Version: 1.1
Date: April 2002

Generic guidance for FOCUS groundwater scenarios

About this document

The report on which this document is based is that of the FOCUS Groundwater Scenarios workgroup, which is an official guidance document in the context of 91/414/EEC [full citation is FOCUS (2000) "FOCUS groundwater scenarios in the EU review of active substances" Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference SANCO/321/2000 rev.2, 202pp]. This document does not replace the official FOCUS report. However, a need was identified to maintain the definition of the FOCUS groundwater 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.

Summary of changes made since the official 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 parameterization documents, which complement the present document. The present document describes the underlying scenario definitions and their use, whilst the model parameterization 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.

Forward by the FOCUS Steering Committee

Dated: April 2000

Background

In accordance with the Council Directive 91/414/EEC concerning the placing of plant protection products on the market, active substances are jointly reviews by Member States at the EU level for inclusion on a positive list provided as Annex I of the Directive. Member States are responsible for the authorisation of formulated plant protection products containing these substances. The work of the FOCUS groups is concerned with providing the tools for estimating environmental concentrations of active substances for the purpose of their evaluation for inclusion in Annex I.

Environmental fate models have been used for many years in a regulatory context to describe the fate and behaviour of plant protection products and their metabolites in soil and water. The use of mathematical modelling in deriving predicted environmental concentrations (PEC) was therefore seen as a critical process in the development of a harmonised EU approach.

In 1993, FOCUS was formed (acronym for the FOrum for the Co-ordination of pesticide fate models and their USe). The remit of FOCUS was to develop consensus amongst the Member States, the European Commission, and industry on the role of modelling in the EU review process of active substances. The FOCUS organisation consists of a steering committee and working groups. The working groups consist of experts from regulatory authorities, from industry and from research institutes. Guidance was firstly developed for leaching to groundwater (FOCUS, 1995) and later for soil persistence and surface water (FOCUS 1996 & 1997). The guidance developed by the workgroups included a description of the relevant models and their strengths and weaknesses. Any PEC model calculation assumes a scenario which is therefore an important element of the guidance. Several Member States had developed national scenarios for the registration of plant protection products but no standard scenarios were at the EU level. Although previous FOCUS workgroups developed recommendations for scenarios, they could not develop standard scenarios within their limited time frame.

Remit of the FOCUS Groundwater Scenarios Workgroup

Standard scenarios are needed because they increase the consistency of the regulatory evaluation process by minimising the subjective influence of the person who performs the PEC calculation. Standard scenarios also make interpretation much easier, and enable the adoption of a consistent scientific process for a Tier 1 evaluation of the leaching potential of substances at the EU level. Therefore the FOCUS Workgroup for Groundwater Scenarios was charged in 1997 by the FOCUS Steering Committee with developing a set of standard scenarios which can be used to assess potential movement of active substances and metabolites of plant protection products to groundwater as part of the EU process for placing active substances on Annex 1. Since this process proceeds at the community level, the standard scenarios have to apply to the whole EU. As a result, their selection criteria necessarily differ from those of the national scenarios used by individual Member States for decision-making on formulated plant protection products in national authorisations: any similarity with existing national scenarios will therefore be purely coincidental.

The FOCUS Steering Committee prescribed that about 10 realistic worst case scenarios should be developed, and that input files for these scenarios should be developed at least for the chromatographic-flow models PELMO, PESTLA (now replaced by PEARL) and PRZM. The intended framework within which the scenarios would be used was also indicated. All relevant scenarios (but not all models - see below) would be run for every active substance as a standardised Tier 1 assessment of leaching potential. In this context the relevant scenarios are defined by the intended use of the substance, and the matrix of significant crop/scenario combinations shown in Table 1.3 of this report. The purpose of this assessment would be to establish if a "safe" scenario exists which is relevant for use of the substance. If one or more of these relevant scenarios result in predicted groundwater concentrations less than 0.1 ug/l, then in principle the active substance could be included on Annex 1 (with restrictions on its use if necessary). The Member States would then further assess the leaching potential of the relevant plant protection products under their own conditions in the process of national authorisations. In addition to modelling, there is also a role for lysimeter or field studies and monitoring data at higher tiers when these data exist.

Use of the FOCUS groundwater scenarios and interpreting results

The FOCUS Groundwater Scenarios Workgroup has now completed its work, which is represented by this report and the associated computer files.

What the standard scenarios do and don't represent

Vulnerability of ground water to contamination resulting from the use of an active substance is represented by nine realistic worst-case scenarios. Collectively, these represent agriculture across Europe, for the purposes of a Tier 1 EU-level assessment of leaching potential. The scenarios do not mimic specific fields, and nor are they necessarily representative of the agriculture at the location after which they are named or in the Member States where they are located.

The purpose of the standard scenarios is to assist in establishing if "safe" scenarios exist which are relevant for use of a substance. Since they form Tier 1 of the assessment, they have been defined to represent a realistic worst case.

Selecting models and scenarios

The scenarios have been defined independently of simulation models, but they have also been implemented in the models PEARL, PELMO and PRZM, and also MACRO in the case of Châteaudun. However it is not the intention that all scenarios should be run in combination with all models. Current practice is to use a single appropriate model, and it is anticipated that this would generally still be adequate when using the FOCUS groundwater scenarios. The notifier should select an appropriate model, and should present the input assumptions and model results in the dossier within the section reserved for the predicted environmental concentration in groundwater (PEC_{GW}). The rapporteur Member State may verify the calculations provided in the dossier but could also choose to run a different FOCUS model as part of preparing the monograph, in which case the choice of a different model should be justified. In all cases, the simulations at Tier 1 by the notifier and rapporteur should be within the framework of the FOCUS scenarios, models and input guidance.

Recommendations for interpretation of results

From this first Tier assessment there are three possible outcomes

1. The critical model output for a substance may exceed 0.1 ug/l for all relevant scenarios
2. It may be less than 0.1 ug/l for all relevant scenarios
3. It may exceed 0.1ug/l for some relevant scenarios and be less than 0.1ug/l for others

- If a substance exceeds 0.1ug/l for all relevant scenarios, then Annex 1 inclusion would not be possible unless convincing higher tier data (e.g. studies, monitoring or more refined modelling) was available to over-ride the modelling results.
- If a substance is less than 0.1ug/l for all relevant scenarios, then the choice of a realistic-worst case definition for the scenarios means that there can be confidence that the substance is safe in the great majority of situations in the EU. This does not exclude the possibility of leaching in highly vulnerable local situations within specific Member States, but such situations should not be widespread and can be assessed at the Member State level when considering national authorisations.
- If a substance is less than 0.1ug/l for at least one but not for all relevant scenarios, then in principle the substance can be included on Annex 1 with respect to leaching to groundwater. As the scenarios represent major agricultural areas of the EU, such a result indicates that "safe" uses have been identified, which are significant in terms of agriculture in the EU. The scenarios which gave results less than 0.1ug/l, along with the results of any higher tier studies which already exist, help to indicate the extent of the "safe" uses which exist for the substance. These higher tier studies could include lysimeter or field leaching studies, monitoring and more refined modelling. The results of the entire leaching assessment at the EU level could then be used to assist local assessments of leaching at the Member State level.

