reflect the EFSA guidance (2017a). Guidance on pesticide property parameter derivation when there is pH dependence was updated to reflect EFSA guidance (2020). A reference was added to the OECD 106 evaluators checklist (EFSA, 2017b) in relation to equilibrium sorption parameters. Information on new options for defining transformation product formation fractions via more recent versions of the PELMO shell have been added. Also chapter 3 includes corrections to errors to periods for Kc values between maximum leaf area and senescence for the crop onions at the Porto and Thiva scenarios that were made in the FOCUS (2009) / European Commission (2014) reports. Finally text was added acknowledging regulatory developments regarding determining aged (non equilibrium) sorption parameters. Note that incorporating aged sorption in simulations does not result in a tier 1 assessment. For transparency changes from Version 2.0 are highlighted in yellow.

Table of CONTENTS

EXECUTIVE SUMMARY

Main features of the FOCUS ground water scenarios

FOCUS (2000, 2009) has defined 125 realistic worst-case ground water scenarios (based on nine locations with 12 to 16 crops each) combinations) to collectively represent agriculture in the EU for the purposes of a Tier 1 EU-level assessment of the leaching potential of active substances.



Soil properties and weather data have been provided for all nine locations and are summarised in the table below. Soil properties have been defined down to the water-table, where such data were available.

Crop information has also been defined for each scenario, including five crops which can be grown across the whole EU, and a further 20 which are particular to specific parts of the EU.

Location	Mean Annual Temp. (°C)	Annual Rainfall (mm)	Topsoil Texture†	Topsoil Organic Matter (%)
Châteaudun	11.3	648 + I*	silty clay loam	2.4
Hamburg	9.0	786	sandy loam	2.6
Jokioinen	4.1	650	loamy sand	7.0
Kremsmünster	8.6	899	loam/silt loam	3.6
Okehampton	10.2	1038	loam	3.8
Piacenza	13.2	857 + I*	loam	2.2
Porto	14.8	1150 + I*	loam	2.5
Sevilla	17.9	493 + I*	silt loam	1.6
Thiva	16.2	500 + I*	loam	1.3

† = USDA classification (USDA, 1975; FAO, 1977)
I* = scenario also includes irrigation

The scenarios as defined do not mimic specific fields, and nor should they be viewed as representative of the agriculture in the Member States where they are located.

The scenario definitions are simply lists of properties and characteristics which exist independently of any simulation model. These scenario definitions have also been used to produce sets of model input files. Input files corresponding to 125 scenarios have been developed for use with the simulation models PEARL, PELMO and PRZM, while input files for crops grown at a single location have also developed for the model MACRO. The models all report concentrations at 1m depth for comparative purposes, but this does not represent ground water. Results can also be produced for depths down to the water-table in cases where the model is technically competent to do so and the soil data is available. The weather data files developed for these models include irrigation in five of the locations, and also include the option of making applications every year, every other year or every third year.

How can the scenarios be used to assess leaching?

Defining scenarios and producing sets of model input files is not enough to ensure a consistent scientific process for evaluating leaching potential in the EU. The user still has to define substance-specific model inputs, and then has to run the models and summarise the outputs. (In this report the term “substance” is used to describe active substances of plant protection products and their metabolites in soil.) Each of these steps can result in inconsistent approaches being adopted by different modellers, resulting in inconsistent evaluations of leaching potential. The work groups have addressed these issues as follows:

Defining substance-specific model inputs

This document provides guidance on the selection of substance-specific input parameters. This includes guidance on

- default values and the substance-specific measurements which may supersede them
- how to derive input values for a substance from its regulatory data package
- selection of representative single input values from a range of measurements
- the differing ways in which individual processes are parameterised in the four models, and differences in units of measurement

Running the FOCUS scenarios in the simulation models

For each of the four models there is a “shell” which has been developed to simplify the process of running the FOCUS scenarios.

Summarising the model outputs

In order to ensure the overall vulnerability of the scenarios, and to also ensure consistency, a single method of post-processing the model outputs has been defined, and is built directly into the model shells.

What benefits does this work deliver to the regulatory process?

The FOCUS ground water scenarios offer a way of evaluating leaching potential across the EU. A consistent process has been defined which is based on best available science at the time of last update.

The anticipated benefits include:

- *Increased consistency.* The primary purpose of defining standard scenarios is to increase the consistency with which industry and regulators evaluate leaching. The standard scenarios, the guidance on substance-specific input parameters, the model shells, and the standard way of post-processing model outputs should together help greatly in achieving this.
- *Speed and simplicity.* Simulation models are complex and are difficult to use properly. Having standard scenarios means that the user has fewer inputs to specify, and the guidance document simplifies the selection of these inputs. The model shells also make the models easier to operate.
- *Ease of review.* Using standard scenarios means that the reviewer can focus on those relatively few inputs which are in the control of the user.
- *Common, agreed basis for assessment.* The FOCUS scenarios provide Member States a common basis on which to discuss leaching issues with substances at the EU level. Registrants will also have greater confidence that their assessments have been done on a basis which the regulators will find acceptable. Debate can then focus on the substance-specific issues of greatest importance, rather than details of the weather data or soil properties, for example.

Will the four models give differing results?

Three possible reasons for differences between the results of the models have been identified and are listed below, together with the measures undertaken to minimise these differences.

- *Different weather, soil and crop data.* This source of variation has been largely eliminated by the provision of standard scenarios.
- *Different ways of summarising the model output.* The standard way of post-processing model outputs, which is built into the model shells, should eliminate this.

- *Different process descriptions within the models.* This is the one source of variation between model results which has not been addressed, since harmonisation of the models was beyond the scope of the work groups. Similarly, validation of the models or of the process descriptions within the models was also beyond the scope of the work groups.

One of the major activities of the FOCUS Ground Water Work Group (FOCUS, 2009) was to harmonise the results of the models by agreeing to common descriptions of dispersion length, crop transpiration, and runoff. The harmonisation effort was largely successful with 90 percent of the PEARL and PELMO values for the proposed scenarios within a factor of three. As shown in FOCUS (2009), this agreement among models for the FOCUS (2009) scenarios is considerably better than observed among the models for the FOCUS (2000) scenarios. Given the current agreement among the models, the FOCUS (2009) recommended that the ground water assessments might be performed with any of the models (PEARL, PELMO, and PRZM) and there was no need to perform the assessments with more than one model. However EFSA PPR (2013a) and European Commission (2014) recommended that the PECgw calculations for decision making should be based on more than one model. Applicants and rapporteurs are advised that they should provide simulations with PEARL and PELMO or PRZM. Where a crop of interest is defined for Châteaudun, MACRO simulations need to be run. (EFSA PPR, 2013a / European Commission, 2014).

There are situations when the differences between the models can be useful, for example there may be a fate process which is important for a particular substance which is not represented in all the models, and this could guide model selection.

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1. DEFINING THE SCENARIOS

1.1 Framework for the FOCUS ground water scenarios

1.1.1 Objectives

One objective of the two FOCUS work groups (FOCUS, 2000; 2009) addressing ground water was to develop a set of standard scenarios which can be used to assess the potential movement of crop protection products and their relevant metabolites to ground water as part of the EU review process for active substances. In order to eliminate the impact of the person performing these simulations as much as possible, one goal was to standardise input parameters, calculation procedures, and interpretation and presentation of results. For ease and uniformity in implementing these standard scenarios computer shells were developed containing the standard scenarios and all of the associated crop, soil, and weather information.

1.1.2 Principal Criteria

The following principles guided the selection and development of the leaching scenarios:

- The number of locations should not exceed 10.
- The combinations of crop, soil, climate, and agronomic conditions should be realistic.
- The scenarios should describe an overall vulnerability approximating the 90^{th} percentile of all possible situations (this percentile is often referred to as a realistic worst case).
- The vulnerability should be split evenly between soil properties and weather.

The exact percentile for the soil properties and weather which will provide an overall vulnerability of the 90^{th} percentile cannot be determined precisely without extensive simulations of the various combinations present in a specific region. After exploratory statistical analysis, FOCUS (2000) decided that the overall 90^{th} percentile could be best approximated by using a 80^{th} percentile value for soil and a 80^{th} percentile value for weather. The 80^{th} percentile for weather was determined by performing simulations using multi-year weather data, while the 80th percentile soil was selected by expert judgement.

1.1.3 Selection of Locations

Locations were selected by an iterative procedure with the objective that they should:

- represent major agricultural regions (as much as possible).
- span the range of temperature and rainfall occurring in EU arable agriculture.
- be distributed across the EU with no more than one scenario per Member State.

The selection process involved an initial proposal of about ten regions derived from examining information from a number of sources (FAO climatic regions, recharge map of Europe, temperature and rainfall tables, land use information, etc.). This proposal was refined by dropping similar climatic regions and adding regions in climatic areas not covered by the original proposal. Some of these added scenarios are not located in major agricultural regions, but they represent areas with a significant percentage of arable agriculture in the EU, albeit diffuse (Table 1.1). The end result was the selection of nine locations (shown in Figure 1.1 and listed in Table 1.2).

The selected locations should also not be viewed as sites representative of agricultural in the countries in which they are located. Instead the sites should be viewed collectively as representative of agricultural areas in climatic zones with significant agriculture in the whole EU.

Table 1.1. Arable agriculture in EU climate zones.

Precipitation (mm)	Mean Annual Temperature (°C)	Arable land * (%)	Total Area * (%)	Representative Locations
601 to 800	5 to 12.5	31	19	Hamburg/Châteaudun
801 to 1000	5 to 12.5	18	13	Kremsmünster
1001 to 1400	5 to 12.5	15	12	Okehampton
601 to 800	>12.5	13	11	Sevilla/Thiva**
801 to 1000	>12.5	9	8	Piacenza
< 600	>12.5	4	4	Sevilla/Thiva
< 600	5 to 12.5	3	2	Châteaudun***
1001 to 1400	>12.5	3	3	Porto
< 600	<5	1	11	Jokioinen
>1400	5 to 12.5	1	1	--
1001 to 1400	<5	1	4	--
601 to 800	<5	1	8	--
801 to 1000	<5	0	3	--
>1400	<5	0	0	--
>1400	>12.5	0	0	--

*Relative to the area of the European Union in 2000 plus Norway and Switzerland.

**Although these locations have less than 600 mm of precipitation, irrigation typically used at these two locations brings the total amount of water to greater than 600 mm.

***Most areas in this climatic zone will be irrigated, raising the total amount of water to greater than 600 mm. Therefore, Châteaudun can be considered representative of agriculture in this climatic zone.

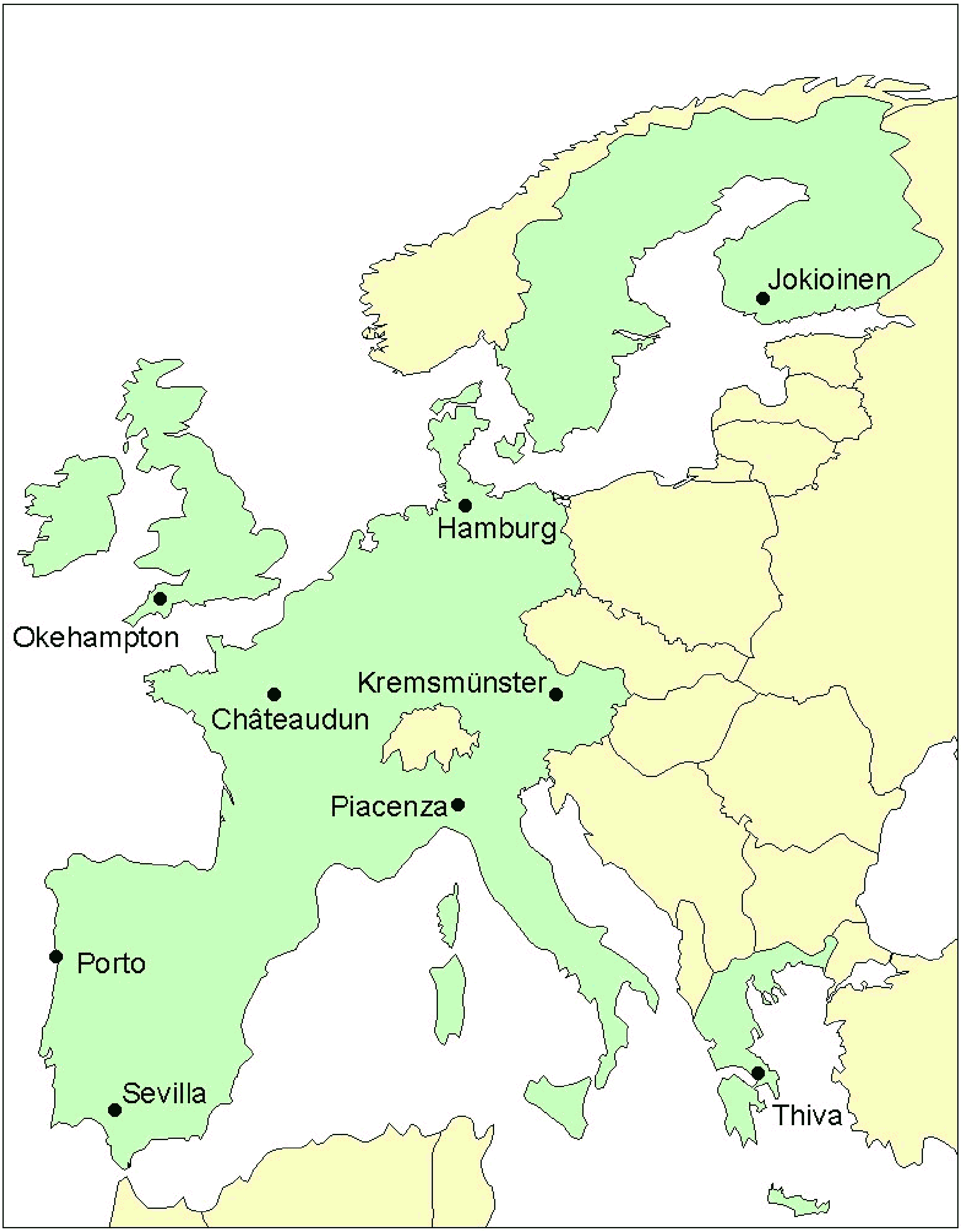

Figure 1.1. Location of the ground water scenarios.

The arable and total land area data in Table 1.1 is based on the work of Knoche *et al*., 1998. Temperature and precipitation boundaries were determined based on weather data of about 5000 stations in Europe from Eurostat (1997) and agricultural use was based on information from USGS *et al*. (1997). As a check, the same area data was also estimated using a second approach based on the data of FAO (1994) and van de Velde (1994). Both of these approaches resulted in very similar estimates.

Since the generation of Table 1.1, the number of countries in the EU has increased significantly. Therefore FOCUS Ground Water Work Group (FOCUS, 2009) assessed whether the FOCUS scenarios ‘covers’ the agricultural area of new member states. A scenario ‘covers’ an area when it represents either the same properties or represents a more vulnerable situation like higher rainfall amounts or lower organic carbon contents. The spatial analysis shows that the current set of FOCUS leaching scenarios is applicable to new member countries for the purpose of Tier 1 screening simulations.

