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FOCUS groundwater scenarios in the EU review of active substances

The report of the work of the Groundwater Scenarios Workgroup of FOCUS (FOrum for the Co-ordination of pesticide fate models and their USe), Version 1 of November 2000.

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Forward by the FOCUS Steering Committee

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 2.3 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

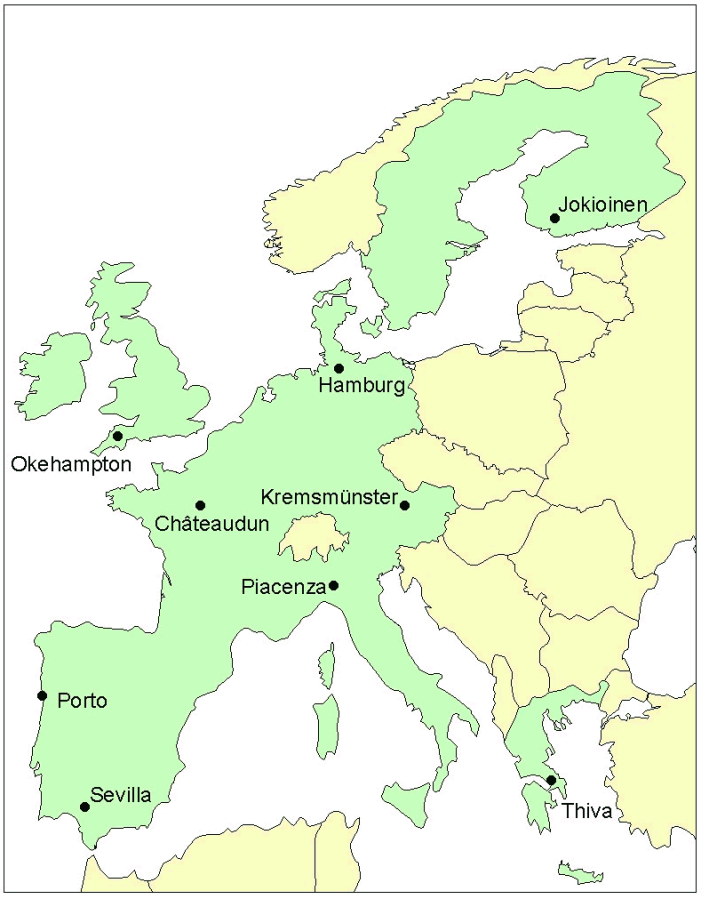
EXECUTIVE SUMMARY

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. INTRODUCTION

This report is structured as follows. Chapter 2 describes the definition of the scenarios, including the principles of the selection and the procedures used for selecting the weather, soil, crop and pesticide data. It contains also a summary of these inputs - details of soil and crop input data can be found in Appendix A. Most of the contents of Chapter 2 and Appendix A are not specific to one particular model. Chapter 3 summarises the parameterisation of the four selected models (details of which can be found in Appendices B to E). Chapter 4 describes the test runs performed with four "dummy" substances and their results. Chapter 5 gives detailed guidance to users on substance-specific input parameters. Chapter 6 contains a general discussion of uncertainties related to the scenarios that have been developed, reflecting all major discussion issues in the working group during the development of the scenarios.

2. DEFINING THE SCENARIOS

2.1 Framework for the FOCUS groundwater scenarios

2.1.1 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.

2.1.2 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).

2.1.3 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 2.1). The end result was the selection of nine locations (shown in Figure 2.1 and listed in Table 2.2).

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.