Support

The FOCUS Steering Committee is currently setting up a mechanism for the professional distribution, maintenance and ongoing support of the FOCUS scenarios. This will include access to the computer files via the Internet, and formal process for version control and updating of the files. Training sessions are also being planned.

References

FOCUS (1995). Leaching Models and EU Registration. European Commission Document 4952/VI/95

FOCUS (1996). Soil Persistence Models and EU Registration. European Commission Document 7617/VI/96

FOCUS (1997). Surface Water Models and EU Registration of Plant Protection Products. European Commission Document 6476/VI/97

CONTENTS

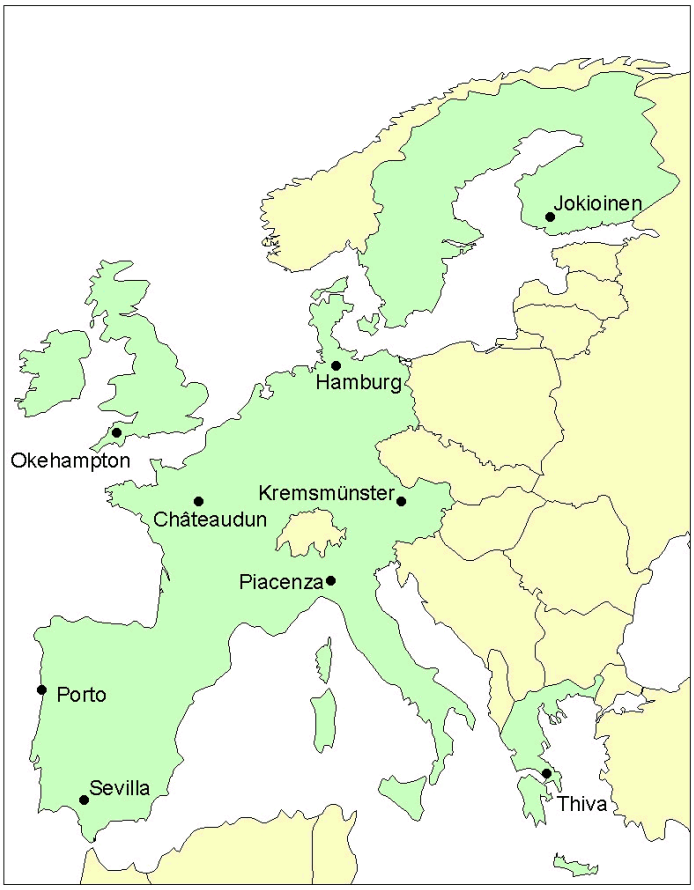
EXECUTIVE SUMMARY

Main features of the FOCUS groundwater scenarios

Nine realistic worst-case groundwater scenarios have been defined, which 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 defined for all scenarios 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 twenty which are particular to specific parts of the EU.



Location	Mean Annual Temp. (°C)	Annual Rainfall (mm)	Topsoil†	Organic Matter (%)
Châteaudun	11.3	648 + I*	silty clay loam	2.4
Hamburg	9.0	786	sandy loam	2.6
Jokioinen	4.1	638	loamy sand	7.0
Kremsmünster	8.6	900	loam/silt loam	3.6
Okehampton	10.2	1038	loam	3.8
Piacenza	13.2	857 + I*	loam	1.7
Porto	14.8	1150	loam	6.6
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. Instead the nine scenarios should be viewed collectively as representing major agricultural areas in the EU.

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 all nine scenarios have been developed for use with the simulation models PEARL, PELMO and PRZM, whilst input files for a single scenario have also developed for the model MACRO. The models all report concentrations at 1m depth for comparative purposes, but this does not represent groundwater. 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 the case of four of the scenarios, 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 invites the possibility of inconsistent approaches being adopted by different modellers, resulting in inconsistent evaluations of leaching potential. The workgroup has 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 groundwater scenarios offer for the first time a way of evaluating leaching potential across the EU. A consistent process has been defined which is based on best available science.

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.** If and when the FOCUS scenarios are adopted for use in the regulatory process then Member States will have 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?

The development of scenario files for the models PELMO, PESTLA and PRZM was specified in the remit provided by the FOCUS Steering Committee (the model PEARL superseded PESTLA during the course of the project).The Workgroup decided to also use MACRO because of its macropore flow routine, which simulates non-chromatographic flow. All these models are already regularly used in the registration processes in various Member States. Three possible reasons for differences between the results of the models have been identified and are listed below, together with the measures undertaken by the Workgroup 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 Workgroup. Similarly, validation of the models or of the process descriptions within the models was also beyond the scope of the Workgroup.

In view of the differences in process descriptions between the four models, it is to be expected that the results produced will not be exactly the same. However, example calculations with dummy substances showed remarkable similarity between the model results in practice. Predicted concentrations for the chromatographic flow models PELMO, PEARL and PRZM were mostly within a factor of two when concentrations were >1 ug/l, and

generally within an order of magnitude for lower concentrations. The macropore flow model MACRO predicted concentrations for the Châteaudun scenario which were about threefold higher than the other models. This difference appeared to be smaller when high concentrations were predicted by chromatographic models and higher when lower concentrations were predicted.

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.

Are there uncertainties in using the FOCUS groundwater scenarios?

Uncertainty will always be present to some degree in environmental risk assessment. As part of the EU review of active substances, the use of the FOCUS scenarios provides a mechanism for assessing leaching potential with an acceptable degree of certainty.

The choice of leaching scenarios, soil descriptions, weather data and parameterisation of simulation models has been made in the anticipation that these combinations should result in realistic worst cases for leaching assessments. It should be remembered, however, that the FOCUS groundwater scenarios are virtual, in that each is a combination of data from various sources designed to be representative of a regional crop, climate and soil situation. As such, none can be experimentally validated.

To further reduce uncertainty, independent quality checks of the scenario files and model shells were performed, and identified problems were removed. An additional check for the plausibility of the scenarios and models is provided by the test model runs made with dummy substances, which have widely differing properties.

Whilst there is still scope for further reductions in uncertainty through the provision of improved soils and weather data at the European level, the FOCUS groundwater scenarios workgroup is confident that the use of the standard scenarios provides a suitable method to assess leaching potential at Tier 1 in the EU review procedure.