1.1.4 Selection of Soils

The selection of the soil was based on the properties of all soils present in the specific agricultural region represented by a location. Thus unrealistic combinations of climatic and soil properties were avoided. The intent was to choose a soil that was significantly more vulnerable than the median soil in the specific agricultural region, but not so extreme as to represent an unrealistic worst case. Soils which did not drain to ground water were excluded when possible, therefore no drainage assumptions were required in the scenario definitions. This is a conservative assumption in terms of predicting leaching. Soil tillage was also ignored. Vulnerability was defined with respect to chromatographic leaching (that is, leaching is greater in low organic matter sandy soils than higher organic matter loams). The selection of appropriate soils was performed by expert judgement, except for the Okehampton location where SEISMIC, an environmental modelling data base for England and Wales, was used to select a suitable soil (Hallett et al., 1995). Soil maps (NOAA, 1992; Fraters, 1996) were used to obtain information on the average sand and clay fractions and the organic matter in a region. Based on these average values, target values for soil texture and organic matter were developed for each location to ensure that they were more vulnerable than the average. In consultation with local experts, soils were selected which met these target values (values for surface parameters are provided in Table 1.2). In some cases special consideration was given to suitable soils at research locations where measurements of soil properties were readily available (Châteaudun, Sevilla and Piacenza). In a few cases the target values had to be re-examined during the process of picking specific soils. The Hamburg scenario was based on the national German scenario. This national scenario was based on a soil survey intended to locate a worst case leaching soil, so the vulnerability associated with this soil significantly exceeds the target of an 80th percentile soil (Kördel et al, 1989). FOCUS (2009) revised the organic matter content of the Piacenza and Porto scenarios based on a spatial analysis of the climatic zones represented by the Porto and Piacenza locations that indicated a change in the organic matter was appropriate to make them fit the vulnerability concept. Detailed soil properties for all scenarios as a function of depth are provided in Section 3.

Table 1.2. Overview of the locations for the ground water scenarios.

Location	Mean Annual Temp. (°C)	Annual Rainfall (mm)	Topsoil Texture†	Topsoil Organic Matter (%)
Châteaudun	11.3	648 + I*	silty clay loam	2.4
Hamburg	9.0	786	sandy loam	2.6
Jokioinen	4.1	650	loamy sand	7.0
Kremsmünster	8.6	899	loam/silt loam	3.6
Okehampton	10.2	1038	loam	3.8
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Sevilla	17.9	493 + I*	silt loam	1.6
Thiva	16.2	500 + I*	loam	1.3

† = USDA classification (USDA, 1975; FAO, 1977)

I* = scenario also includes irrigation

1.1.5 Climatic Data

As part of the scenario selection process, targets for annual rainfall were also developed for each site based on tables of annual rainfall (Heyer, 1984). These target values were used by FOCUS (2000) to identify appropriate climatic data for a 20 year period. The resulting average values for rainfall at each site are shown in Table 1.2. Five locations (Châteaudun, Piacenza, Porto, Sevilla, and Thiva) were identified as having irrigation normally applied to at least some crops in the region.

1.1.6 Macropore Flow

The question of macropore flow was discussed at length in FOCUS (2000) and they decided to develop parameters for one scenario to be able to compare differences between simulations with and without macropore flow to help demonstrate to Member States the effect of macropore flow. The Châteaudun location was chosen for this scenario because soils at this site are heavier than at most of the other sites and because experimental data were available for calibrating soil parameters. The macropores in the profile at Châteaudun are present to about 60 cm depth. Note that macropore flow is just one form of preferential flow. Forms of preferential flow other than macropore flow are not considered by current models and were not considered by the workgroup.

1.1.7 Crop Information

FOCUS (2000) decided to make the scenarios as realistic as possible by including most major European crops (except rice which was excluded since scenarios for this crop are being developed elsewhere and the regulatory models being used are not suitable for predicting leaching under these flooded conditions). Crop parameters were obtained for five crops grown in all nine locations and for a further 20 crops grown in at least one location (Table 1.3). Sometimes parameters for a crop not typically grown in a specific area (for example, sugar beets in Okehampton) were included because such crops might be grown in similar soils and climates. Crops for each scenario were identified and cropping parameters were developed with the help of local experts. Some crops not included in this table can be simulated using these same parameters, e.g. pears map onto apples. On the other hand some crops and land uses cannot be mapped onto the crops in Table 1.3, e.g. Christmas trees, fallow land and rotational grassland.

The scenarios assume that the same crop is grown every year. For three of the crops (cabbage, vegetable beans, and carrots) there are multiple crops grown per season at some locations, with the standard practice for applications to be made to both crops. Some crops (such as potatoes) are rarely grown year after year. Therefore, an option was added to allow applications every year, every other year, or every third year. In order to conduct comparable evaluations, the simulation period was extended to 40 and 60 years for applications made every other year and every third year respectively (by repeating the 20 year weather dataset, with a date offset). The specification of applications to be made every other year or every third year is also applicable to products for which annual applications are excluded by a label restriction. Crop rotations are not explicitly simulated for reasons of technical difficulty.

The use of various crops for each location necessitated the development of crop-specific irrigation schedules for the five irrigated locations, namely Châteaudun, Piacenza, Porto, Sevilla, and Thiva.

Table 1.3. Crops included in FOCUS scenarios by location.

Crop	C	H	J	K	N	P	O	S	T
apples	+	+	+	+	+	+	+	+	+
grass (+ alfalfa)	+	+	+	+	+	+	+	+	+
potatoes	+	+	+	+	+	+	+	+	+
sugar beets	+	+	+	+	+	+	+	+	+
winter cereals	+	+	+	+	+	+	+	+	+
beans (field)		+		+	+				
beans (vegetables)							+		+
bush berries			+						
cabbage	+	+	+	+			+	+	+
carrots	+	+	+	+			+		+
citrus						+	+	+	+
cotton								+	+
linseed					+				
maize	+	+		+	+	+	+	+	+
oilseed rape (summer)			+		+		+		
oilseed rape (winter)	+	+		+	+	+	+		
onions	+	+	+	+			+		+
peas (animals)	+	+	+		+				
soybean						+			
spring cereals	+	+	+	+	+		+		
strawberries		+	+	+				+	
sunflower						+		+	
tobacco						+			+
tomatoes	+					+	+	+	+
vines	+	+		+		+	+	+	+

C Châteaudun, H Hamburg, J Jokioinen, K Kremsmünster, N Okehampton, P Piacenza, O Porto, S Sevilla, T Thiva.

1.1.8 Information on Crop Protection Products and Metabolites

Information on the chemical properties of crop protection products and their metabolites, application rates, and application timing are left to the user to provide. A more detailed discussion appears in Section 2.4, including recommendations for selecting values of the parameters required by the various models. Because the vulnerability of the scenarios is to be reflected in the soil properties and climatic data rather than in the properties chosen for the crop protection products and their metabolites, and because each simulation consists of twenty repeat applications, mean or median values (using a geometric mean of the sample population as the best estimate of the median of the whole population) are recommended for these parameters.

1.1.9 Implementation of Scenarios

Models. The remit of the workgroup was to develop scenarios generally suitable for evaluating potential movement to ground water. The intent was not to produce model-specific scenarios but rather describe a set of conditions that can continue to be used as existing models are improved and better models developed. However, simulating any of these scenarios with an existing model also requires the selection of many model-specific input parameters. Therefore, for uniform implementation of these standard scenarios, computer shells were developed to generate the input files needed for the various computer models. Such shells, which include all scenarios, were developed for three widely used regulatory models (PELMO, PEARL, and PRZM). A shell for MACRO, another widely used model (and the most widely used considering macropore flow), was developed for the macropore flow scenario at Châteaudun. These shells also included post-processors to calculate and report the annual concentrations used as a measure of the simulation results.

Simulation Period. As mentioned earlier, a simulation period of 20 years should normally be used to evaluate potential movement to ground water. When applications are made only every other year or every third year the simulation period should be increased to 40 and 60 years, respectively. In order to appropriately set soil moisture in the soil profile prior to the simulation period and because residues may take more than one year to leach (especially for persistent compounds with moderate adsorption to soil), a six year “warm-up” period has been added to the start of the simulation period. Simulation results during the warm-up period are ignored in the assessment of leaching potential.

Calculation of Annual Concentrations. The method for calculating the mean annual concentration for a crop protection product or associated metabolites is the same for all models. The mean annual concentration moving past a specified depth is the integral of the solute flux over the year (total amount of active substance or metabolite moving past this depth during the year) divided by the integral of the water flux over the year (total annual water recharge). In years when the net recharge past the specified depth is zero or negative, the annual mean concentration should be set to zero. All mean concentrations are based on a calendar year. When applications are made every other year or every third year, the mean concentrations for each of the 20 two or three year periods are determined by averaging the annual concentrations in each two or three year period on a flux-weighted basis.

In equation form, the average concentration past a specified depth is calculated as follows:

$$C_i = (\sum_{i,\ i+j} J_s) / (\sum_{i,\ i+j} J_w)$$

where C_i is the average (flux) concentration of substance at the specified depth (mg/L) for the period starting on day i, J_s the daily substance leaching flux (mg/m2/day), J_w the daily soil water drainage (l/m2/day) and j the number of days considered in the averaging period (365 or 366 days for a 20 year scenario; 730 or 731 for a 40 year scenario; 1095 or 1096 for a 60 year scenario).

For the Richard's equation based models (PEARL and MACRO), this average concentration includes the negative terms due to upward flow of water and solute. Therefore, when degradation is occurring below the specified depth, the upward movement can artificially increase the calculated average solute concentration at the specified depth. In these cases, the simulations should be conducted at the deepest depth which is technically feasible to minimise this effect. Alternatively, PELMO or PRZM could be used.

Simulation Depth. All simulations have to be conducted to a sufficient depth in order to achieve an accurate water balance. For capacity models such as PRZM and PELMO, this means that simulations must be conducted at least to the maximum depth of the root zone. For Richard’s equations models such as PEARL and MACRO, the simulations should be conducted to the hydrologic boundary. With respect to concentrations of active substances and metabolites, the EU Uniform Principles (product authorisation decision making criteria) refer to concentrations in ground water. However, a number of factors can make simulations of chemical transport in subsoils difficult. These include lack of information on subsoil properties, lack of information of chemical-specific properties of crop protection products and their metabolites, model limitations, and sometimes fractured rock or other substrates which cannot be properly simulated using existing models. Information on degradation of active substance and metabolites in subsoils is especially important, since in the absence of degradation the main change in concentration profiles is only the result of dispersion. Therefore, all model shells report integrated fluxes of water and relevant compounds at a depth of 1 m. Models may also report integrated fluxes at deeper depths such as at the hydrologic boundary or water table, where technically appropriate. As more information becomes available and improvements to models occur, the goal is to be able to simulate actual concentrations in ground water. Soil properties below 1 m are included in the soil property files for each scenario, along with the depth to ground water.

Model Output. The model shells rank the twenty mean annual concentrations from lowest to highest. The average between the sixteenth and seventeenth value (fourth and fifth highest) is used to represent the 80th percentile value associated with weather for the specific simulation conditions (and the overall 90th percentile concentration considering the vulnerability associated with both soil and weather). When applications are made every other or every third year, the 20 concentrations for each two or three year period are ranked and the average of the sixteenth and seventeenth values selected.

In addition to the concentration in water moving past 1 m, the outputs also include at a minimum a listing of the input parameters and annual water and chemical balances for each of the simulation years. Water balance information includes the annual totals of rainfall plus irrigation, evapotranspiration, runoff, leaching below 1 m, and water storage to 1 m. Chemical balances (for the active substance and/or relevant metabolites) include the annual totals of the amount applied (or produced in the case of metabolites), runoff and erosion losses, plant uptake, degradation, volatilisation losses, leaching below 1 m, and storage to 1 m. All variables may additionally be reported at a depth greater than 1 m, as discussed previously.

1.2 Weather and irrigation data for the FOCUS scenarios

Section 2.2 of the original FOCUS Groundwater Scenarios report (FOCUS, 2000) still stands as a description of how the weather data were derived and implemented, so repeating it here is not necessary. Refinements made by FOCUS (2009) were the use of FAO rather than MARS reference evapotranspiration and the evaporation from bare soil in PELMO and PRZM (see Section 11.5 in FOCUS, 2009).

The current irrigation routines are described in Section 11.5.3 of FOCUS (2009) / European Commission (2014). FOCUS (2009) decided that irrigation schedules should be developed for individual crops in Châteaudun, Piacenza, Porto, Seville, and Thiva. These irrigation schedules provide irrigation from the time of planting until start of senescence and are generated using irrigation routines in PEARL and PELMO, which apply irrigation once a week on a fixed day to bring the root zone up to field capacity. However, irrigation was applied only if the amount required exceeded 15 mm. Because of the minor differences remaining in the water balance (primarily evapotranspiration), the irrigation routines for PEARL and PELMO predict somewhat different amounts. However, using different irrigation routines tends to compensate for evapotranspiration differences to provide closer estimates between the two models for the amount of water moving below the root zone, which is the key water balance parameter affecting leaching. The irrigation amounts generated by PELMO are used directly in PRZM. While allowing PRZM to generate irrigation amounts is also possible, the work group decided that this added a level of complexity that was not needed, given the similarity of PELMO and PRZM. In PEARL 5.5.5 and PELMO 6.6.4 and later versions irrigation is applied at the soil surface and not the crop canopy (as was the case in earlier versions) for the permanent ‘row’ crops apples, citrus and vines.

1.3 Soil and crop data

Section 2.3 of FOCUS (2000) describes how the soil and crop data were derived and implemented. Sections 11.3 and 11.5 of FOCUS (2009) / European Commission (2014) describe refinements in this information. All of this data is provided in the tables in Chapter 3 of this report, with the exception of the crop interception data, which the user needs in order to adjust the application rate correctly. Note Chapter 3 includes corrections to errors to periods for Kc values between maximum leaf area and senescence for onions at the Porto and Thiva scenarios made in the FOCUS (2009) and European Commission (2014) reports.

Tables 1.4 and 1.5 give interception data for distinguished growth stages of different crops. The origin of these values is EFSA (2014). Note that the interception data in Tables 1.4 and 1.5 are only valid for applications made directly onto the crop. Examples where these data do not apply include herbicide applications made beneath orchard crops and vines, directly onto bare soil; for such applications zero interception should be assumed, and simulations should be made with the field-averaged application rate.

Table 1.4. Interception (%) by apples, bushberries, citrus and vines dependent on growth stage.

Crop	Stage				
	BBCH# 0–9	BBCH# 10–69		BBCH# 71–75	BBCH# 76–89
Apples	without leaves 50	flowering 60		early fruit development 65	full canopy 65
	BBCH# 0–9	BBCH# 10–69			BBCH# 71–89
Bushberries	without leaves 40	flowering 60		flowering 60	full foliage 75
Citrus	all stages 80				
	BBCH# 0–9	BBCH# 11–13	BBCH# 14–19	BBCH# 53–69	BBCH# 71–89
Vines	without leaves 40	first leaves 50	leaf development 60	flowering 60	ripening 75

#The BBCH code is indicative (Meier, 2001).

Table 1.5. Interception by other crops dependent on growth stage.

Crop	Bare – emergence	Leaf development	Stem elongation	Flowering	Senescence Ripening
	BBCH[#]				
	0– 09	**10–19**	**20–39**	**40–89**	**90–99**
Beans (field + vegetable)	0	25	40	70	80
Cabbage	0	25	40	70	90
Carrots	0	25	60	80	80
Cotton	0	30	60	75	90
Grass[##]	0	40	60	90	90
Linseed	0	30	60	70	90
Maize	0	25	50	75	90
Oil seed rape (summer)	0	40	80	80	90
Oil seed rape (winter)	0	40	80	80	90
Onions	0	10	25	40	60
Peas	0	35	55	85	85
Potatoes	0	15	60	85	50
Soybean	0	35	55	85	65
Spring cereals	0	0	BBCH 20–29*: 20 BBCH 30–39*: 80	BBCH 40–69: 90 BBCH 70–89: 80	80
Strawberries	0	30	50	60	60
Sugar beets	0	20	70 (rosette)	90	90
Sunflower	0	20	50	75	90
Tobacco	0	50	70	90	90
Tomatoes	0	50	70	80	50
Winter cereals	0	0	BBCH 20–29*: 20 BBCH 30–39*: 80	BBCH 40–69: 90 BBCH 70–89: 80	80

The BBCH code is indicative (Meier, 2001).

A value of 90 is used for applications to established turf

* BBCH code of 20-29 for tillering and 30-39 for elongation

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2. PESTICIDE INPUT PARAMETER GUIDANCE

2.1 Summary of Main Recommendations

This section contains detailed guidance on the input of substance-specific parameters for four different models that are recommended for use with some or all of the FOCUS scenarios. Much of this guidance is based upon a number of more general principles and recommendations. To help the modeller be aware of these, they are summarised below:

1. The scenarios are intended for tier one risk assessment, and therefore the guidance on the substance-specific input parameters aims to provide a degree of standardisation. This inevitably leads to over-simplification in some cases and hence, where more detailed data may be appropriate for higher tier modelling (e.g. the change of degradation rate with depth), this has been noted.
2. Simulations with the worst case intended use pattern requested for review must be undertaken but simulations can additionally be undertaken using the most typical intended use pattern.
3. Where there are a number of experimental values (e.g. degradation rate, sorption constants etc.) then the mean or median (as estimated by a geometric mean) values should generally be used rather than the extreme value. This is because the vulnerability of the scenarios has been shared between the soil and weather data, and so should not rest also with the substance properties (FOCUS, 2000).
4. Degradation rates used in the models should be determined using the procedures outlined by FOCUS (2006) and EFSA (2014).
5. The increase of sorption with time is a phenomenon that is widely accepted to occur. Guidance for incorporating non-equilibrium sorption is provided in Section 7.1.6 of FOCUS (2009) and European Commission (2014). The area of obtaining the parameters for modelling to describe increasing sorption with time from experimental measurements, has been an area where regulatory guidance has been developed. I.e. European Commission (2021).
6. Interception of the substance by the crop canopy should be determined by reference to the interception data provided in Tables 1.4 and 1.5 and a corrected application rate should be calculated. The substance should then be applied directly to the ground in all models, thus avoiding the internal interception routines in the models.
7. It is inevitable that different results will sometimes be produced by different models. However, the FOCUS workgroups have not attempted to reduce these simply by recommending the use of input data that simplify the individual model sub-routines to the lowest common denominator (dumb down). Even after the work of FOCUS (2009), the results are not sufficiently similar, so model simulations need to be performed with

PEARL and PELMO or PRZM. Where a crop of interest is defined for Châteaudun MACRO simulations need to be run. (EFSA PPR, 2013a and European Commission, 2014).

2.2 Introduction

The scenarios developed by the FOCUS are aimed to assist the risk assessment required for the review of active substances under Directive 91/414/EEC and Regulation (EC) No 1107/2009. A number of Member States (MS; Germany [Resseler *et al*., 1997], The Netherlands [Brouwer *et al*., 1994], UK [Jarvis, 1997]) have already produced guidance for modelling under their national plant protection product legislation and this has been taken into account in the current document. Unsurprisingly MS have historically differing views over the most appropriate input values for models. Therefore, our task is to provide clear guidance to users on appropriate values to input into models for risk assessment under Directive 91/414/EEC and Regulation (EC) No 1107/2009, at Tier 1, while still retaining the support of the MS.

The aim of these scenarios is to be a first tier to the risk assessment and this does not exclude the possibility of more detailed modelling at subsequent times. As a first tier, a high degree of standardisation of the model inputs has been undertaken. For instance, the model input values for the nine selected soils have been fixed and are not subject to user variability. Similarly the crop, weather and much of the agricultural practice data have been provided as set inputs. The modeller therefore has only to input various substance-specific parameters in order to achieve consistent results for the substance of interest in the scenarios provided.

Comparative modelling exercises have shown that the modeller can be a significant variable in the range of output data obtained from the same available information for input (Brown *et al*., 1996, Boesten, 2000). Therefore we consider it important to attempt to reduce still further the amount of variation introduced. By necessity, individual users must provide their own input values for their substance of interest. However, this provides the opportunity for different users to input different substance-specific information into the models, even though they have the same range of data available to them.

This chapter aims to provide further advice to users to help them select a representative single input value from a range that may be available and to help less experienced users to be aware of the most appropriate form of the data to use in particular models. It is important in this context that the user recognises that the quality of the experimental data may vary and this should be taken into account when selecting input parameters for modelling. The guidance cannot be exhaustive in considering all substance-specific factors but it attempts to highlight the major differences between models where it is likely to have a significant effect on the results of the simulation. Note that this guidance is aimed specifically for Tier 1 FOCUS ground water scenarios and is not necessarily appropriate for the wider use of the models. Any user is also advised to check their proposed input data prior to running the model to ensure that the totality of the substance-specific input values results in a realistic reflection of the general behaviour of the compound.

In developing these scenarios FOCUS has chosen to include three different models for all scenarios and a further model for a macropore flow scenario. It is inevitable that some differences in the outputs will occur between the differing models. To some extent this is a strength of the project since differing models treat the varying transport and transformation processes in different manners and hence for specific situations some models are likely to account for substance behaviour better than others. It is not within the FOCUS remit to validate the various model sub-routines nor is it our aim to reduce all the processes simulated to the lowest common denominator with the intention of producing the same result from all models. Therefore where models deal with processes such as volatilisation in differing manners, this guidance does not attempt to artificially manipulate the recommended input data with a view to reducing variability of the results. In these cases the best guidance and sources of information are provided for each of the different processes. In the majority of cases however, recommendations for standardised inputs are made (i.e. when the same input parameter is required by different models but in differing units etc.).

Finally, these scenarios have been developed to provide realistic worst case situations for the EU review process. The user should recognise that vulnerability is being covered by the choice of soils and climates and, therefore, choices of extreme values of substance-specific parameters would result in model predictions beyond the 90^{th} percentile.

2.3 General guidance on parameter selection

Directive 91/414/ EEC and Regulation (EC) No 1107/2009 require that estimations of PECgw are made for both the active substance and metabolites or transformation products. (Levels triggering ground water assessment for metabolites are presented in Sanco/221/2000-rev.10 25 February 2003). Historically most models and modellers have principally addressed the leaching of the parent compound but routines are now available in many models (including those used with the FOCUS scenarios) to directly assess the mobility of metabolites if required. In order to use these routines it is necessary to have information on either, the proportion of each metabolite formed (kinetically derived formation fraction), or on the individual rate constants for the formation of each metabolite. If this information is not available, a less sophisticated, but nonetheless valid, method is to substitute the metabolite data for the parent compound in the model and adjust the application rate to correspond to the amount of metabolite formed in the experimental studies. This method may lead to underestimation of leaching concentrations, especially when the parent is rather mobile and the user should be aware of this. In either situation the guidance in this document applies equally to the parent or metabolite.

The ground water leaching scenarios have been provided for four models; PRZM (PRZM 3.0 Manual; Carsel *et al*., 1998), PELMO (Jene 1998), PEARL (Leistra *et al*, 2000), and MACRO (Jarvis and Larsson, 1998). Each of these models requires the same general information regarding the most important substance properties (e.g. degradation rate, sorption). However, all input these data in slightly different ways. This section addresses general information such as the broader availability of input data and the follow section addresses specific parameters. Further information on the differences between earlier versions of the models can be obtained from FOCUS (1995). However, the reader should be aware that some significant changes may have occurred in more recent versions of the models.

Regardless of the particular model, the amount of data available from which to select the model input varies significantly from parameter to parameter. For a number of the input parameters, such as diffusion coefficients, degradation rate correction factors for temperature and moisture and transpiration stream concentration factor (TSCF), substance-specific data is unlikely to be available or alternatively is unlikely to be more reliable than a generic average. Default values for such parameters are recommended by FOCUS (2000, 2009) and European Commission (2014).

For a further number of the input parameters, such as the physico-chemical properties, and the management-related information, the values are generally straightforward to input into the models. The physico-chemical property data are generally available as single values from standard experiments conducted as part of the registration package. The management related parameters can be obtained from the intended Good Agricultural Practice (GAP). For the management related parameters the worst case supported must be used (i.e. highest application rates, most vulnerable time for leaching etc.). In addition, the most typical uses can also be simulated if significantly different.

For the remaining parameters, such as degradation rate, kinetic formation fraction of metabolites, and soil sorption, a number of experimental values are generated as part of the registration package. Determining which single value should be used as input for each parameter is difficult and contentious since the relevant output data can vary significantly depending on which of the range of possible values are used as input.

The environmental fate data requirement annexes to Directive 91/414/EEC (95/36/EC) and data required for Regulation (EC) no 1107/2009 require that reliable degradation rate endpoints are available from a minimum of four soils for the parent compound and three soils for metabolites (laboratory studies initially and then, if necessary, field studies). (The trigger levels for assessing metabolites are defined in the data requirements for Regulation (EC) no 1107/2009 and in Sanco/221/2000-rev.10 25 February 2003.) Therefore FOCUS (2000, 2006) recommends that where reliable endpoints for the parent compound are available in a minimum of four different soils it is generally acceptable to use the geometric mean of the degradation rates as input into the model. Similarly, FOCUS (2000, 2006) recommends that where reliable endpoints for metabolites are available in a minimum of three different soils it is generally acceptable to use the geometric mean of the degradation rate as input into the model. EFSA (2014) also prescribes that a geometric mean value is selected as input, except when degradation rate is correlated with soil properties such as pH. FOCUS (2000, 2006) also provides for the exception when degradation rate is correlated with soil properties. Further guidance on using substance properties other than the geomean, if there is a significant change in substance properties within a soil pH range 5.1–8.0 was provided in the FOCUS Surface Water Repair report (EFSA, 2020) which is also applicable to groundwater simulations. This recommends performing two simulations at ‘contrasting pH values’, so assuming substance properties representative for a soil $pH_{(water)}$ of 5.1 and 8.0, respectively, and to report the results from both runs. In situations where less than the required number of reliable degradation rates from different soils can be derived further experimental data should be generated (EFSA, 2014).

For the kinetic formation fractions of metabolites from their precursor/s FOCUS (2006) recommends an arithmetic mean is used.

Reliable soil sorption results (K_{Foc}, K_{oc} or K_{Fom}, K_{om}) are also required in a minimum of four soils for parent compound and in a minimum of three soils for metabolites that reach levels defined in Sanco/221/2000-rev.10 25 February 2003 and/or the environmental fate data requirement annexes to Directive 91/414/EEC and data required for Regulation (EC) No 1107/2009. Where these are all representative agricultural soils, EFSA (2014) prescribes that the geometric mean value of the sorption constant normalised for organic carbon (K_{Foc}, K_{oc}, K_{om} or K_{Fom}) be input to the models, unless the sorption is indicated to be pH-or other soil property dependent. In situations where there are reliable results from less than the required number of different agricultural soils then further experimental data should be generated.

When characterising sorption behaviour of ionic compounds, the value will vary depending on the pH and a geometric mean value is no longer appropriate. For some compounds, both sorption and degradation are pH dependent. Under these conditions, use of linked values of Koc and degradation rates is appropriate. Inputs should be selected with the aim of obtaining a realistic rather than an extreme situation and the values used should be justified in the report.

Though FOCUS (2000, 2009) recommended a first approach for compounds with pH dependent sorption of running the scenarios with the soil pH defined for the specific FOCUS scenarios (provided in the tables in Chapter 3), EFSA PPR (2013a) / European Commission (2014) considered that this was not appropriate. Therefore Tier 1 simulations for consideration of EU approval should select adsorption values, chosen to represent a realistic worst case considering the pH of the soils in the EU that are used for the production of the pertinent crop. Normally this pH would be selected to minimise sorption; however, there are certain compounds for which lower sorption results in faster degradation. In addition to choosing adsorption values that represent a realistic worst case applicants might also provide simulations for all scenarios selecting a contrasting adsorption value associated for a more best case, considering the pH of the soils in the EU that are used for the production of the pertinent crop. Decision makers would then get a view on the range of recharge concentrations that can result depending on the average pH of the soils overlying a confined aquifer in a particular region. As an example, for a compound with a single ionisable functional group that follows a typical S shaped relationship for adsorption with pH, such as a weak acid, two contrasting pH values for which best and worst case adsorption estimates could be selected would be associated with a soil pH (measured in water) of 5.1 and 8.0 respectively if the crop could grow in this range of soil pH. If the pH relationship was more ∩ or U shaped, adsorption associated with an intermediate pH as the best or worst case respectively could be justified. Using correct pH maps and using soil column pH descriptions to parameterise scenarios in case of pH dependent substance properties, was considered more important in assessments at the national level rather than the EU level by the EFSA PPR panel (EFSA PPR, 2013a).

Further guidance on using substance properties other than the geomean, if there is a significant change in substance properties within a soil pH range 5.1–8.0 was provided in the FOCUS Surface Water Repair report (EFSA, 2020) which is also applicable to groundwater simulations. This recommends performing two simulations at ‘contrasting pH values’, so assuming substance properties representative for a soil $pH_{(water)}$ of 5.1 and 8.0, respectively, and to report the results from both runs.

Representative substance properties for soil pH values of 5.1 and pH 8.0, respectively, may be obtained by: (i) applying a sigmoid equation (as outlined in EFSA, 2017a, particularly for weak acid substances), (ii) applying a linear or any other suitable mathematical equation and calculating substance properties at pH 5.1 and pH 8.0 on the basis of this equation, or (iii) splitting the data into two subsets and calculating mean sorption values for both subsets. Because of the median pH values in the EU being close to a pH(water) of 6.5, it is recommended to set the split point close to this pH value, if applicable. In principle, these approaches apply to both the sorption constant (K_d, K_{oc} or K_{Foc}) and the Freundlich sorption exponent (1/n) as well as to the formation fraction and the properties of any metabolites. In any case, the correlation between substance properties and soil pH should be proven to be significant by means of adequate statistical tests (e.g. Kendall's tau-b (τ_b) test, two-sided or Pearson's test for small samples sizes). Note that pH values measured in matrices other than water (e.g. $CaCl_2$ or KOH) should be converted into pH values measured in water applying a suitable transfer equation (e.g. Boesten *et al*., 2012). Care should be taken if experimental data do not cover the entire pH range avoiding extensive extrapolation.

For all model inputs derived from the regulatory data package, only studies of acceptable quality should be considered.

2.4 Guidance on substance-specific input parameters

2.4.1 Physico chemical parameters

Molecular Weight. In PELMO this can be used to estimate the Henry's law constant if required. In PELMO and PEARL these data are also required to correct concentrations for the differing molecular weights of parents and metabolites.

Solubility in Water. In PEARL this is required for the model (units: mg/L) to calculate the Henry's law constant (this is only appropriate for non-ionised compounds). In PELMO this can be used to determine the Henry's law constant if this value is not input directly (see below).

Vapour Pressure. In PEARL this is required for the model (units: Pa) to subsequently calculate the Henry's law constant. In PELMO this can be used to determine the Henry's law constant if this value is not input directly (see below).

pK_a-Value (if acid or base). The pK_a value has an effect on the sorption of a compound at different pH values (i.e. dissociated acidic molecules are more mobile than the uncharged acid conjugates). When simulating the behaviour of compounds which dissociate, the user should thoroughly describe which charge transfer is given by the pK_a value (i.e. $H_2A \rightarrow HA^-$,

$HA^- \rightarrow A^{2-}$ etc.). PELMO and PEARL can account directly for the effect of changing ionisation with pH. PELMO requires both the pK_a value and the reference pH at which the K_{oc} was obtained in order to adjust the sorption for pH in the profile. PEARL requires both the pK_a value and the two extreme K_{om} values (one at very low pH and one at very high pH). MACRO_DB also has a similar routine if this is used to parameterise MACRO.