References

FAO, 1977. Guidelines for soil profile description. Food and Agriculture Organization of the United Nations, Rome. ISBN 92-5-100508-7.

USDA, 1975. Soil Taxonomy. A basic system of soil classification for making and interpreting soil surveys. Agriculture Handbook no. 436. Soil Conservation Service, USDA, Washington DC.

1. DEFINING THE SCENARIOS

1.1 Framework for the FOCUS groundwater scenarios

1.1.1 Objectives

The FOCUS Groundwater Scenarios Workgroup was charged by the FOCUS Steering Committee with developing a set of standard scenarios which can be used to assess the potential movement of crop protection products and their relevant metabolites to groundwater 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, the workgroup developed computer shells containing the standard scenarios and all of the associated crop, soil, and weather information.

1.1.2 Principal Criteria

The Groundwater Scenarios Workgroup followed these principles for 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 90th 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 90th percentile cannot be determined precisely without extensive simulations of the various combinations present in a specific region. After exploratory statistical analysis, the workgroup decided that the overall 90th percentile could be best approximated by using a 80th percentile value for soil and a 80th percentile value for weather (Sections 6.3 & 6.4.6). The 80th percentile for weather was determined by performing simulations using multi-year weather data (Section 2.1.9), whilst the 80th percentile soil was selected by expert judgement (Section 2.1.4).

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 the whole EU.

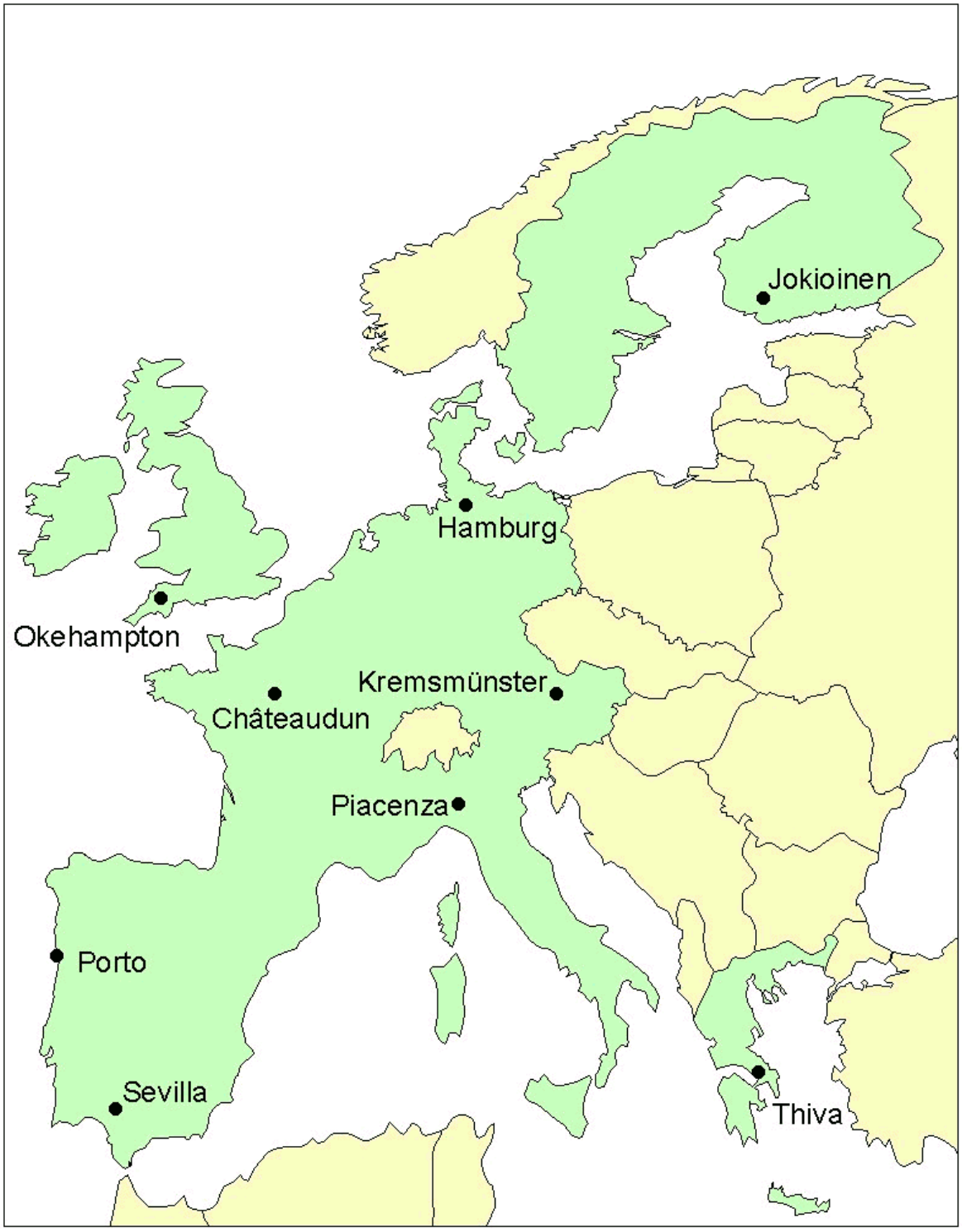
Table 1.1 Arable agriculture in EU climate zones.

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 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.

The arable and total land area data in this table 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.

Figure 1.1 Location of the nine groundwater scenarios.



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 chose 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 groundwater 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). Detailed soil properties for all scenarios as a function of depth are provided in Section 2.3 and Appendix A.

Table 1.2 Overview of the nine groundwater scenarios. (Soil texture is based on FAO, 1977, and USDA, 1975; I indicates that rainfall is supplemented by irrigation.)

			Surface Soil Properties	
	Mean Annual Temp.	Annual Rainfall	Texture	Organic Matter
Location	**(°C)**	**(mm)**		**(%)**
Châteaudun	11.3	648 + I	silty clay loam	2.4
Hamburg	9.0	786	sandy loam	2.6
Jokioinen	4.1	638	loamy sand	7.0
Kremsmünster	8.6	900	loam/silt loam	3.6
Okehampton	10.2	1038	loam	3.8
Piacenza	13.2	857 + I	loam	1.7
Porto	14.8	1150	loam	6.6
Sevilla	17.9	493 + I	silt loam	1.6
Thiva	16.2	500 + I	loam	1.3

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 the weather subgroup to identify appropriate climatic data (procedures are described in Section 2.2) for a 20 year period. The resulting average values for rainfall at each site are

shown in Table 1.2. Four locations (Châteaudun, Piacenza, 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. The main reason for including it is that macropore flow can be an important process, especially in structured soils. Macropore transport is more affected by site characteristics and less by compound-specific properties than chromatographic flow. Reasons for not considering macropore flow would include

- although great progress have been made in the past few years, current estimation procedures for crucial macropore flow parameters are not yet sufficiently robust in comparison to chromatographic-flow models
- few of the normal regulatory models consider macropore flow, and
- sensitive sites for chromatographic flow are usually not the sites most sensitive to macropore flow (sites most sensitive to macropore flow are often finer-textured soils with drainage systems).