FOCUS (2009) decided to make the pH-H_2O values of the FOCUS groundwater scenarios available electronically because most of the values provided for the soil profiles were pH-H_2O values (FOCUS, 2000). Models may now be used to describe the sorption of substances showing pH dependent sorption, however the modelling report should demonstrate that the adsorption values predicted by the model fit the experimental data. Using an experimental adsorption value appropriate for the soil pH of the relevant FOCUS scenario is not considered an acceptable method of including pH dependent sorption into the FOCUS scenarios when used for applications to support EU level decision making. This is because these scenarios cannot be considered to possess the FOCUS-defined vulnerability as the FOCUS (2000) (as updated by FOCUS (2009)) scenario selection procedure did not consider pH effects as a variable when defining 80th percentile soil column descriptions. Defining scenario vulnerability using correct pH maps in case of pH dependent sorption was considered more important in assessments at the national level rather than the EU level by the EFSA PPR panel (EFSA PPR, 2013a).

When introducing a measured K_{oc}-pH relationship into the FOCUS leaching models, the pH-H_2O measuring method must be consistent with that used for analysing the sorption measurements. If the pH-H_2O is not available for the soils from the adsorption studies, it can be calculated as follows (Boesten *et al*., 2012):

$$\text{pH-}H_2O = 0.860\ \text{pH-KCl} + 1.482$$

$$\text{pH-}H_2O = 0.982\ \text{pH-}CaCl_2 + 0.648$$

where pH-KCl is the pH measured in an aqueous solution of 1 mol/L of KCl and where pH-$CaCl_2$ is the pH measured in an aqueous solution of 0.01 mol/L of $CaCl_2$.

Reference pH-Value at which K_{oc}-Value was Determined. This is required for PELMO only (see above).

Dimensionless Henry's Law Constant. The Henry's law constant can be used as a direct input in PRZM and PELMO (in PEARL the model calculates the value from input values of water solubility and vapour pressure; see above). This value (H; in its dimensioned form of

Pa m³ mol^{-1}) should be available for the active substance as it is required as part of the substance dossier for review under Directive 91/414/EEC and Regulation (EC) No 1107/2009. Care should be taken with the units of the Henry's law constant. In PRZM the Henry's law constant value is dimensionless (this is also often stated as the air/water partition coefficient, K_{aw} i.e. has no units due to concentrations in the gas and liquid phases being expressed in the same units, usually mol/m³) but in PELMO the units are Pa m³ mol^{-1} (equivalent to J/mol). The conversion factor from K_{aw} (dimensionless) to H (Pa m³ mol^{-1}) is as follows $H = K_{aw} R T$, where R is the universal gas constant (8.314 Pa m³ mol^{-1} K^{-1}) and T is in K.

The Henry's law constant is used to calculate the volatility of the substance once in the soil. MACRO does not include this parameter and is unable to simulate volatilisation of substance, so this model may not be the most appropriate for compounds which possess significant volatility.

If the soil degradation rate is a value derived from field studies (see below) it will incorporate all relevant degradation/dissipation processes, including volatilisation. Therefore care should be taken regarding the use of the Henry's law constant input. This is particularly important for substances which show some volatility.

Diffusion Coefficient in Water. This is required for MACRO and PEARL only. The suggested default value is 4.3 x 10^{-5} m²/day (Jury, 1983; PEARL units) which is equivalent to 5.0 x 10^{-10} m²/sec (MACRO units). This is generally valid for molecules with a molecular mass of 200-250. If necessary, a more accurate estimate can be based on the molecular structure of the molecule using methods as described by Reid & Sherwood (1966).

Gas Diffusion Coefficient. This is required for PELMO, PRZM and PEARL. The suggested default value is 0.43 m²/day (Jury, 1983; PEARL units) which is equivalent to 4300 cm²/day (PRZM units) and 0.050 cm²/sec (PELMO units). This is generally valid for molecules with a molecular mass of 200-250. If necessary, a more accurate estimate can be based on the molecular structure of the molecule using methods as described by Reid & Sherwood (1966).

Molecular Enthalpy of Dissolution. This is required for PEARL. The suggested default value is 27 kJ/mol.

Molecular Enthalpy of Vaporisation. This is required for PEARL and PRZM. The suggested value is 95 kJ/mol (PEARL) which is equivalent to 22.7 kCal/mol (PRZM).

2.4.2 Degradation parameters of the active substance/metabolite

Degradation Rate or Half-Life in Bulk Topsoil at Reference Conditions. The guidance in EFSA (2014) that also relies on FOCUS (2006) provides guidance for determining degradation rates for both laboratory and field studies. With either type of data, the degradation rates should be normalised to reference conditions. The procedure for normalising laboratory data to reference conditions (moisture of 10kPa (pF2) and temperature of 20°C) is provided later in this section. FOCUS (2006) provides the procedure for normalising field data. EFSA (2014) recommends that the time step normalisation procedure from FOCUS (2006) is used. When using field data, the degradation must be parameterised in such a way as to avoid duplicating degradation processes. Either laboratory degradation or field degradation or combined laboratory and field degradation rates should be used following a consideration of the available data as outlined in EFSA (2014). In addition the modeller should take into account the effect of this decision on the parameterisation of the model. PEARL, PELMO, PRZM (PRZM 3.15+ only), and MACRO all have the ability to operate using degradation rates normalised to reference conditions.

Degradation of compound in soil may not be suitably described in all cases with single first order kinetics models. In these cases non-equilibrium sorption approaches in FOCUS models with linked sorption and degradation routines (see Section 7.1.6 of FOCUS, 2009 / European Commission (2014)) should be checked to see if they are capable of describing the behaviour of the compound and therefore suitable for use in predicting leaching to ground water. Information on this subject is also given in FOCUS (2006) (see especially Section 7.1.2.2.1 and Appendix 4).

Metabolism Scheme (if Necessary with Transformation Fractions (parent to metabolites). PRZM, PELMO and PEARL are capable of directly simulating the behaviour of metabolites through a transformation scheme within the model. To undertake this, the models require all the same substance information for the metabolite as for the parent and, in addition, input is required on the nature of the degradation pathway. MACRO is able to simulate parent plus one metabolite, but a metabolite file must be created during a simulation with the parent compound. This file can then be used as the input data for a subsequent simulation for the metabolite.

PRZM and PEARL require information regarding the sequence of compound formation and what fraction of the parent ultimately degrades to the metabolite (for PEARL and PRZM this fraction is required for each parent-daughter pair). MACRO also requires information on the fraction of the parent that degrades to the metabolite. PELMO uses the rate constants for each degradation pathway (therefore if the parent degraded to two metabolites, rate constants for the degradation of the parent to each of the compounds is used in simulations). Each of the two forms of data used by the different models is easily converted to the other. Note that in FOCUS PELMO 6.6.4 and later versions, the user has the option to input the kinetic formation fraction from precursor(s) via the FOCUS PELMO shell. I.e. analogous to the approach of the FOCUS shells of MACRO, PELMO and PRZM. When the user chooses the approach of entering the rate constant in the shell of FOCUS PELMO 6.6.4 and later, a stoichiometric factor can be entered which can be different to 1. This facilitates the execution of a single run for a metabolism scheme where mass is generated by the simulation, as can be achieved when the sum of two formation fractions from the same precursor is > 1, when using formation fraction entry. Previous versions of PELMO were not able to generate mass in simulations, so multiple runs were needed when the regulatory modelling approach needed this situation to be simulated. Degradation rates of parent and metabolites are usually estimated by a computer fitting program based on the percentages of each compound present at each timepoint and a proposed (by the user) route of degradation. Further guidance on best practice for these procedures is included in FOCUS (2006). FOCUS (2006) recommends arithmetic mean kinetic formation fractions are derived from these estimates made by the pertinent computer fitting program and associated pertinent compartment model, when this is feasible. Guidance is also given in FOCUS (2006) on approaches, when robust kinetic formation fractions made by the pertinent computer fitting program prove problematic.

Reference Temperature. Where laboratory data have been obtained in line with current EU guidelines (95/36/EC), the reference temperature will be 20°C. Degradation rates obtained at other temperatures should be corrected to this value before averaging (using the procedures described later in this section) or being used directly in model simulations.

Reference Soil Moisture (gravimetric; volumetric; pressure head). Guidelines for laboratory degradation studies require that these are undertaken at a moisture content of 40-50% MWHC (maximum water holding capacity; SETAC, 1995) or matric potential of pF 2-2.5 (OECD 307, 2002). Additional data provided in study reports may include the actual moisture content of the soil during the study as volumetric (% volume/volume), or as gravimetric (% mass/mass). Other studies may define the reference soil moisture in terms of; % field capacity (FC), or as other matric potential values such as kPa or Bar.

The availability of water within a soil profile, and therefore its effect on the rate of pesticide degradation, depends on the texture of the soil. Heavier soils contain a larger percentage of water before it becomes "available" than do lighter soils. For this reason studies are usually undertaken at defined percentages of the MWHC or FC, or at defined matric potentials, to attempt to ensure that experimental conditions are equivalent. However, by strict principles of soil physics some of these values have no definition (and some have no consistent definition), hence it is very difficult to relate them to each other directly. It is only via the actual water contents associated with some of these terms that comparisons can be made between values.

There is however, little advantage in simply using the actual water content from the experimental study as input into the model, as the DT50 used is likely to be an average from a number of soils. The solution to this problem is not straightforward but, since the concept of matric potential is independent of soil type and can be related to volumetric water content, a reference moisture content of 10kPa (pF2) must be used with the FOCUS scenarios. It is further recommended that for the purposes of this guidance, this value be considered as field capacity for PELMO and PRZM and in any study report where field capacity is specified without any reference to the matric potential or actual moisture content.

This requires that a complex procedure is undertaken to normalise the DT50 values from all laboratory studies before an average value (geometric mean) can be calculated.

(i) The moisture content of each soil must first be converted to a volumetric or gravimetric value (The soil moisture correction is based on a ratio (θ/θ_{REF}) and hence the actual water content units are unimportant as long as they are consistent). If these values are not available in the study report then Tables 2.1 and 2.2 provide guidance on conversion methods based on average properties for the stated soil types (Wösten *et al*., 1998; PETE). If more than one of the available methods of measurement is given in the study report then it is recommended that the value that appears first in Table 2.1 be used for the conversion process.

Note that the optimal data to use are the specific moisture content at which the experiment was undertaken and the moisture content at 10kPa for the given soil as stated in the study report. All conversions stated in Table 2.1 are approximations based on generic properties of soil types and these could, on occasion, produce anomalous results. Therefore the user should also consider any transformed water contents in comparison to the original study data to ensure the derived data provide reasonable results.

Table 2.1. Generic methods for obtaining soil moisture contents for subsequent DT50 standardisation.

Units provided	Required unit for soil moisture normalisation			
	%v/v (volumetric)		% g/g dry weight (gravimetric)	
	Value used in experiment	Value at field capacity (10kPa)	Value used in experiment	Value at field capacity (10kPa)
% FC (assumed 10kPa)	Conversion to volumetric or gravimetric water content unnecessary since fraction of FC can be input directly into Walker equation (i.e. = θ/θ_{REF})			
% g/g (gravimetric)			As stated	Use default gravimetric value at field capacity for texture type given in Table 2.2
% v/v (volumetric)	As stated	Use default volumetric value at field capacity for texture type given in Table5.2		
kPa	In reality the only values are likely to be 5 or 10kPa. 10kPa is the defined value of field capacity and therefore no correction is required. 5 kPa is slightly wetter than field capacity but the assumption is made that degradation rates do not change at water contents between field capacity and saturation therefore these values also do not need a moisture correction. Note: If water contents are given as fractions of 5 or 10 kPa then they can be treated in the same manner as fractions of field capacity			
pF	In reality, the only values are likely to be 2 or 2.5 (10 and 33kPa respectively). pF 2 (10 kPa) is the defined value of field capacity and therefore no correction is required.			
			For pF 2.5 (also given as 33kPa or 1/3 Bar) Use default gravimetric value at pF 2.5 for texture type given in Table 2.2	Use default gravimetric value at field capacity for texture type given in Table 2.2
Bar	In reality the only values are likely to be 75% of 1/3 bar.			
			Use default gravimetric value for texture type at 1/3 Bar given in Table 2.2. Calculate % gravimetric at given % of 1/3 Bar	Use default gravimetric value at field capacity for texture type given in Table 2.2
% MWHC (Maximum water holding capacity; assumed 1kPa, i.e. pF1)			Use default gravimetric value for texture type at MWHC given in Table 2.2. Calculate % gravimetric at given % of MWHC	Use default gravimetric value at field capacity for texture type given in Table 2.2

Table 2.2 Default values for moisture contents for soils at field capacity, maximum water holding capacity and 1/3 Bar (based on HYPRES [Wösten *et al*., 1998]; PETE)*.

USDA classification	Proposed UK/BBA equivalent classification	Volumetric water content at 10 kPa (field capacity) (θ_{v10}) (%)	Gravimetric water content at 10 kPa (field capacity) (W_{10}) (%)	Gravimetric water content at 1/3 Bar (pF 2.5, 33kPa) (W_{33}) (%)	Gravimetric water content at MWHC (1kPa) (%)
Sand	Sand	17	12	7	24
Loamy sand	Loamy sand	20	14	9	24
Sandy loam	Sandy loam	27	19	15	27
Sandy clay loam	Sandy clay loam	31	22	18	28
Clay loam	Clay loam	38	28	25	32
Loam	Sandy silt loam	34	25	21	31
Silt loam		36	26	21	32
Silty clay loam	Silty clay loam	40	30	27	34
Silt	Silt loam	37	27	21	31
Sandy clay	Sandy clay	40	35	31	41
Silty clay	Silty clay	46	40	36	44
Clay	Clay	50	48	43	53

* The PETE database gives average topsoil organic carbon content and undisturbed soil bulk density based on over 3000 UK soil profiles. The average of these bulk density values and those predicted by HYPRES (using mid-range sand, silt and clay percentage for the given soil classes) was used for the calculations. The pedotransfer functions from HYPRES were used to determine the soil water content at the given matric potentials based on bulk density, organic carbon content and particle size characteristics. It has been assumed that these data from undisturbed soil profiles provide an acceptable approximation to disturbed profile data which are generally stated in regulatory reports (water contents in disturbed soil profiles are likely to be higher and hence the generic data provided above would lead to more conservative [longer] standardisations of the DT_{50})

(ii) The water content at 10kPa (pF2) for the given soil is also determined. For the purposes of FOCUS this can be considered equivalent to field capacity. If this information is not provided it can be approximated as shown in Tables 2.1 and 2.2.

(iii) Once the moisture content data are converted to water contents (ensuring units are the same), then the DT50 can be manually corrected to that at 10kPa (pF2) using the same moisture dependent correction equation as used in the models. The correction factor is expressed as $(f) = (\theta/\theta_{REF})^B$ (see relevant section of this guidance). Each DT50 is then multiplied by this factor to obtain values normalised to 10kPa (pF2). In cases where the water content of the experimental soil is calculated to be above field capacity then the DT50 should be considered to be the same as that at field capacity (i.e. no correction required)

(iv) The average DT50 (geometric mean or for large data sets median value) can then be calculated from each individual value normalised to 10kPa.

PELMO and PRZM allow reference water contents to be input as % FC. Therefore, following the normalisation procedure a value of 100% should be used. The default option in PEARL implies that the degradation rate was measured at a matric potential of –10 kPa (-100 hPa). It is also possible to specify the reference water content in kg/kg but this option is not used for FOCUS. For further information the actual volumetric water content at 10kPa for each scenario is provided in Table 2.3.

Table 2.3. Topsoil volumetric water contents of the FOCUS scenario locations at field capacity (10kPa).

C	H	J	K	N	P	O	S	T
37.4	29.2	30.4	33.4	35.8	33.9	44.3	36.4	34.0

Recent versions of MACRO allow the degradation rate to be specified at a reference moisture content of pF 1 or 2 (i.e.10kPa).

This results in an equivalent DT50 value being used as input for each scenario and each model.

To provide some clarity to this normalisation procedure an example is given as follows. A study is undertaken in 4 soils at 45% MWHC and 20°C and the results are shown below:

Soil Type (USDA classification)	DT50	Gravimetric Water Content at MWHC
Sandy loam	100	34
Sand	150	27
Clay loam	85	47
Silt	80	41

1. Since the gravimetric water content at MWHC is measured it is most appropriate to use these soil specific values as the basis of the normalisation process. 45% MWHC (the moisture content under study conditions) is therefore 15.3, 12.2, 21.2 and 18.5% g/g in the sandy loam, sand, clay loam and silt soils respectively.
2. No data regarding the water content at 10kPa is provided and therefore the default data from Tables 2.1 & 2.2 are used to obtain approximated values for these soil types i.e. 19, 12, 28, 26% g/g for the sandy loam, sand, clay loam and silt soils respectively.
3. Using the Walker equation, a correction factor (f) for the degradation rate at 10 kPa can be worked out as follows (f)= $(\theta/\theta_{REF})^{0.7}$.
   f = $(15.3/19)^{0.7}$ = 0.86 for the sandy loam soil
   The default data suggest that the sandy soil is above field capacity therefore a value of 1 (i.e. no correction for moisture content) is used

$f = (21.2/28)^{0.7} = 0.82$ for the clay loam soil

$f = (18.5/26)^{0.7} = 0.79$ for the silt soil

4. Multiplying the DT50 values by the appropriate factors gives values of 86, 150, 70 and 63 days for the sandy loam, sand, clay loam and silt soils respectively at 10 kPa. The geometric mean of these values is 87 days.
5. The input onto the relevant model would be a DT50 of 87 days at the field capacity (10kPa, pF 2) of the soil.

Factors or Function for the Adjustment of Degradation rates in Different Depths. This parameter can have a large effect on the amount of substance simulated to leach to ground water and is required for all four models. Unfortunately experimental data are rarely available and hence estimation methods are usually required. Consideration should be given to whether degradation is predominantly chemical or microbial. If the substance degrades solely (or predominantly) by chemical processes (i.e. hydrolysis) then the rate of degradation does not need to change dramatically down the profile (unless degradation is pH sensitive, in which case further consideration may be required). In this case the modeller should provide a justified argument and proceed to more specific (Tier 2) modelling. The scenarios provided by FOCUS have assumed that degradation is microbially mediated and have provided default factors which should not be altered by the user unless specific experimental data are available. The group considers that, in the light of current understanding, the most appropriate factors by which to multiply the degradation rate with depth (i.e. increase the half life) are as follows (Boesten and van der Pas, 2000; Di *et al*, 1998; Fomsgaard, 1995; Helweg, 1992; Jones and Norris, 1998; Koch *et al*, 1979; Kruger *et al*, 1993 & 1997; Lavy *et al*, 1996; Smelt *et al*, 1978ab; Vaughan *et al*, 1999):

0-30 cm	1
30-60 cm	0.5
60-100 cm	0.3
>100 cm	no degradation

Due to slightly varying horizon depths in the nine soils selected, there are some minor adjustments to these values and these are provided with the soils data for the scenarios (See Chapter 3).

This parameter is input into the models in two differing manners. MACRO and PRZM require the degradation rates at each depth to be input directly (after the changes with depth have been manually estimated – this is done automatically in the PRZM and MACRO shells according to the specifications above). PEARL and PELMO require a factor to be input for each depth, which is then used by the model to provide a degradation rate relative to that in the topsoil.

If any modeller possesses degradation rate data at depths below 1 m which they intend to use to increase the realism of a higher tier simulation, then they should be aware of a potential anomaly that could occur in the results at 1m depth. For the Richards equation based models (PEARL and MACRO) the average concentration at 1m includes the negative terms due to upward movement of water and solute. Therefore, when degradation is occurring below the specified depth, the upward movement can artificially inflate the solute concentration. In these cases the simulations should be conducted at the deepest depth which is technically feasible to minimise this effect. Alternatively, PELMO or PRZM could be used.

Parameters Relating Degradation Rate to Soil Temperature. The four models require different factors to relate degradation rate to soil temperature but all are related. The user should ensure that equivalent values are used if any comparison of model outputs is undertaken ($\gamma = \alpha = (\ln Q_{10})/10$).

The Q10 factor is required for PELMO and PRZM (versions 3.15+), and the recommended default value is 2.58. The alpha factor (a) value is required for MACRO and the recommended default value is 0.0948 K^{-1}. These factors can also be derived from the Arrhenius activation energy. PEARL uses the Arrhenius activation energy directly, for which the recommended default value is 65.4 kJ mol^{-1}.

Parameter Relating Degradation to Soil Moisture. The B value is required for all four models except the most recent releases of FOCUS_MACRO (FOCUS_MACROv5.5.3 and above) and early versions of PRZM that predated the FOCUS tools. The B value is derived from the Walker equation ($f = (\theta/\theta_{REF})^B$, Walker, 1974). The recommended default value is 0.7, which is the geometric mean of a number of values found in the literature (Gottesbüren, 1991). In FOCUS_MACROv5.5.3 and above the MACRO ‘exponent for moisture response’ should be set to 0.49 to simulate a comparable degradation rate soil moisture relationship to that produced by the Walker equation with a B value of 0.7. Though FOCUS_MACROv5.5.3 and above simulations must use an exponent of 0.49, due to the moisture correction equation implemented in MACRO 5.5.3 and above, laboratory degradation rates and when possible field degradation rates, derived from the studies should always be normalised to the reference soil moisture (pF2) using the Walker equation, with its B value of 0.7.

2.4.3 Sorption parameters

K_{oc}-/K_{om}-value or K_F-values in Different Depths. PEARL, PELMO, PRZM and MACRO now all use the Freundlich adsorption coefficient (K_F), however previous versions of PRZM use

the linear partition coefficient (K_d). The Freundlich adsorption coefficient is defined as x= K_F c_{ref} $(c/c_{ref})^{1/n}$ where x is the content of substance sorbed (mg/kg) and c is the concentration in the liquid phase (mg/L). C_{ref} is the reference concentration which is usually 1 mg/L.

In PRZM and PELMO the sorption coefficient (K_d or K_F) can be set for each layer down the profile or a single K_{Foc} (the Freundlich sorption constant normalised for organic carbon content) value can be given, with appropriate organic carbon contents down the profile and the model will automatically correct the sorption with depth. PEARL has the same options, but uses organic matter rather than organic carbon for input and hence K_{om} rather than K_{oc} (%OC = %OM/1.724; K_{oc} = 1.724 * K_{om}). MACRO requires K_d to be set for each layer whilst PEARL requires a single K_{Fom} value and organic matter content in each soil layer.

Exponent of the Freundlich Isotherm. The FOCUS models require the Freundlich adsorption coefficient (see above), so the exponent of the isotherm (1/n, sometimes also referred to as N) is also required and this is determined in each laboratory sorption experiment. Where the results of a number of adsorption coefficient determinations are averaged (geometric mean) to derive the single coefficient value to use as model input, the arithmetic mean value of 1/n should be used as model input. When there is no data, a default value of 0.9 should be used. If a linear relation for sorption has been determined the value may be set to 1[1].

When checking the reliability of equilibrium sorption parameters the OECD 106 evaluators checklist should be applied (EFSA, 2017b).

Non-Equilibrium Sorption Parameters. Results from non equilibrium sorption studies can be used when data are available. Guidance on the studies needed to generate these data and how endpoints should be derived from them is available (European Commission, 2021). When using non-equilibrium sorption a corresponding DT50 (fitted representing just the equilibrium domain ($DegT50_{EQ}$) as opposed to usual DegT50 (that is estimated by fitting of the total extractable mass of substance in soil) must be used. Information on the application of non-equilibrium sorption is provided in Section 7.1.6 in FOCUS (2009) and European

[1] The origin of the last sentence in this paragraph is the FOCUS Surface Water Scenarios workgroup report. Applicants should be aware that with the aim of harmonising regulatory exposure assessments, Member State fate and behaviour experts from the competent authorities have agreed the following as a practical way of applying 'If a linear relation for sorption has been determined the value may be set to 1'. They have interpreted this sentence to mean that where an applicant has chosen to carry out a batch adsorption experiment investigating only a single concentration (i.e. just screening experiments in the OECD 106 test guideline), that the applicant has started with the assumption (i.e. text from section 2.4.3 "has determined") that a linear relation for sorption in that soil is reasonable, so a 1/n of 1 should be ascribed for that soil. In the situation where the available experiments investigated the relationship between soil solution concentration and sorption, but it was not possible to determine a reliable 1/n value, (i.e. text from section 2.4.3 "where there is no data") the default value of 0.9 has been ascribed to the pertinent soils.

Commission (2014). However using the default values mentioned in Section 7.1.6 in FOCUS (2009) and European Commission (2014) when data are unavailable is not recommended (EFSA PPR Panel, 2018). Note using Non-Equilibrium (aged) Sorption Parameters in simulations does not result in a tier 1 assessment.

2.4.4 Crop related substance parameters

TSCF (Transpiration Stream Concentration Factor). This value is required for PEARL and MACRO. Equations produced by Briggs *et al.* (1982) for non-ionic compounds provide a relationship between TSCF and octanol:water partition coefficient with the maximum value for TSCF given as 0.8. The recommended default value is 0 for all compounds. When a reliable measured octanol:water partition coefficient for neutral pH is available, the equation:

$TSCF = 0.784 \exp\{(-[\log(Kow) - 1.78]^2 / 2.44)\}$

produced by Briggs *et al.* (1982) should be used to calculate the TSCF. (EFSA PPR, 2013b / European Commission, 2014)

PRZM and PELMO require a plant uptake factor. The TSCF should be used for this value.

2.4.5 Management related substance parameters

Number of Applications. These should be from the GAP. Worst case options should be used, but realistic values may be used for additional simulations.

Dosages (Application Rates). Worst case options should be used, but realistic values may be used for additional simulations. For all models, the dose should be corrected for the amount of crop interception occurring (see below). This means that the dose input into the model should be that which actually reaches the soil according to experimental crop interception data.

Note that 100% of the dose should be applied and not 99% as occurs in the US (i.e. allowing 1% loss through drift).

Application Dates. These should be from the GAP. Worst case options should be used, but realistic values may be used for additional simulations.

Incorporation Depth. The majority of applications in agriculture are likely to be to foliage or the soil surface and the depth of incorporation is therefore unnecessary. However some compounds may be incorporated and in such cases the label recommendation for incorporation depth (usually *ca.* 20 cm) should be used as input

PELMO incorporates switches that determine whether application is to soil or to foliage. If the soil method is used then an incorporation depth can be specified (if application is to the soil surface the incorporation depth should be specified as 0).

PRZM works by specifying CAM values (Chemical Application Method) and associated values such as depth . This allows for different soil distributions from a variety of application methods (CAM 1 is application direct to soil, although a 4 cm incorporation depth is automatically assumed, to account for surface roughness).

PEARL incorporates switches that determine whether application is to soil, to foliage, incorporated or injected. If the incorporation option is used, an incorporation depth can be specified.

MACRO cannot directly simulate soil incorporation of plant protection products. It requires a plant protection product to be applied in a minimal amount of irrigation water (suggested 0.1 mm) to the soil surface. The user therefore needs to calculate the concentration of the substance in the irrigation water such that it equals the application rate in kg/ha (from the GAP).

For the purposes of the FOCUS scenarios all applications will be to soil (see below), either incorporated or to the surface.

Factor Accounting for Interception by Crops. When application is made to bare soil according to the GAP, crop interception is clearly not required. However, much of the application is to plants and therefore, in practice, some interception will occur.

The methods to account for foliar interception in PELMO and PRZM are based on a simple model of ground cover and that in MACRO and PEARL based on LAI. For reasons of consistency, simplicity and accuracy, FOCUS (2000) recommends that the internal interception routines in all models are disabled and the application rate is manually corrected for interception. Experimental values of interception for all the crops have been provided earlier in this report (Tables 1.4 and 1.5), based on Becker *et al.* (1999), van de Zande *et al.* (1999), van Beinum & Beulke (2010) and Olesen & Jensen (2013). These should be used to calculate the effective application rate to the soil. If the timing of the substance application might be in one of two or more growth stage windows, then the worst case interception assumption should be used.

2.5 References

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3. DEFINITION OF THE FOCUS SCENARIOS

3.1 Châteaudun

Table 3-1. Crop parameters for Châteaudun.

Crop	Growth Stage				Max. LAI		Root Depth (m)
	Planting (dd/mm)	Emergence (dd/mm)	Senescence (dd/mm)	Harvest (dd/mm)	($m^2\ m^{-2}$)	(dd/mm)	
apples	perennial	01/04@	01/09	01/10#	4	31/05	1.0
grass + alfalfa	perennial$	01/04 16/05 01/07 16/08	NA	15/05 30/06 15/08 30/09	5 5 5 5	15/05 30/06 15/08 30/09	0.5 0.5 0.5 0.5
potatoes	15/04	30/04	02/08	01/09	4	15/06	0.6
sugar beets	25/03	16/04	05/09	15/10	5	15/07	1.0
winter cereals	20/10	26/10*	20/06	15/07	7.5	31/05	0.8
cabbage		20/04& 31/07&	20/06 30/09	15/07 15/10	3 3	31/05 05/09	0.6 0.6
carrots	28/02 30/06	10/03 10/07	01/05 21/08	31/05 20/09	3 3	20/04 10/08	0.8 0.8
maize	20/04	01/05	01/09	01/10	4.5	15/08	0.8
oil seed rape (win)	30/08	07/09**	10/06	10/07	4	20/04	1.0
onions	15/04	25/04	18/07	01/09	3	30/06	0.6
peas (animals)	25/03	05/04	31/07	15/08	4	07/06	0.6
spring cereals	20/02	10/03	30/06	20/07	5	10/06	0.6
tomatoes		10/05&	26/07	25/08	6	30/06	0.8
vines	perennial	01/04	13/08	01/11	6	31/07	1.0

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth

& transplanted from seedbed - date indicates day of transplantation.

* spring point of 15/4.

** spring point of 11/3.

Table 3-2. Crop Kc factors for Châteaudun.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	01/10-31/03	1.00	01/04-30/05	1.05	31/05-31/08	1.10	01/09-30/09	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	01/09-29/04	1.00	30/04-14/06	1.05	15/06-01/08	1.10	02/08-31/08	0.90
sugar beets	15/10-15/04	1.00	16/04-14/07	1.05	15/07-04/09	1.10	05/09-14/10	0.85
winter cereals	15/07-25/10	1.00	26/10-30/05	1.05	31/05-19/06	1.10	20/06-14/07	0.70
cabbage	15/10-19/04 15/07-30/07	1.00	20/04-30/05 31/07-04/09	1.00	31/05-19/06 05/09-29/09	1.00	20/06-14/07 30/09-14/10	0.93
carrots	20/09-09/03 31/05-09/07	1.00	10/03-19/04 10/07-09/08	1.03	20/04-30/04 10/08-20/08	1.05	01/05-30/05 21/08-19/09	0.90
maize	01/10-30/04	1.00	01/05-14/08	1.05	15/08-31/08	1.10	01/09-30/09	0.83
oil seed rape (win)	10/07-06/09	1.00	07/09-19/04	1.00	20/04-09/06	1.00	10/06-09/07	0.93
onions	01/09-24/04	1.00	25/04-29/06	0.98	30/06-17/07	0.95	18/07-31/08	0.85
peas (animals)	15/08-04/04	1.00	05/04-06/06	1.05	07/06-30/07	1.10	31/07-14/08	1.05
spring cereals	20/07-09/03	1.00	10/03-09/06	1.05	10/06-29/06	1.10	30/06-19/07	0.70
tomatoes	25/08-09/05	1.00	10/05-29/06	1.05	30/06-25/07	1.10	26/07-24/08	0.85
vines	01/11-31/03	1.00	01/04-30/07	0.88	31/07-12/08	0.75	13/08-31/10	0.65

Table 3-3. Soil parameters for Châteaudun.