The work group 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

The workgroup 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 (see Chapter 1.3). 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 two of the crops (cabbage and carrots) there are multiple crops grown per season, 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 four irrigated locations, namely Châteaudun, Piacenza, Sevilla and Thiva (see Chapter 1.2).

Table 1.3 Crops included in FOCUS Scenarios by location.
C Châteaudun, H Hamburg, J Jokioinen, K Kremsmünster, N Okehampton, P Piacenza, O Porto, S Sevilla, T Thiva.

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	+	+		+		+	+	+	+

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 4.2, 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 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 groundwater. 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 3.2, PEARL 1.1, and PRZM 3.2). A shell for MACRO 4.2, 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 will normally be used to evaluate potential movement to groundwater. When applications are made only every other year or every third year the simulation period will 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 (Annex VI to Directive 91/414/EEC) refer to concentrations in groundwater. 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 one metre. 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 groundwater. Soil properties below 1 m are included in the soil property files for each scenario, along with the depth to groundwater.

Model Output

The model shells rank the twenty mean annual concentrations from lowest to highest. The seventeenth value (fourth highest) is used to represent the 80^{th} percentile value associated with weather for the specific simulation conditions (and the overall 90^{th} 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 seventeenth value 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.

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1.2 Weather data for the FOCUS scenarios

Chapter 2.2 of the original FOCUS Groundwater Scenarios report still stands as a description of how the weather data were derived and implemented, and it is not necessary to repeat that here. However, the closing words of that chapter provide specific information and guidance that the user should be familiar with when using the scenarios, and so this part is repeated below. Additionally the weather and irrigation data themselves form part of scenario definition – these data are available from the FOCUS website.

The irrigated weather files are applied to all crops as follows:

- potatoes
- sugar beet
- alfalfa - applies also to grass
- apples - applies also to citrus and vines
- maize - applies also to sunflower, tobacco, cotton and soybeans
- tomatoes - applies also to onions, strawberries, cabbage, carrots and vegetable beans
- no irrigation - winter and spring cereals, winter oilseed rape and peas (for animals)

For crops where irrigated weather files are provided, they should be used.

1.3 Soil and crop data

Chapter 2.3 of the original FOCUS Groundwater Scenarios report still stands as a description of how the soil and crop data were derived and implemented, and it is not necessary to repeat that all here. However, two small portions are repeated here. Firstly, the crop kc-factors, which in essence form a part of the definition of the scenarios. Secondly, the crop interception data, which the user needs in order to adjust the application rate correctly.

Crop kc factors

Table 1.4 lists the kc-factors for all crops considered; a kc-factor is assumed constant for a crop and therefore independent from the soil – climate – location.

Table 1.4 kc-factors relating crop evapotranspiration to a reference evapotranspiration.

Crop	kc_season	kc_year
Perennial		
Apples	0.98	0.99
Grass	1.00	1.00
Vines	0.79	0.89
Strawberries	1.00	1.00
Bushberries	1.00	1.00
Citrus	0.73	0.73
Field and vegetable crops		
Potatoes	0.83	0.94
Sugarbeet	0.87	0.93
Winter cereals	0.74	0.84
Beans	0.73	0.89
Cabbage	0.87	0.97
Carrots	0.85	0.96
Maize	0.86	0.94
Oilseed rape (summer)	0.85	0.93
Oilseed rape (winter)	0.74	0.78
Onions	0.76	0.91
Peas	0.89	0.96
Spring cereals	0.80	0.92
Tomatoes	0.88	0.97
Linseed	0.69	0.84
Soybean	0.81	0.92
Sunflower	0.70	0.86
Tobacco	0.94	0.98
Cotton	0.87	0.95

Interception

Tables 1.5 and 1.6 give interception data for distinguished growth stages of different crops. Note that the interception data in Tables 1.5 and 1.6 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 1.5 Interception (%) by apples, bushberries, citrus and vines dependent on growth stage.

Crop	stage				
Apples	without leaves 50	flowering 65		foliage development 70	full foliage 80
Bushberries	without leaves 50	flowering 65		flowering 65	full foliage 80
Citrus	all stages 70				
Vines	without leaves 40	first leaves 50	leaf development 60	flowering 70	ripening 85

Table 1.6 Interception by other crops dependent on growth stage.

Crop	Bare – emergence	Leaf development	Stem elongation	Flowering	Senescence Ripening
	BBCH[#]				
	00 - 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	50	80	50
Soybean	0	35	55	85	65
Spring cereals	0	25	50 (tillering) 70 (elong.)*	90	90
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	25	50 (tillering) 70 (elong.)*	90	90

[#] The BBCH code is indicative (BBCH, 1994).
[##] A value of 90 is used for applications to established turf
* BBCH code of 20-29 for tillering and 30-39 for elongation

1.3.2 References

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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/median value 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 (Sections 2.1.2, 6.3 & 6.4.6).
4. Decisions on the use of laboratory or field degradation/dissipation rates can only be made on a case by case basis. However, when deciding which rate to use, particular attention should be paid to whether the method of determining the rates is compatible with the method assumed by the model (e.g. first order) and whether any other model sub-routines should be disabled (e.g. volatilisation).
5. The increase of sorption with time is a phenomenon that is widely accepted to occur, however data to quantify this are not generally available. If specific data are available for the substance then this can be taken into account during the modelling but otherwise a default of “no increase with time” should be used.
6. Interception of the substance by the crop canopy should be determined by reference to the interception data provided by FOCUS 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 workgroup has 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).

2.2 Introduction

The scenarios developed by the FOCUS groundwater scenarios group are aimed to assist the risk assessment required for the review of active substances under Directive 91/414/EEC. 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, at Tier 1, whilst 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.

Recent 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. It should be noted that this guidance is aimed specifically for first tier FOCUS groundwater 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 have 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 90th percentile (Section 6.4.6).

2.3 General guidance on parameter selection

Directive 91/414/EEC requires that estimations of PEC_{gw} are made for both the active substance and relevant metabolites. 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, 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 depending on how much metabolite is 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 groundwater leaching scenarios have been provided for four models; PRZM 3.2 (PRZM 3.0 Manual; Carsel *et al*., 1998), PELMO 3.2 (Jene 1998), PEARL 1.1 (Leistra *et al*, 2000) and MACRO 4.2 (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 the FOCUS report entitled "Leaching Models and EU Registration" (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 the FOCUS group.

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 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.

A German group consisting of Regulatory and Industry representatives have provided recommendations for use in the German regulatory process (Resseler *et al*., 1997). Where a range of degradation rates are available, they have proposed that mean kinetics from field tests or laboratory studies should be used in preference to the worst case value. However, they note that if there are few results which are too scattered to make an average meaningful, then a single value from a field test comparable with the intended field of use should be used.

The environmental fate annexes to Directive 91/414/EEC (95/36/EC) recommend that degradation rate studies are undertaken in four soils for the parent compound and three soils for relevant metabolites (laboratory studies initially and then, if necessary, field studies). Therefore the FOCUS group recommend that where the parent compound has been studied in a minimum of four soils it is generally acceptable to use the mean degradation rate as input into the model. Similarly, the FOCUS group recommend that where the relevant metabolite has been studied in a minimum of three soils it is generally acceptable to use the mean degradation rate as input into the model. In cases where a large number of additional data points are available, a median value may be more appropriate. In some cases the range of the results may be too large for this to be acceptable. This should be judged on a case by case basis and in this situation a value from a single study should be used, with appropriate justification of the study chosen. In situations where less than the recommended number of soils have been studied it is generally appropriate to use the worst case result which is generated in a soil of agricultural use.

Soil sorption results (Kfoc, Koc or Kfom, Kom) are also required in four soils for parent compound and in three soils for relevant metabolites according to the environmental fate annexes to Directive 91/414/EEC (95/36/EC). Where these are all agricultural soils, the FOCUS group recommend that it is generally acceptable to use the mean value of the sorption constant normalised for organic carbon (Kfoc, Koc, Kom or Kfom) to derive the input to the model, unless the sorption is known to be pH-dependent. In situations where there are results from less than the recommended number of agricultural soils then it is generally appropriate to use the worst case result (lowest sorption). In cases where a large number of additional data points are available, a median value may be more appropriate. When characterising sorption behaviour of ionic compounds, the value will vary depending on the pH and a mean or median value is no longer appropriate. In this situation it is recommended that the choice of input parameter is made in relation to the pH of the soils in the scenario in the first instance.

In addition there will be certain compounds for which sorption and degradation are pH dependent and the values are linked (e.g. lower sorption at high pH but faster degradation). Under these conditions it is appropriate to use linked values of Koc and half life rather than average values of either. 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.

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).

pKa-value (if acid or base)
The pKa 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 pKa 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 pKa value and the reference pH at which the Koc was obtained in order to adjust the sorption for pH in the profile. PEARL requires both the pKa value and the two extreme Kom 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. Since the pH throughout the profile varies by less than 1 pH unit in the soils selected for the FOCUS scenarios, it is usually more appropriate to input a single experimental value at a relevant pH rather than relying on the theoretical relationships in PELMO and PEARL to calculate such a value.

For MACRO, PEARL and PRZM, sorption data obtained at a comparable pH to the relevant soil in the simulation scenario, should be used as input.

Reference pH-value at which Koc-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 should be available as it is required as part of the substance dossier for review under Directive 91/414/EEC (H; in its dimensioned form of Pa m^3 mol^{-1}). 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/mole). 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 / under field conditions
It is important to clearly distinguish between degradation rates/half lives at reference conditions (laboratory) and those under field conditions. Either approach (laboratory degradation or field degradation/dissipation rates) may be defensible depending on the circumstances (Section 6.4.5), but in all cases the modeller must justify the approach taken (an example of how the use of field data might be justified is given by CTB, 1999). 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 first order laboratory degradation rates which the model then corrects for the temperature and moisture content effects (the reader should particularly also see the reference soil moisture section of this guidance where it is recommended that laboratory degradation rates are normalised to –10kPa prior to any averaging of the results) during the simulation. In addition, PRZM 3.2 also allows a biphasic degradation rate (with a break point) to be input if the degradation rate is not simple first order.

The PRZM model has often been used with field data (at least in Europe) and to do this the model must be parameterised in such a way as to avoid duplicating degradation processes (so called "double dipping"). Therefore processes such as volatilisation and photolysis should be disabled in the case where field degradation/dissipation rates are used. Additionally, the moisture content and temperature corrections for degradation rate would need to be disabled (Appendices B-E and model shell User Manuals) unless the modeller attempts to standardise the results accounting for differences between field and reference soil temperature/moisture. In principle, the same approach can be taken in PELMO, PEARL and MACRO and the models simplified to run using a field degradation/dissipation rate. This approach will function in a consistent way for PRZM. However, for MACRO, PEARL and PELMO it will result in no degradation below 0°C, and reduced degradation below 5°C for MACRO. This is because of the form of the degradation rate vs. temperature function built into these models, and will result in a conservative assessment.

It is also essential to assess whether the method used to determine degradation rates from the experimental data is compatible with the method assumed by the models (usually simple first order kinetics). Degradation rates for both laboratory and field experiments can be calculated using various different methods (advice on appropriate methods is provided in Doc 9188/VI/97). Where methods are not compatible, consideration should be given on a case by case basis to the most suitable approach. In some cases this could include re-fitting the experimental data to a first order kinetic, but only if this still gives an acceptable (though inferior) fit.

Reference temperature
Where laboratory data have been obtained in line with current EU guidelines (95/36/EC), the reference temperature will be 20°C.

Where older studies are used, degradation may have been studied at a range of temperatures and care should be taken in the use of both the reference temperature and the degradation rate. Where degradation rates have been obtained at a temperature other than 20°C (e.g. 25°C) then the relevant temperature can be used as input for the reference temperature for PEARL, PELMO, MACRO and PRZM (if using the temperature correction option). The degradation rate can also be manually normalised to 20°C by use of the temperature dependence correction equations (see relevant section of this guidance).

When attempting to determine an appropriate degradation rate for input into a model, a realistic comparison of the range of available results can only be undertaken if they were all obtained under the same temperature conditions. It is therefore essential to ensure that a correction to a common temperature has been undertaken prior to any comparison.

Reference soil moisture (gravimetric; volumetric; pressure head)
Current EU guidelines for laboratory degradation studies require that these are undertaken at a moisture content of 40-50% MWHC (maximum water holding capacity; SETAC, 1995). 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 matric potential values such as pF, 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 an 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, it is recommended that a reference moisture content of 10kPa (pF2) should 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 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 & 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.