Horizon	Depth (cm)	Classification	pH-H_2O*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
					<2	2-50	>50				
Ap	0-25	silty clay loam	8.0	7.3	30	67	3	2.4	1.39	1.3	1.0
B1	25-50	silty clay loam	8.1	7.4	31	67	2	1.6	0.93	1.41	0.5
B2	50-60	silt loam	8.2	7.5	25	67	8	1.2	0.7	1.41	0.5
II C1	60-100	limestone#	8.5	7.8	26	44	30	0.5	0.3	1.37	0.3
II C1	100-120	limestone#	8.5	7.8	26	44	30	0.5	0.3	1.37	0
II C2	120-190	limestone#	8.5	7.8	24	38	38	0.46	0.27	1.41	0
M	190-260	limestone#	8.3	7.6	31	61	8	0.36	0.21	1.49	0

The limestone is cryoturbated in the C-horizons and powdery in the M-horizon.

* Measured at a soil solution ratio of 1:5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.

The profile is overlying an aquitanian limestone. The depth of the ground water table is around 12 m.

Table 3-4. Soil hydraulic properties for Châteaudun, Van Genuchten/Mualem parameters (restricted form, m=1-1/n).

Depth (cm)	θ_s ($m^3\ m^{-3}$)	θ_r ($m^3\ m^{-3}$)	α (m^{-1})	n	Water Content		Ksat ($m\ s^{-1}*10^{-6}$)	λ	AW[@] (mm)
					10kPa ($m^3\ m^{-3}$)	1600kPa ($m^3\ m^{-3}$)			
0-25	0.43	0.0	5.00	1.080	0.374	0.253	20.00	0.50	30.25
25-50	0.44	0.0	5.00	1.095	0.372	0.235	30.00	0.50	34.25
50-60	0.44	0.0	5.00	1.095	0.372	0.235	50.00	2.50	13.70
60-100	0.44	0.0	1.50	1.160	0.386	0.185	12.00	-2.00	80.40
100-120	0.44	0.0	1.50	1.160	0.386	0.185	12.00	-2.00	-
120-190	0.49	0.0	1.07	1.280	0.417	0.116	9.06	-1.50	-
190-260	0.42	0.0	1.91	1.152	0.362	0.176	14.81	-1.18	-

[@] Plant available water in the soil layer.

Plant available water in the top 1 m is 158.6 mm.

For the MACRO model a few additional parameters are needed. These are obtained from the same original dataset. In order to avoid confusion these parameters are not included here.

3.2 Hamburg

Table 3-5. Crop parameters for Hamburg.

Crop	Growth Stage				Max. LAI		Root Depth (m)
	Planting (dd/mm)	Emergence (dd/mm)	Senescence (dd/mm)	Harvest (dd/mm)	($m^2\ m^{-2}$)	(dd/mm)	
apples	perennial	15/04@	30/09	30/10#	4	01/07	1.0
grass + alfalfa	perennial	25/03$ 01/06 16/07	NA	31/05 15/07 31/08	5 5 5	31/05 15/07 31/08	0.6 0.6 0.6
potatoes	01/05	10/05	16/08	15/09	3	20/07	0.7
sugar beets	01/04	15/04	08/09	08/10	4.2	30/08	1.0
winter cereals	12/10	01/11*	16/07	10/08	3.8	01/06	1.0
beans (field)	25/03	10/04	05/08	25/08	4	10/07	0.9
cabbage		20/04& 31/07&	30/06 30/09	15/07 15/10	3 3	31/05 05/09	0.7 0.7
carrots	28/02 30/06	10/03 10/07	01/05 21/08	31/05 20/09	3 3	20/04 10/08	0.8 0.8
maize	20/04	05/05	21/08	20/09	4.2	30/07	1.0
oil seed rape (win)	25/08	02/09**	28/06	28/07	4	05/05	1.0
onions	15/04	25/04	18/07	01/09	3	30/06	0.7
peas (animals)	25/03	10/04	10/08	25/08	4	10/07	0.9
spring cereals	10/03	01/04	31/07	20/08	3.9	05/06	0.9
strawberries	perennial	15/03	01/08	31/08^	2.5	30/04	0.7
vines	perennial	01/05	11/08	30/10	3	15/07	1.0

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

& transplanted from seedbed - date indicates day of transplantation.

^ crop removed from field.

* spring point of 4/5.

** spring point of 18/4.

Table 3-6. Crop Kc factors for Hamburg.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	30/10-14/04	1.00	15/04-30/06	1.05	01/07-29/09	1.10	30/09-29/10	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	15/09-09/05	1.00	10/05-19/07	1.05	20/07-15/08	1.10	16/08-14/09	0.90
sugar beets	08/10-14/04	1.00	15/04-29/08	1.05	30/08-07/09	1.10	08/09-07/10	0.85
winter cereals	10/08-31/10	1.00	01/11-05/31	1.05	01/06-15/07	1.10	16/07-09/08	0.70
beans (field)	25/08-09/04	1.00	10/04-09/07	1.05	10/07-04/08	1.10	05/08-24/08	0.70
cabbage	15/10-19/04 15/07-30/07	1.00	20/04-30/05 31/07-04/09	1.00	31/05-29/06 05/09-29/09	1.00	30/06-14/07 30/09-15/10	0.93
carrots	20/09-09/03 31/05-09/07	1.00	10/03-19/04 10/07-09/08	1.03	20/04-4/30 10/08-20/08	1.05	01/05-30/05 21/08-19/09	0.90
maize	20/09-04/05	1.00	05/05-29/07	1.05	30/07-20/08	1.10	21/08-19/09	0.83
oil seed rape (win)	28/07-01/09	1.00	02/09-04/05	1.00	05/05-27/06	1.00	28/06-27/07	0.93
onions	01/09-24/04	1.00	25/04-29/06	0.98	30/06-17/07	0.95	18/07-31/08	0.85
peas (animals)	25/08-09/04	1.00	10/04-09/07	1.05	10/07-09/08	1.10	10/08-24/08	1.05
spring cereals	20/08-31/03	1.00	01/04-04/06	1.05	05/06-30/07	1.10	31/07-19/08	0.70
strawberries	31/08-14/03	1.00	15/03-29/04	1.00	30/04-7/31	1.00	01/08-30/08	1.00
vines	30/10-30/04	1.00	01/05-14/07	0.88	15/07-10/08	0.75	11/08-29/10	0.65

Table 3-7. Soil parameters for Hamburg.

Horizon	Depth (cm)	Classification	pH-H_2O*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
					<2	2-50	>50				
Ap	0-30	sandy loam	6.4	5.7	7.2	24.5	68.3	2.6	1.5	1.5	1.0
BvI	30-60	sandy loam	5.6	4.9	6.7	26.3	67	1.7	1	1.6	0.5
BvII	60-75	sand	5.6	4.9	0.9	2.9	96.2	0.34	0.2	1.56	0.3
Bv/Cv	75-90	sand	5.7	5	0	0.2	99.8	0	0	1.62	0.3
Cv	90-100	sand	5.5	4.8	0	0	100	0	0	1.6	0.3
Cv	100-200	sand	5.5	4.8	0	0	100	0	0	1.6	0.0

† These values are estimated from the measured KCl values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

* Measured at a soil solution ratio of 1:2.5

@ The depth factor indicates the relative transformation rate in the soil layer.

Ground water depth of 2 m (estimated by IUCT).

Table 3-8. Soil hydraulic properties for Hamburg, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s ($m^3\ m^{-3}$)	θ_r ($m^3\ m^{-3}$)	α (m^{-1})	n	m	Water Content		Ksat ($m\ s^{-1} \cdot 10^{-6}$)	λ	AW[@] (mm)
						10kPa ($m^3\ m^{-3}$)	1600kPa ($m^3\ m^{-3}$)			
0-30	0.3910	0.0360	1.491	1.4680	0.3188	0.292	0.064	23.330	0.500	68.4
30-60	0.3700	0.0300	1.255	1.5650	0.3610	0.277	0.047	31.670	0.500	69.0
60-75	0.3510	0.0290	1.808	1.5980	0.3742	0.229	0.040	28.330	0.500	28.4
75-90	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	21.2
90-100	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	14.1
100-200	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	

[@] Plant available water in the soil layer.

Plant available water in the top 1 m is 201 mm.

3.3 Jokioinen

Table 3-9. Crop parameters for Jokioinen.

Crop	Growth Stage				Max. LAI		Root Depth (m)
	Planting (dd/mm)	Emergence (dd/mm)	Senescence (dd/mm)	Harvest (dd/mm)	($m^2\ m^{-2}$)	(dd/mm)	
apples	perennial	10/05[@]	15/09	15/10[#]	4	25/05	1.0
grass + alfalfa	perennial[$]	15/04[$] 16/06 16/07	NA	15/06 15/07 25/08	7 7 7	15/06 15/07 25/08	0.9 0.9 0.9
potatoes	15/05	05/06	05/09	25/09	5	30/08	0.6
sugar beets	10/05	25/05	05/09	15/10	5	10/08	0.9
winter cereals	10/09	20/09*	21/07	15/08	4.8	25/06	0.95
bush berries	perennial	10/05	06/08	25/10	4	25/05	0.6
cabbage		20/05[&]	05/09	20/09	5	05/09	0.9
carrots	15/05	01/06	05/09	05/10	4	05/09	0.6
oil seed rape (sum)	10/05	20/05	31/07	30/08	3.8	05/07	0.8
onions	10/05	20/05	01/07	15/08	4	25/06	0.3
peas (animals)	10/05	25/05	10/08	25/08	4	30/06	0.8
spring cereals	07/05	18/05	05/08	25/08	4.5	30/06	0.8
strawberries	perennial	15/05	16/08	15/09^	2.5	25/06	0.3

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

& transplanted from seedbed - date indicates day of transplantation.

^ crop removed from field.

* spring point of 14/5.

Table 3-10. Crop Kc factors for Jokioinen.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	15/10-09/05	1.00	10/05-24/05	1.05	25/05-14/09	1.10	15/09-14/10	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	25/09-04/06	1.00	05/06-29/08	1.05	30/08-04/09	1.10	05/09-24/09	0.90
sugar beets	15/10-24/05	1.00	25/05-09/08	1.05	10/08-04/09	1.10	05/09-14/10	0.85
winter cereals	15/08-19/09	1.00	20/09-24/06	1.05	25/06-20/07	1.10	21/07-14/08	0.70
bush berries	25/10-09/05	1.00	10/05-24/05	0.88	25/05-05/08	0.75	06/08-24/10	0.65
cabbage	20/09-19/05	1.00	20/05-04/09	1.00			05/09-19/09	0.93
carrots	05/10	1.00	01/06-04/09	1.03			05/09-04/10	0.95
oil seed rape (sum)	30/08-19/05	1.00	20/05-04/07	1.00	05/07-30/07	1.00	31/07-29/08	0.93
onions	15/08-19/05	1.00	20/05-24/06	0.98	25/06-30/06	0.95	01/07-14/08	0.85
peas (animals)	25/08-24/05	1.00	25/05-29/06	1.05	30/06-09/08	1.10	10/08-24/08	1.05
spring cereals	25/08-17/05	1.00	18/05-29/06	1.05	30/06-04/08	1.10	05/08-24/08	0.70
strawberries	15/09-14/05	1.00	15/05-24/06	1.00	25/06-15/08	1.00	16/08-14/09	1.00

Table 3-11. Soil parameters for Jokioinen.

Horizon	Depth (cm)	Classification	pH-H_2O^*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
					<2	2-50	>50				
Ap	0-30	loamy fine sand	6.2	5.5	3.6	23.2	73.2	7.0	4.06	1.29	1.0
Bs	30-60	loamy fine sand	5.6	4.9	1.8	12.2	86.0	1.45	0.84	1.52	0.5
BC1	60-95	loamy fine sand	5.4	4.7	1.2	14.9	83.9	0.62	0.36	1.64	0.3
BC2	95-100	loamy fine sand	5.4	4.7	1.7	18.9	79.4	0.50	0.29	1.63	0.3
BC2	100-120	loamy fine sand	5.4	4.7	1.7	18.9	79.4	0.50	0.29	1.63	0.0
Cg	120-150	fine sand	5.3	4.6	1.9	8.6	89.5	0.36	0.21	1.66	0.0

* Measured at a soil solution ratio of 1:2.5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.

The ground water level is approximately 1.52 m below soil surface.

Table 3-12. Soil hydraulic properties for Jokioinen, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s ($m^3\ m^{-3}$)	θ_r ($m^3\ m^{-3}$)	α (m^{-1})	n	m	Water Content 10kPa ($m^3\ m^{-3}$)	Water Content 1600kPa ($m^3\ m^{-3}$)	Ksat ($m\ s^{-1}*10^{-6}$)	λ	AW[@] (mm)
0-30	0.4519	0.0100	3.900	1.2745	0.2154	0.304	0.086	4.165	-0.646	65.4
30-60	0.3890	0.0100	6.650	1.4849	0.3266	0.158	0.023	5.686	-0.060	40.5
60-95	0.3632	0.0100	6.000	1.5007	0.3336	0.151	0.021	4.294	0.833	45.5
95-100	0.3636	0.0100	5.600	1.4778	0.3233	0.162	0.024	4.142	0.957	6.9
100-120	0.3636	0.0100	5.600	1.4778	0.3233	0.162	0.024	4.142	0.957	
120-150	0.3432	0.0100	7.250	1.5472	0.3537	0.121	0.017	4.834	1.036	

[@] Plant available water in the soil layer.

Plant available water in top meter is 158.3 mm.

3.4 Kremsmünster

Table 3-13. Crop parameters for Kremsmünster.

Crop	Growth Stage: Planting (dd/mm)	Emergence (dd/mm)	Senescence (dd/mm)	Harvest (dd/mm)	Max. LAI ($m^2\ m^{-2}$)	Max. LAI (dd/mm)	Root Depth (m)
apples	perennial	15/04[@]	30/09	30/10[#]	4	01/07	1.0
grass + alfalfa	perennial	10/04[$] 26/05 16/07	NA	25/05 15/07 20/09	5 5 5	25/05 15/07 20/09	0.5 0.5 0.5
potatoes	01/05	10/05	16/08	15/09	3.5	20/07	0.7
sugar beets	01/04	15/04	31/08	10/10	4.2	30/08	1.0
winter cereals	25/10	05/11*	16/07	10/08	4	05/06	1.0
beans (field)	25/03	10/04	05/08	25/08	4	10/07	0.8
cabbage		20/04[&] 31/07[&]	30/06 30/09	15/07 15/10	3 3	31/05 05/09	0.6 0.6
carrots	28/02 30/06	10/03 10/07	01/05 21/08	31/05 20/09	3 3	20/04 10/08	0.7 0.7
maize	20/04	05/05	21/08	20/09	4.2	30/07	1.0
oil seed rape (win)	25/08	02/09**	28/06	28/07	4	05/05	1.0
onions	15/04	25/04	18/07	01/09	3	30/06	0.6
spring cereals	10/03	01/04	31/07	20/08	3.9	05/06	0.9
strawberries	perennial	15/03	01/08	31/08^	2.5	30/04	0.7
vines	perennial	01/05	11/08	30/10	3	15/07	1.0

@ leaf emergence

leaf fall

$ "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

& transplanted from seedbed - date indicates day of transplantation.

^ crop removed from field.

* spring point of 24/4.