It is important to 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 & 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 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

Previous versions of MACRO did not have an input value for the reference soil moisture, it assumed that the degradation rate was measured at the volumetric water content at the boundary between the macropore and micropore flow domains (i.e. XMPOR). The latest version of MACRO (December 1999) allows 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)	DT_{50}	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 average of these values is 92 days.
5. The input onto the relevant model would be a DT50 of 92 days at the field capacity (10kPa, pF 2) of the soil.

Factors or function for the adjustment of degradation rate in different depths
This parameter can have a large effect on the amount of substance simulated to leach to groundwater 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 & van der Pas, 2000; Di *et al*, 1998; Fomsgaard, 1995; Helweg, 1992; Jones & Norris, 1998; Koch *et al*, 1979; Kruger *et al*, 1993 & 1997; Lavy *et al*, 1996; Smelt *et al*, 1978a&b; 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 Appendix A of this report).

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 shell 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 2.2 (FOCUS, 1996). The alpha factor (a) value is required for MACRO and the recommended default value is 0.079 K^{-1}. These factors can also be derived from the Arrhenius activation energy. PEARL 1.1 uses the Arrhenius activation energy directly, for which the recommended default value is 54 kJ mol^{-1} (FOCUS 1996)

Parameter relating degradation rate to soil moisture

The B value is required for all four models (only in versions 3.15+ for PRZM) and 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).

2.4.3 Sorption parameters

Koc-/Kom-value or Kf-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 Kom rather than Koc (%OC = %OM/1.724; Koc = 1.724 * Kom). 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
For models which require the Freundlich adsorption coefficient (see above) the exponent of the isotherm (1/n) is also required and this is determined in each experiment. However where the results of a number of adsorption coefficient determinations are averaged then the average value of 1/n should also be used (note that 1/n is sometimes also referred to as N). When there is no data, a default value of 0.9 should be used.

Increase of the sorption coefficient with time or parameters describing non-equilibrium sorption
Although it is generally accepted that sorption increases with time there are no available generic data to use as a default and there can be problems in the manner in which the models simulate this phenomenon. If substance-specific data are available they should be used but otherwise a default assumption of no increased sorption with time should be made.

PELMO has an input for a simple increase in sorption with time (percentage increase/yr) However this only works for a single substance application and the original sorption value cannot be reverted to in following years for further applications of substances. In addition, the increasing sorption with time can only be undertaken for the first soil layer.

PEARL (version 1.1) assumes that the total content sorbed consists of two parts: the equilibrium content and the non-equilibrium content. The sorption at the non-equilibrium site is described with a first order rate equation assuming also a Freundlich isotherm for the non-equilibrium site. This results in consistent description of the non-equilibrium sorption in the case of repeated application. However, there may be some difficulty in obtaining these data as they are not part of the regulatory requirements.

PRZM 3.2 can include a flag to increase sorption with time (KDFLAG=3). Values to increase sorption by certain factors at specified times after application then need to be provided as input. The aged sorption is reset to the initial sorption after each subsequent application and hence existing substance in the soil profile is again treated as unaged.

Metabolism scheme (if necessary) with transformation fractions (parent -> 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 (range 0-1; for PEARL 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 requires the input of 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 would be required). This information is 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.

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.* (1983) for non-ionic compounds provide a relationship between TSCF and octanol:water partition coefficient with the maximum value for TSCF given as 0.8. Based on the data in this reference, the recommended default value is 0.5 for systemic compounds and 0 for non-systemic compounds if these equations are not utilised.

PRZM and PELMO require a plant uptake factor. It is recommended that the TSCF is used for this value.

2.4.5 Management related substance parameters

Number of applications
As per the GAP. Worst case options should be used, but realistic values may be used for additional simulations.

Dosages
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)

Dates of application
As per 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).

PRZM3.2 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 requires the dosage and incorporation depth to be set in the input file. If application to the soil surface is required the incorporation depth should be set to 0**.**

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 recommend 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 are provided in Chapter 1.3 based on Becker *et al.* (1999) and van de Zande *et al.* (1999). 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. SPECIFICATION OF THE FOCUS SCENARIOS

3.1 FOCUS groundwater scenario for Châteaudun

Table 3.1 Crop parameters for Châteaudun

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	m^2 m^{-2}	(dd/mm)	m
apples	perennial	01/04[@]	01/10[#]	4	31/05	1.9
grass + alfalfa	perennial[$]	01/04	15/05	5	15/05	0.5
		16/05	30/06	5	30/06	0.5
		01/07	15/08	5	15/08	0.5
		16/08	30/09	5	30/09	0.5
potatoes	15/04	30/04	01/09	4	15/06	0.6
sugar beets	25/03	16/04	15/10	5	15/07	1.0
winter cereals	20/10	26/10	15/07	7.5	31/05	0.8
cabbage		20/04[&]	15/07	3	31/05	0.6
		31/07[&]	15/10	3	05/09	0.6
carrots	28/02	10/03	31/05	3	20/04	0.8
	30/06	10/07	20/09	3	10/08	0.8
maize	20/04	01/05	01/10	4.5	15/08	0.8
oil seed rape (win)	30/08	07/09	10/07	4	20/04	1.0
onions	15/04	25/04	01/09	3	30/06	0.6
peas (animals)	25/03	05/04	15/08	4	07/06	0.6
spring cereals	20/02	10/03	20/07	5	10/06	0.6
tomatoes		10/05[&]	25/08	6	30/06	0.8
vines	perennial	01/04	01/11	6	31/07	1.9

[@] 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 3.2 Soil parameters for Châteaudun

Horizon	depth	classification	pH-H_2O*	pH-KCl†	texture µm			om	oc	bulk density	depth factor@
	cm				<2	2-50	>50	%	%	g cm^{-3}	-
Ap	0-25	silty clay loam	8.0	7.3	30	67	3	2.4	1.39	1.3	1
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 groundwater table is around 12 m.

Table 3.3 Soil hydraulic properties, Van Genuchten/Mualem parameters (restricted form, m=1-1/n)

depth	θ_s	θ_r	α	n	Water content		Ksat	λ	AW@
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	10kPa	1600kPa	m s^{-1}	-	mm
					$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
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 FOCUS groundwater scenario for Hamburg

Table A4 Crop parameters for Hamburg

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	m^2 m^{-2}	(dd/mm)	m
apples	perennial	15/04[@]	30/10[#]	4	01/07	1.6
grass + alfalfa	perennial	25/03[$] 01/06 16/07	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	15/09	3	20/07	0.7
sugar beets	01/04	15/04	08/10	4.2	30/08	1.2
winter cereals	12/10	01/11	10/08	3.8	01/06	1.1
beans (field)	25/03	10/04	25/08	4	10/07	0.9
cabbage		20/04[&] 31/07[&]	15/07 15/10	3 3	31/05 05/09	0.7 0.7
carrots	28/02 30/06	10/03 10/07	31/05 20/09	3 3	20/04 10/08	0.8 0.8
maize	20/04	05/05	20/09	4.2	30/07	1.2
oil seed rape (win)	25/08	02/09	28/07	4	05/05	1.1
onions	15/04	25/04	01/09	3	30/06	0.7
peas (animals)	25/03	10/04	25/08	4	10/07	0.9
spring cereals	10/03	01/04	20/08	3.9	05/06	0.9
strawberries	perennial	15/03	31/08*	2.5	30/04	0.7
vines	perennial	01/05	30/10	3	15/07	2.4

[@] 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 seed bed - date indicates day of transplantation, * crop removed from field.