** spring point of 15/4.

Table 3-14. Crop Kc factors for Kremsmünster.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	30/10-14/04	1.00	15/04-30/06	1.05	01/07-29/09	1.10	30/09-29/10	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	15/09-09/05	1.00	10/05-19/07	1.05	20/07-15/08	1.10	16/08-14/09	0.90
sugar beets	10/10-14/04	1.00	15/04-29/08	1.05	30/08	1.10	31/08-09/10	0.85
winter cereals	10/08-04/11	1.00	05/11-04/06	1.05	05/06-15/07	1.10	16/07-09/08	0.70
beans (field)	25/08-09/04	1.00	10/04-09/07	1.05	10/07-04/08	1.10	05/08-24/08	0.70
cabbage	15/10-19/04 15/07-30/07	1.00	20/04-30/05 31/07-04/09	1.00	31/05-29/06 05/09-29/09	1.00	30/06-14/07 30/09-14/10	0.93
carrots	20/09-09/03 31/05-09/07	1.00	10/03-19/04 10/07-09/08	1.03	20/04-30/04 10/08-20/08	1.05	01/05-30/05 21/08-19/09	0.90
maize	20/09-04/05	1.00	05/05-29/07	1.05	30/07-20/08	1.10	21/08-19/09	0.83
oil seed rape (win)	28/07-01/09	1.00	02/09-04/05	1.00	05/05-27/06	1.00	28/06-27/07	0.93
onions	01/09-24/04	1.00	25/04-29/06	0.98	30/06-17/07	0.95	18/07-31/08	0.85
spring cereals	20/08-31/03	1.00	01/04-04/06	1.05	05/06-30/07	1.10	31/07-19/08	0.70
strawberries	31/08-14/03	1.00	15/03-29/04	1.00	30/04-31/07	1.00	01/08-30/08	1.00
vines	30/10-30/04	1.00	01/05-14/07	0.88	15/07-10/08	0.75	11/08-29/10	0.65

Table 3-15. Soil parameters for Kremsmünster.

Depth (cm)	Classification	pH-H_2O*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
				<2	2-50	>50				
0-30	loam/silt loam	7.7	7.0	14	50	36	3.6	2.1	1.41	1.0
30-50	loam/silt loam	7.0	6.3	25	50	25	1.0	0.6	1.42	0.5
50-60	loam/clay loam	7.1	6.4	27	44	29	0.5	0.3	1.43	0.5
60-100	loam/clay loam	7.1	6.4	27	44	29	0.5	0.3	1.43	0.3
100-200	loam/clay loam	7.1	6.4	27	44	29	0.5	0.3	1.43	0.0

† These values are estimated from the measured KCl values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

* Measured at a soil solution ratio of 1:2.5

@ The depth factor indicates the relative transformation rate in the soil layer.

The depth of ground water is around 1.6 m, for apples and vines a deeper ground water level has to be assumed. At a depth of approximately 3.3 m a rather impermeable layer is present.

Layer below 1 m copied from 60 - 100 cm layer.

Layer 0 - 30 cm is Ap horizon, 30 - 100 cm is Bwg horizon.

Table 3-16. Soil hydraulic properties for Kremsmünster, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s ($m^3 m^{-3}$)	θ_r ($m^3 m^{-3}$)	α (m^{-1})	n	m	Water Content		Ksat ($m\ s^{-1}*10^{-6}$)	λ	AW[@] (mm)
						10kPa ($m^3 m^{-3}$)	1600kPa ($m^3 m^{-3}$)			
0-30	0.4246	0.0100	2.440	1.2186	0.1794	0.334	0.123	1.769	-2.080	63.3
30-50	0.4446	0.0100	2.700	1.1659	0.1423	0.365	0.169	2.780	-2.404	39.2
50-60	0.4430	0.0100	3.080	1.1578	0.1363	0.361	0.173	2.459	-2.065	18.8
60-100	0.4430	0.0100	3.080	1.1578	0.1363	0.361	0.173	2.459	-2.065	75.2
100-200	0.4430	0.0100	3.080	1.1578	0.1363	0.361	0.173	2.459	-2.065	

[@] Plant available water in soil layer.

Plant available water in top meter is 196.5 mm.

Layer 100 - 200 cm copied from layer 60 - 100 cm because of lacking information.

3.5 Okehampton

Table 3-17. Crop parameters for Okehampton.

Crop	Growth Stage				Max. LAI		Root Depth (m)
	Planting (dd/mm)	Emergence (dd/mm)	Senescence (dd/mm)	Harvest (dd/mm)	($m^2 m^{-2}$)	(dd/mm)	
apples	perennial	25/03[@]	16/08	15/09[#]	2.5	15/06	1.0
grass + alfalfa	perennial	10/02[$] 16/05 16/07	NA	15/05 15/07 15/09	4.5 4.5 4.5	15/05 15/07 15/09	0.45 0.45 0.45
potatoes	15/04	30/04	02/08	01/09	4	15/07	0.6
sugar beets	10/04	25/04	15/09	25/10	3	30/08	0.8
winter cereals	07/10	17/10*	07/07	01/08	7.5	15/05	0.8
beans (field)	01/03	15/03	26/08	15/09	4	07/06	0.45
linseed	25/03	30/03	18/08	25/09	3	25/06	0.6
maize	07/05	25/05	18/08	07/10	7	15/07	0.8
oil seed rape (sum)	25/03	30/03	21/07	20/08	3	15/05	0.6
oil seed rape (win)	07/08	14/08**	21/06	21/07	4.5	30/04	0.85
peas (animals)	25/03	05/04	31/07	15/08	4.0	07/06	0.45
spring cereals	25/03	01/04	31/07	20/08	4.5	22/05	0.6

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

* spring point of 21/4.

** spring point of 9/4.

Table 3-18. Crop Kc factors for Okehampton.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	15/09-24/03	1.00	25/03-14/06	1.05	15/06-15/08	1.10	16/08-14/09	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	01/09-29/04	1.00	30/04-14/07	1.05	15/07-01/08	1.10	02/08-31/08	0.90
sugar beets	25/10-24/04	1.00	25/04-29/08	1.05	30/08-14/09	1.10	15/09-24/10	0.85
winter cereals	01/08-16/10	1.00	17/10-14/05	1.05	15/05-06/07	1.10	07/07-31/07	0.70
beans (field)	15/09-14/03	1.00	15/03-06/06	1.05	07/06-25/08	1.10	26/08-14/09	0.70
linseed	25/0929/03	1.00	30/03-24/06	1.03	25/06-17/08	1.05	18/08-24/09	0.65
maize	07/10-24/05	1.00	25/05-14/07	1.05	15/07-17/08	1.10	18/08-06/10	0.83
oil seed rape (sum)	20/08-29/03	1.00	30/03-14/05	1.00	15/05-20/07	1.00	21/07-19/08	0.93
oil seed rape (win)	21/07-13/08	1.00	14/08-29/04	1.00	30/04-20/06	1.00	21/06-20/07	0.93
peas (animals)	15/08-04/04	1.00	05/04-06/06	1.05	07/06-30/07	1.10	31/07-14/08	1.05
spring cereals	20/08-31/03	1.00	01/04-21/05	1.05	22/05-30/07	1.10	31/07-19/08	0.70

Table 3-19. Soil parameters for Okehampton.

Horizon	Depth (cm)	Classification	pH-H_2O*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
					<2	2-50	>50				
A	0-25	loam	5.8	5.1	18	43	39	3.8	2.2	1.28	1.0
Bw1	25-55	loam	6.3	5.6	17	41	42	1.2	0.7	1.34	0.5
BC	55-85	sandy loam	6.5	5.8	14	31	55	0.69	0.4	1.42	0.3
C	85-100	sandy loam	6.6	5.9	9	22	69	0.17	0.1	1.47	0.3
C	100-150	sandy loam	6.6	5.9	9	22	69	0.17	0.1	1.47	0.0

* Measured at a soil solution ratio of 1:2.5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.

The depth of ground is about 20 m.

Table 3-20. Soil hydraulic properties for Okehampton, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s ($m^3\ m^{-3}$)	θ_r ($m^3\ m^{-3}$)	α (m^{-1})	n	m	Water Content 10kPa ($m^3\ m^{-3}$)	Water Content 1600kPa ($m^3\ m^{-3}$)	Ksat ($m\ s^{-1}*10^{-6}$)	λ	AW[@] (mm)
0-25	0.4664	0.0100	3.550	1.1891	0.1590	0.358	0.148	3.484	-2.581	52.5
25-55	0.4602	0.0100	3.640	1.2148	0.1768	0.340	0.125	4.887	-2.060	64.5
55-85	0.4320	0.0100	4.560	1.2526	0.2017	0.290	0.090	4.838	-1.527	60.0
85-100	0.4110	0.0100	5.620	1.3384	0.2528	0.228	0.050	4.449	-0.400	26.7
100-150	0.4110	0.0100	5.620	1.3384	0.2528	0.228	0.050	4.449	-0.400	

[@] Plant available water in the soil layer.

Plant available water in top meter is 203.7 mm.

3.6 Piacenza

Table 3-21. Crop parameters for Piacenza.

Crop	Growth Stage: Planting (dd/mm)	Growth Stage: Emergence (dd/mm)	Growth Stage: Senescence (dd/mm)	Growth Stage: Harvest (dd/mm)	Max. LAI ($m^2\ m^{-2}$)	Max. LAI (dd/mm)	Root Depth (m)
apples	perennial	01/04[@]	02/09	01/11[#]	5	31/05	1.0
grass + alfalfa	perennial[$]	28/02[$] 16/05 16/07	NA	15/05 15/07 20/09	4 4 4	15/05 15/07 20/09	0.8 0.8 0.8
potatoes	01/04	20/04	11/08	10/09	5	01/06	0.5
sugar beets	01/03	20/03	27/07	15/09	4	30/06	0.8
winter cereals	25/11	01/12*	01/06	01/07	7	10/05	1.0
citrus	perennial	evergreen	NA	NA	5	31/05	1.0
maize	30/04	15/05	30/09	30/10	5	31/07	1.0
oil seed rape (win)	30/09	05/10**	21/05	20/06	3.5	15/04	0.6
soybean	25/04	10/05	10/09	05/10	6.5	31/07	0.6
sunflower	01/04	20/04	26/08	20/09	4	20/06	1.0
tobacco		20/05[&]	25/09	05/10	4	20/07	1.0
tomatoes		10/05[&]	26/07	25/08	6	30/06	1.0
vines	perennial	01/04	13/08	01/11	6	31/07	1.0

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

& transplanted from seedbed - date indicates day of transplantation.

* spring point of 19/3.

** spring point of 7/3.

Table 3-22. Crop Kc factors for Piacenza.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	01/11-31/03	1.00	01/04-30/05	1.05	31/05-01/09	1.10	02/09-31/10	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	10/09-19/04	1.00	20/04-31/05	1.05	01/06-10/08	1.10	11/08-09/09	0.90
sugar beets	15/09-19/03	1.00	20/03-29/06	1.05	30/06-26/07	1.10	27/07-14/09	0.85
winter cereals	01/07-30/11	1.00	01/12-09/05	1.05	10/05-31/05	1.10	01/06-30/06	0.70
citrus	NA		NA		All year	0.60	NA	
maize	30/10-14/05	1.00	15/05-30/07	1.05	31/07-29/09	1.10	30/09-29/10	0.83
oil seed rape (win)	20/06-04/10	1.00	05/10-14/04	1.00	15/04-20/05	1.00	21/05-19/06	0.93
soybean	05/10-09/05	1.00	10/05-30/07	1.03	31/07-09/09	1.05	10/09-04/10	0.75
sunflower	20/09-19/04	1.00	20/04-19/06	1.05	20/06-25/08	1.10	26/08-19/09	0.75
tobacco	05/10-19/05	1.00	20/05-19/07	1.00	20/07-24/09	1.00	25/09-04/10	0.93
tomatoes	25/08-09/05	1.00	10/05-29/06	1.05	30/06-25/07	1.10	26/07-24/08	0.85
vines	01/11-31/03	1.00	01/04-30/07	0.88	31/07-12/08	0.75	13/08-31/10	0.65

Table 3-23. Soil parameters for Piacenza.

Horizon	Depth (cm)	Classification	pH-H_2O^*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
					<2	2-50	>50				
Ap	0-30	loam	7	6.3	15	45	40	2.17	1.26	1.3	1.0
Ap	30-40	loam	7	6.3	15	45	40	2.17	1.26	1.3	0.5
Bw	40-60	silt loam	6.3	5.6	7	53	40	0.80	0.47	1.35	0.5
Bw	60-80	silt loam	6.3	5.6	7	53	40	0.80	0.47	1.35	0.3
2C	80-100	sand	6.4	5.7	0	0	100	0	0	1.45	0.3
2C	100-170	sand	6.4	5.7	0	0	100	0	0	1.45	0.0

* Measured at a soil solution ratio of 1:2.5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.

The depth of ground water is 1.5 m (range 1.30-1.70 m).

Table 3-24. Soil hydraulic properties for Piacenza, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s ($m^3 m^{-3}$)	θ_r ($m^3 m^{-3}$)	α (m^{-1})	n	m	Water Content		Ksat ($m s^{-1}*10^{-6}$)	λ	AW[@] (mm)
						10kPa ($m^3 m^{-3}$)	1600kPa ($m^3 m^{-3}$)			
0-30	0.4622	0.0100	3.13	1.238	0.1993	0.341	0.113	4.269	-2.037	68.4
30-40	0.4622	0.0100	3.13	1.238	0.1993	0.341	0.113	4.269	-2.037	22.8
40-60	0.4543	0.0100	2.31	1.3531	0.261	0.317	0.065	6.138	0.109	50.4
60-80	0.4543	0.0100	2.31	1.3531	0.261	0.317	0.065	6.138	0.109	50.4
80-100	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	28.2
100-170	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	

[@] Plant available water in the soil layer.

Plant available water in top meter is 220.2 mm.

3.7 Porto

Table 3-25. Crop parameters for Porto.

Crop	Growth Stage				Max. LAI		Root Depth (m)
	Planting (dd/mm)	Emergence (dd/mm)	Senescence (dd/mm)	Harvest (dd/mm)	($m^2 m^{-2}$)	(dd/mm)	
apples	perennial	15/03[@]	1/09	31/10[#]	3	30/06	1.0
grass + alfalfa	perennial	28/02[$] 16/05 16/07	NA	15/05 15/07 20/09	4 4 4	15/05 15/07 20/09	0.8 0.8 0.8
potatoes (sum)	28/02	15/03	08/06	15/06	4	30/05	0.7
sugar beets	28/02	15/03	12/06	01/08	5	30/04	1.0
winter cereals	15/11	30/11	31/05	30/06	6.5	30/04	1.0
beans (vegetable)	28/02	10/03	11/08	31/08	4	15/05	0.5
cabbage		28/02[&] 31/07[&]	16/06 31/10	01/07 15/11	4 4	15/05 31/08	0.5 0.5
carrots	15/02 15/07	28/02 22/07	11/05 25/09	31/05 15/10	4 4	01/05 15/09	0.5 0.5
citrus	perennial	evergreen	NA	NA	6	31/05	1.0
maize	20/04	01/05	01/09	01/10	4.5	15/08	0.8
oil seed rape (sum)	15/03	22/03	26/07	25/08	3	31/05	0.9
oil seed rape (win)	30/08	07/09	10/06	10/07	4	20/04	1.0
onions	15/02	28/02	21/05	31/05	3.5	15/05	0.5
spring cereals	20/02	10/03	30/06	20/07	5	10/06	0.6
tomatoes		15/03[&]	01/08	31/08	5	15/06	0.5
vines	perennial	15/03	31/07	30/09	4	31/07	1.0

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

& transplanted from seedbed - date indicates day of transplantation.