Table 3.5 Soil texture

Horizon	depth	classification	pH-H_2O[†]	pH-KCl[*]	texture			om	oc	bulk density	depth factor[@]
	cm				<2	2-50	>50	%	%	g cm^{-3}	-
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.
Level of groundwater 2 m (estimated by IUCT).

Table 3.6 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW @
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
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	

@ AW Plant available water in the layer.

The cumulative amount over the top 1m soil is 201 mm.

3.3 FOCUS groundwater scenario for Jokioinen

Table 3.7 Crop parameters for Jokioinen

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	m^2 m^{-2}	(dd/mm)	m
apples	perennial	10/05[@]	15/10[#]	4	25/05	1.2
grass + alfalfa	perennial[$]	15/04[$]	15/06	7	15/06	0.9
		16/06	15/07	7	15/07	0.9
		16/07	25/08	7	25/08	0.9
potatoes	15/05	05/06	25/09	5	30/08	0.6
sugar beets	10/05	25/05	15/10	5	10/08	0.9
winter cereals	10/09	20/09	15/08	4.8	25/06	0.95
bush berries	perennial	10/05	25/10	4	25/05	0.6
cabbage		20/05[&]	20/09	5	05/09	0.9
carrots	15/05	01/06	05/10	4	05/09	0.6
oil seed rape (sum)	10/05	20/05	30/08	3.8	05/07	0.8
onions	10/05	20/05	15/08	4	25/06	0.3
peas (animals)	10/05	25/05	25/08	4	30/06	0.8
spring cereals	07/05	18/05	25/08	4.5	30/06	0.8
strawberries	perennial	15/05	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 seed bed - date indicates day of transplantation, * crop removed from field.

Table 3.8 Soil parameters for Jokioinen

Horizon	depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
	cm				<2	2-60	>60	%	%	g cm^{-3}	-
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 groundwater level is approximately 1.52 m below soil surface.

Table 3.9 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
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 soil layer.

Plant available water in top meter is 158.3 mm.

3.4 FOCUS groundwater scenario for Kremsmünster

Table 3.10 Crop parameters for Kremsmünster

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	15/04[@]	30/10[#]	4	01/07	1.6
grass + alfalfa	perennial	10/04[$] 26/05 16/07	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	15/09	3.5	20/07	0.7
sugar beets	01/04	15/04	10/10	4.2	30/08	1.2
winter cereals	25/10	05/11	10/08	4	05/06	1.1
beans (field)	25/03	10/04	25/08	4	10/07	0.8
cabbage		20/04[&] 31/07[&]	15/07 15/10	3 3	31/05 05/09	0.6 0.6
carrots	28/02 30/06	10/03 10/07	31/05 20/09	3 3	20/04 10/08	0.7 0.7
maize	20/04	05/05	20/09	4.2	30/07	1.2
oil seed rape (win)	25/08	02/09	28/07	4	05/05	1.1
onions	15/04	25/04	01/09	3	30/06	0.6
spring cereals	10/03	01/04	20/08	3.9	05/06	0.9
strawberries	perennial	15/03	31/08*	2.5	30/04	0.7
vines	perennial	01/05	30/10	3	15/07	2.4

[@] 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 seed bed - date indicates day of transplantation, * crop removed from field.

Table 3.11 Soil parameters for Kremsmünster

depth	classification	pH-H_2O[†]	pH-KCl[*]	texture µm			om	oc	bulk density	depth factor[@]
cm				<2	2-50	>50	%	%	g cm^{-3}	
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.

Level of groundwater (range) around 1.6 m, for apples and vines a deeper groundwater 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 3.12 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
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 FOCUS groundwater scenario for Okehampton

Table 3.13 Crop parameters for Okehampton

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2 m^{-2}$	(dd/mm)	m
apples	perennial	25/03[@]	15/09[#]	2.5	15/06	1.5
grass + alfalfa	perennial	10/02[$]	15/05	4.5	15/05	0.45
		16/05	15/07	4.5	15/07	0.45
		16/07	15/09	4.5	15/09	0.45
potatoes	15/04	30/04	01/09	4	15/07	0.6
sugar beets	10/04	25/04	25/10	3	30/08	0.8
winter cereals	07/10	17/10	01/08	7.5	15/05	0.8
beans (field)	01/03	15/03	15/09	4	07/06	0.45
linseed	25/03	30/03	25/09	3	25/06	0.6
maize	07/05	25/05	07/10	7	15/07	0.8
oil seed rape (sum)	25/03	30/03	20/08	3	15/05	0.6
oil seed rape (win)	07/08	14/08	21/07	4.5	30/04	0.85
peas (animals)	25/03	05/04	15/08	4.0	07/06	0.45
spring cereals	25/03	01/04	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.

Table 3.14 Soil parameters for Okehampton

Horizon	depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
	cm				<2	2-50	>50	%	%	g cm^{-3}	(-)
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.
Level of groundwater circa 20 m.

Table 3.15 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
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 layer.

Plant available water in top meter is 203.7 mm.

3.6 FOCUS groundwater scenario for Piacenza

Table 3.16 Crop parameters for Piacenza

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	01/04[@]	01/11[#]	5	31/05	1.5
grass + alfalfa	perennial[$]	28/02[$] 16/05 16/07	15/05 15/07 20/09	4 4 4	15/05 15/07 20/09	0.8 0.8 0.8
potatoes	¼	20/04	10/09	5	01/06	0.5
sugar beets	01/03	20/03	15/09	4	30/06	0.8
winter cereals	25/11	01/12	01/07	7	10/05	1.0
citrus	perennial	evergreen	15/12	5	31/05	1.5
maize	30/04	15/05	30/10	5	31/07	1.0
oil seed rape (win)	30/09	05/10	20/06	3.5	15/04	0.6
soybean	25/04	10/05	05/10	6.5	31/07	0.6
sunflower	¼	20/04	20/09	4	20/06	1.0
tobacco		20/05[&]	05/10	4	20/07	1.0
tomatoes		10/05[&]	25/08	6	30/06	1.0
vines	perennial	01/04	01/11	6	31/07	2.0

[@] 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 seed bed - date indicates moment of transplantation.

Table 3.17 Soil parameters for Piacenza

Horizon	depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
	cm				<2	2-50	>50	%	%	g cm^{-3}	
Ap	0-30	loam	7	6.3	15	45	40	1.72	1.00	1.3	1.0
Ap	30-40	loam	7	6.3	15	45	40	1.72	1.00	1.3	0.5
Bw	40-60	silt loam	6.3	5.6	7	53	40	0.64	0.37	1.35	0.5
Bw	60-80	silt loam	6.3	5.6	7	53	40	0.64	0.37	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.
Level of groundwater 1.5 m (range 1.30-1.70 m).

Table 3.18 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θs	θr	α	n	m	Water content		Ksat	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-30	0.4632	0.0100	3.050	1.2487	0.1992	0.339	0.107	4.666	-1.906	69.6
30-40	0.4632	0.0100	3.050	1.2487	0.1992	0.339	0.107	4.666	-1.906	23.2
40-60	0.4546	0.0100	2.270	1.3605	0.2650	0.317	0.063	6.217	0.316	50.8
60-80	0.4546	0.0100	2.270	1.3605	0.2650	0.317	0.063	6.217	0.316	50.8
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 soil layer.
Plant available water in top meter is 222.6 mm.

3.7 FOCUS groundwater scenario for Porto

Table 3.19 Crop parameters for Porto

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2 m^{-2}$	(dd/mm)	m
apples	perennial	15/03[@]	31/10[#]	3	30/06	1.2
grass + alfalfa	perennial	28/02[$]	15/05	4	15/05	0.8
		16/05	15/07	4	15/07	0.8
		16/07	20/09	4	20/09	0.8
potatoes (sum)	28/02	15/03	15/06	4	30/05	0.7
sugar beets	28/02	15/03	01/08	5	30/04	1.0
winter cereals	15/11	30/11	30/6	6.5	30/04	1.0
beans (vegetable)	28/02	10/03	31/08	4	15/05	0.5
cabbage		28/02[&]	01/07	4	15/05	0.5
		31/07[&]	15/11	4	31/08	0.5
carrots	15/02	28/02	31/05	4	01/05	0.5
	15/07	22/07	15/10	4	15/09	0.5
citrus	perennial			6	31/05	1.5
maize	20/04	01/05	01/10	4.5	15/08	0.8
oil seed rape (sum)	15/03	22/03	25/08	3	31/05	0.9
oil seed rape (win)	30/08	07/09	10/07	4	20/04	1.0
onions	15/02	28/02	31/05	3.5	15/05	0.5
spring cereals	20/02	10/03	20/07	5	10/06	0.6
tomatoes		15/03[&]	31/08	5	15/06	0.5
vines	perennial	15/03	30/09	4	31/07	2.0

[@] 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 3.20 Soil texture for Porto

depth	classification	pH-H_2O [*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
cm				<2	2-50	>50	%	%	g cm^{-3}	-
0 - 35	loam	4.9	4.2	10	48	42	6.6	3.8	0.89	1.0
35 - 60	sandy loam	4.8	4.1	8	31	61	3.7	2.1	1.25	0.5
60 - 100	sandy loam	4.8	4.1	8	31	61	3.7	2.1	1.25	0.3
100 - 120	sandy loam	4.8	4.1	8	31	61	3.7	2.1	1.25	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.
Level of groundwater: summer lower than 2 m, winter 0.7 - 1.2 m.
Top layer is Ap horizon, other layers C1 horizon.

Table 3.21 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-35	0.5780	0.0100	4.830	1.1588	0.1370	0.443	0.208	2.885	-1.630	82.25
35-60	0.4720	0.0100	4.340	1.2123	0.1751	0.339	0.125	3.142	-1.350	53.50
60-100	0.4720	0.0100	4.340	1.2123	0.1751	0.339	0.125	3.142	-1.350	85.60
100-120	0.4720	0.0100	4.340	1.2123	0.1751	0.339	0.125	3.142	-1.350	

[@] Plant available water in the soil layer.

Plant available water in top meter is 221.35 mm.

3.8 FOCUS groundwater scenario for Sevilla

Table 3.22 Crop parameters for Sevilla

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

[@] 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 seed bed - date indicates day of transplantation.

Table 3.23 Soil parameters for Sevilla

depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
cm				<2	2-50	>50	%	%	g cm^{-3}	-
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 groundwater level is approximately 2.4 m below soil surface. If necessary the bottom soil layer can be extended to this depth.

Table 3.24 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θs	θr	α	n	m	Water content		Ksat	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
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 soil layer
Plant available water in top meter is 253.6 mm.

3.9 FOCUS groundwater scenario for Thiva

Table 3.25 Crop parameters for Thiva

Crop	Growth stage			LAI		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	15/03[@]	20/10[#]	5	30/06	1.5
grass + alfalfa	perennial	15/04[$]	30/06	4	30/06	0.6
		01/07	15/08	4	15/08	0.6
		16/08	30/09	4	30/09	0.6
		01/10	15/11	4	15/11	0.6
potatoes	15/02	01/03	30/07	4	30/04	0.6
sugar beets	15/04	01/05	30/09	5	30/06	0.9
winter cereals	15/11	30/11	30/06	7.5	30/03	0.8
beans (vegetables)	25/03	01/04	15/06	4	01/05	0.6
	01/07	08/07	30/9	4	08/08	0.6
cabbage		15/08[&]	30/11	4	30/09	0.6
carrots	01/03	15/03	22/05	4	15/04	0.6
	01/06	15/06	10/09	4	15/07	0.6
citrus	perennial		30/11	5		1.5
cotton	01/05	15/05	30/08	5	15/07	0.8
maize	01/04	20/04	15/09	4.5	15/06	0.8
onions	15/02	10/04	30/06	4	15/06	0.6
tobacco		01/05[&]	30/09	5	15/08	0.6
tomatoes	na	10/04[&]	10/09	4	30/05	0.6
vines	perennial	15/03	20/10	4	30/06	2.0

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] crops are transplanted from seed beds - in the column emergence the date of transplantation is given.

Table 3.26 Soil texture

Horizon	depth	classification	pH-H_2O[†]	pH-KCl[*]	texture			%om	%oc	bulk density	depth factor
					<2	2-50	>50	%	%	g cm^{-3}	-
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.

Level of groundwater > 5 m.

Table 3.27 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
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 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 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**, pp93 - 99.