Table 3-26. Crop Kc factors for Porto.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	31/10-14/03	1.00	15/03-29/06	1.05	30/06-08/31	1.10	01/09-30/10	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	15/06-14/03	1.00	15/03-29/05	1.05	30/05-07/06	1.10	08/06-14/06	0.90
sugar beets	01/08-15/03	1.00	15/03-29/04	1.05	30/04-11/06	1.10	12/06-31/07	0.85
winter cereals	30/06-29/11	1.00	30/11-29/04	1.05	30/04-30/05	1.10	31/05-29/06	0.70
beans (vegetable)	31/08-09/03	1.00	10/03-14/05	1.05	15/05-10/08	1.10	11/08-30/08	0.70
cabbage	15/11-27/02 01/07-30/07	1.00	28/02-14/05 31/07-30/08	1.00	15/05-15/06 31/08-30/10	1.0	16/06-30/06 31/10	0.93
carrots	15/10-27/02 31/05-21/07	1.00	28/02-30/04 22/07-14/09	1.03	01/05-10/05 15/09-24/09	1.05	11/05-30/05 25/09-14/10	0.90
citrus	NA		NA		All year	0.60	NA	
maize	01/10-30/04	1.00	01/05-14/08	1.05	15/08-31/08	1.10	01/09-30/09	0.83
oil seed rape (sum)	25/08-21/03	1.00	22/03-30/05	1.00	31/05-25/07	1.00	26/07-24/08	0.93
oil seed rape (win)	10/07-06/09	1.00	07/09-19/04	1.00	20/04-09/06	1.00	10/06-09/07	0.93
onions	31/05-27/02	1.00	28/02-14/05	0.98	15/05-20/05	0.95	21/05-30/05	0.85
spring cereals	20/07-09/03	1.00	10/03-09/06	1.05	10/06-29/06	1.10	30/06-19/07	0.70
tomatoes	31/08-14/03	1.00	15/03-14/06	1.05	15/06-31/07	1.10	01/08-30/08	0.85
vines	30/09-14/03	1.00	15/03-30/07	0.88			31/07-29/09	0.65

Table 3-27. Soil parameters for Porto.

Depth (cm)	Classification	pH-H_2O*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
				<2	2-50	>50				
0-35	loam	4.9	4.2	10	48	42	2.45	1.42	1.09	1.0
35-60	sandy loam	4.8	4.1	8	31	61	1.35	0.78	1.45	0.5
60-100	sandy loam	4.8	4.1	8	31	61	1.35	0.78	1.45	0.3
100-120	sandy loam	4.8	4.1	8	31	61	1.35	0.78	1.45	0.0

* Measured at a soil solution ratio of 1:2.5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.

Depth of ground water: summer lower than 2 m, winter 0.7 - 1.2 m.

Top layer is Ap horizon, other layers C1 horizon.

Table 3-28. Soil hydraulic properties for Porto, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s ($m^3 m^{-3}$)	θ_r ($m^3 m^{-3}$)	α (m^{-1})	n	m	Water Content 10kPa ($m^3 m^{-3}$)	Water Content 1600kPa ($m^3 m^{-3}$)	Ksat ($m s^{-1}*10^{-6}$)	λ	AW@ (mm)
0-35	0.5230	0.0100	2.30	1.2888	0.2241	0.388	0.103	6.504	-1.949	99.75
35-60	0.4183	0.0100	4.29	1.3078	0.2354	0.262	0.065	4.774	-0.9972	49.25
60-100	0.4183	0.0100	4.29	1.3078	0.2354	0.262	0.065	4.774	-0.9972	78.80
100-120	0.4183	0.0100	4.29	1.3078	0.2354	0.262	0.065	4.774	-0.9972	

@ Plant available water in the soil layer.

Plant available water in top meter is 227.8 mm.

3.8 Sevilla

Table 3-29. Crop parameters for Sevilla.

Crop	Growth Stage: Planting (dd/mm)	Growth Stage: Emergence (dd/mm)	Growth Stage: Senescence (dd/mm)	Growth Stage: Harvest (dd/mm)	Max. LAI ($m^2 m^{-2}$)	Max. LAI (dd/mm)	Root Depth (m)
apples	perennial	15/03@	16/08	15/10#	6	31/05	1.0
grass + alfalfa	perennial$	31/01$ 16/04 16/06 16/08	NA	15/04 15/06 15/08 15/10	4 4 4 4	15/04 15/06 15/08 15/10	0.5 0.5 0.5 0.5
potatoes	15/01	31/01	01/05	31/05	4	31/03	0.5
sugar beets	31/10	10/11	12/05	01/07	5	15/04	0.6
winter cereals	15/11	30/11	01/05	31/05	7	28/02	0.40
cabbage		01/03& 15/06&	17/05 31/08	01/06 15/09	3 3	01/05 15/08	0.5 0.5
citrus	evergreen	evergreen	NA	NA	6	31/05	1.5
cotton	25/03	05/04	06/06	31/07	5	30/04	0.6
maize	28/02	07/03	01/07	31/07	6	15/06	0.4
strawberries	perennial	30/11&	01/08	31/08*	3	30/04	0.25
sunflower	01/03	10/03	20/06	15/07	4	15/06	0.60
tomatoes		15/04&	01/06	01/07	6	30/05	0.8
vines	perennial	31/03	11/09	30/11	5	15/06	1.0

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

& transplanted from seedbed - date indicates day of transplantation.

Table 3-30. Crop Kc factors for Sevilla.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	15/10-14/03	1.00	15/03-30/05	1.05	31/05-15/08	1.10	16/08-15/10	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	31/05-30/01	1.00	31/01-30/03	1.05	31/03-30/04	1.10	01/05-30/05	0.90
sugar beets	01/07-9/11	1.00	10/11-14/04	1.05	15/04-11/05	1.10	12/05-30/06	0.85
winter cereals	31/05-29/11	1.00	30/11-27/02	1.05	28/02-30/04	1.10	01/05-30/05	0.70
cabbage	15/09-01/03 01/06-14/06	1.00	02/03-30/04 15/06-14/08	1.00	01/05-16/05 15/08-30/08	1.00	17/05-31/05 31/08-14/09	0.93
citrus	NA		NA		All year	0.60	NA	
cotton	31/07-04/04	1.00	05/0429/04	1.08	30/04-05/06	1.15	06/06-30/7	0.90
maize	31/07-06/03	1.00	07/03-14/06	1.05	15/06-6/30	1.10	01/07-30/7	0.83
strawberries	31/08-29/11	1.00	30/11-29/04	1.00	30/04-31/07	1.00	01/08-30/08	1.00
sunflower	15/07-09/03	1.00	10/03-14/06	1.05	15/0619/06	1.10	20/0614/07	0.75
tomatoes	01/07-14/04	1.00	15/04-29/05	1.05	30/05-31/05	1.10	01/06-30/06	0.85
vines	30/11-30/03	1.00	31/03-14/06	0.88	15/06-10/09	0.75	11/09-29/11	0.65

Table 3-31. Soil parameters for Sevilla.

Depth (cm)	Classification	pH-H_2O*	pH-KCl†	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
				<2	2-50	>50				
0-10	silt loam	7.3	6.6	14	51	35	1.6	0.93	1.21	1.0
10-30	silt loam	7.3	6.6	13	52	35	1.6	0.93	1.23	1.0
30-60	silt loam	7.8	7.1	15	51	34	1.2	0.70	1.25	0.5
60-100	clay loam	8.1	7.4	16	54	30	1.0	0.58	1.27	0.3
100-120	clay loam	8.1	7.4	16	54	30	1.0	0.58	1.27	0.0
120-180	clay loam	8.2	7.5	22	57	21	0.85	0.49	1.27	0.0

* Measured at a soil solution ratio of 1:2.5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.

The ground water depth is approximately 2.4 m below the soil surface. If necessary the bottom soil layer can be extended to this depth.

Table 3-32. Soil hydraulic properties for Sevilla, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s (m^3 m^{-3})	θ_r (m^3 m^{-3})	α (m^{-1})	n	m	Water Content 10kPa (m^3 m^{-3})	Water Content 1600kPa (m^3 m^{-3})	Ksat (m s^{-1}*10^{-6})	λ	AW[@] (mm)
0-10	0.4904	0.0100	2.500	1.2688	0.2119	0.364	0.106	4.819	-1.496	25.8
10-30	0.4836	0.0100	2.450	1.2767	0.2167	0.358	0.101	4.362	-1.374	51.4
30-60	0.4798	0.0100	2.500	1.2695	0.2123	0.356	0.104	4.596	-1.465	75.6
60-100	0.4747	0.0100	2.360	1.2673	0.2109	0.357	0.105	3.911	-1.423	100.8
100-120	0.4747	0.0100	2.360	1.2673	0.2109	0.357	0.105	3.911	-1.423	
120-180	0.4795	0.0100	2.280	1.2297	0.1868	0.377	0.131	3.350	-1.858	

[@] Plant available water in the soil layer.

Plant available water in top meter is 253.6 mm.

3.9 Thiva

Table 3-33. Crop parameters for Thiva.

Crop	Growth Stage Planting (dd/mm)	Growth Stage Emergence (dd/mm)	Growth Stage Senescence (dd/mm)	Growth Stage Harvest (dd/mm)	Max. LAI (m^2 m^{-2})	Max. LAI (dd/mm)	Root Depth (m)
apples	perennial	15/03[@]	21/08	20/10[#]	5	30/06	1.0
grass + alfalfa	perennial	15/04[$] 01/07 16/08 01/10	NA	30/06 15/08 30/09 15/11	4 4 4 4	30/06 15/08 30/09 15/11	0.6 0.6 0.6 0.6
potatoes	15/02	01/03	30/06	30/07	4	30/04	0.6
sugar beets	15/04	01/05	11/08	30/09	5	30/06	0.9
winter cereals	15/11	30/11	31/05	30/06	7.5	30/03	0.8
beans (vegetables)	25/03 01/07	01/04 08/07	26/05 10/09	15/06 30/9	4 4	01/05 08/08	0.6 0.6
cabbage		15/08[&]	15/11	30/11	4	30/09	0.6
carrots	01/03 01/06	15/03 15/06	02/05 21/08	22/05 10/09	4 4	15/04 15/07	0.6 0.6
citrus	perennial	evergreen	NA	NA	5		1.0
cotton	01/05	15/05	15/07	30/08	5	15/07	0.8
maize	01/04	20/04	16/08	15/09	4.5	15/06	0.8
onions	15/02	10/04	21/06	30/06	4	15/06	0.6
tobacco		01/05[&]	20/09	30/09	5	15/08	0.6
tomatoes	na	10/04[&]	11/08	10/09	4	30/05	0.6
vines	perennial	15/03	01/08	20/10	4	30/06	1.0

@ leaf emergence

leaf fall

$ “harvest” and “emergence” dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

& transplanted from seedbed - date indicates day of transplantation.

Table 3-34. Crop Kc factors for Thiva.

Crop	Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm)							
	Harvest to Emergence		Emergence to Maximum LAI		Maximum LAI to Senescence		Senescence to Harvest	
	Period	Kc	Period	Kc	Period	Kc	Period	Kc
apples	20/10-14/03	1.00	15/03-29/06	1.05	30/06-20/08	1.10	21/08-19/10	0.98
grass + alfalfa	NA		NA		All year	1.00	NA	
potatoes	30/07-01/03	1.00	02/03-29/04	1.05	30/04-29/06	1.10	30/06-29/07	0.90
sugar beets	30/09-30/04	1.00	01/05-29/06	1.05	30/06-10/08	1.10	11/08-29/09	0.85
winter cereals	30/06-29/11	1.00	30/11-29/03	1.05	30/03-30/05	1.10	31/05-29/06	0.70
beans (vegetables)	30/9-31/03 15/06-07/07	1.00	01/04-4/30 08/07-07/08	1.05	01/05-25/05 08/08-09/09	1.10	26/05-14/06 10/09-29/09	0.70
cabbage	30/11-14/08	1.00	15/08-29/09	1.00	30/09-14/11	1.00	15/11-29/11	0.93
carrots	10/09-14/03 22/05-14/06	1.00	15/03-14/04 15/06-14/07	1.03	15/04-01/05 15/07-20/08	1.05	02/05-21/05 21/08-09/09	0.90
citrus	NA		NA		All year	0.60	NA	
cotton	30/08-14/05	1.00	15/05-14/07	1.08			15/07-29/08	0.90
maize	15/09-19/04	1.00	20/04-14/06	1.05	15/06-15/08	1.10	16/08-14/09	0.83
onions	30/06-09/04	1.00	10/04-14/06	0.98	15/06-20/06	0.95	21/06-29/06	0.85
tobacco	30/09-30/04	1.00	01/05-14/08	1.00	15/08-19/09	1.00	20/09-29/09	0.93
tomatoes	10/09-09/04	1.00	10/04-29/05	1.05	30/05-10/08	1.10	11/08-09/09	0.85
vines	20/10-14/03	1.00	15/03-29/06	0.88	30/06-31/07	0.75	01/08-19/10	0.65

Table 3-35. Soil parameters for Thiva.

Horizon	Depth (cm)	Classification	pH-H_2O^*	pH-$KCl^\dagger$	Texture (μm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
					<2	2-50	>50				
Ap1	0-30	loam	7.7	7.0	25.3	42.8	31.9	1.28	0.74	1.42	1.0
Ap2	30-45	loam	7.7	7.0	25.3	42.8	31.9	1.28	0.74	1.42	0.5
Bw	45-60	clay loam	7.8	7.1	29.6	38.7	31.7	0.98	0.57	1.43	0.5
Bw	60-85	clay loam	7.8	7.1	31.9	35.7	32.3	0.53	0.31	1.48	0.3
Ck1	85-100	clay loam	7.8	7.1	32.9	35.6	31.5	0.31	0.18	1.56	0.3
Ck1	100-???	clay loam	7.8	7.1	32.9	35.6	31.5	0.31	0.18	1.56	0.0

† These values are estimated from the measured KCl values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

* Measured at a soil solution ratio of 1:2.5

@ The depth factor indicates the relative transformation rate in the soil layer.

Depth of ground water > 5 m.

Table 3-36. Soil hydraulic properties for Thiva, Van Genuchten/Mualem parameters.

Depth (cm)	θ_s ($m^3 m^{-3}$)	θ_r ($m^3 m^{-3}$)	α (m^{-1})	n	m	Water Content		Ksat ($m s^{-1}*10^{-6}$)	λ	AW[@] (mm)
						10kPa ($m^3 m^{-3}$)	1600kPa ($m^3 m^{-3}$)			
0-30	0.4341	0.01	3.33	1.1804	0.15283	0.340	0.147	3.48	-3.162	58.02
30-45	0.4341	0.01	3.33	1.1804	0.15283	0.340	0.147	3.48	-3.162	29.01
45-60	0.4412	0.01	3.58	1.1330	0.117387	0.365	0.196	2.28	-3.402	25.43
60-85	0.4279	0.01	3.62	1.1252	0.111269	0.357	0.199	1.83	-3.312	39.70
85-100	0.4041	0.01	3.37	1.1145	0.102737	0.345	0.202	1.26	-3.259	21.44
100-???	0.4041	0.01	3.37	1.1145	0.102737	0.345	0.202	1.26	-3.259	

[@] Plant available water in the soil layer.

Plant available water in top meter of soil is 142.9 mm.

Layer 100 - ??? cm copied from layer 85 - 100 cm; this layer can be extended according to the needs of the models.

3.10 Latitude and longitude of the FOCUS Scenario Locations

Table 3-37. Latitude and longitude of the FOCUS scenario locations.

Location	Latitude	Longitude
Châteaudun	47° 98’ N	1° 75’ E
Hamburg	53° 63’ N	10° 00’ E
Jokioinen	60° 82’ N	23° 50’ E
Kremsmünster	48° 05’ N	14° 13’ E
Okehampton	50° 80’ N	3° 80’ W
Piacenza	44° 92’ N	9° 73’ E
Porto	41° 23’ N	8° 68’ W
Sevilla	37° 42’ N	5° 88’ W
Thiva	37° 97’ N	23° 72’ E

3.11 Reference

Barrere, C., Bastide, J., Coste, C.M. 1988. Relations entre la vitesse de degradation du propyzamide et les proprietes physicochimique des sols. Weed research 28:93-99.