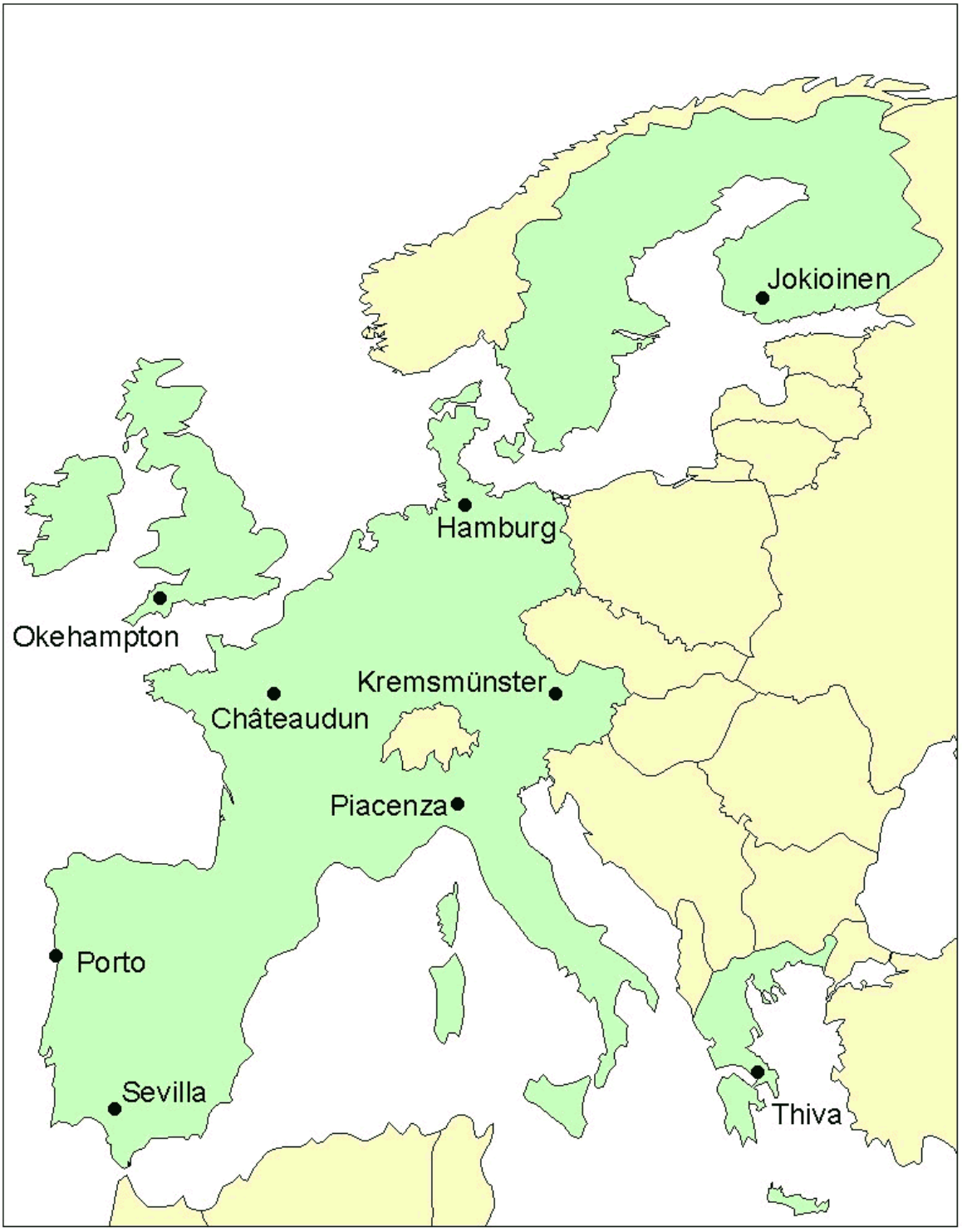
Table 2.1 Arable agriculture in EU climate zones.

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 2.1 Location of the nine groundwater scenarios.



2.1.4 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 2.2). 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 2.2 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

2.1.5 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 2.2. Four locations (Châteaudun, Piacenza, Sevilla, and Thiva) were identified as having irrigation normally applied to at least some crops in the region.

2.1.6 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.

2.1.7 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 2.3). 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 2.3). 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 2.3, 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 2.2).

Table 2.3 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	+	+		+		+	+	+	+

2.1.8 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.

2.1.9 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 80th percentile value associated with weather for the specific simulation conditions (and the overall 90th percentile concentration considering the vulnerability associated with both soil and weather). When applications are made every other or every third year, the 20 concentrations for each two or three year period are ranked and the 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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2.2 Weather data for the FOCUS scenarios

This Chapter describes the procedures used to develop weather datasets for the FOCUS scenarios. Firstly the criteria used to determine the suitability of datasets are described. Once selection criteria were established and a suitable data source identified, then the model input files had to be developed from this data source. Finally the procedures used to develop irrigated datasets are described.

2.2.1 Criteria for selecting weather datasets

Defining the scenarios and the target values

The general approach for establishing the FOCUS groundwater scenarios was to select locations in major agricultural regions that covered the diversity of EU agriculture (see Chapter 2.1). As a part of the process for defining scenario locations, target values for the mean annual rainfall and temperature were set based on climatic maps and tables (Heyer, 1984; FAO, 1994; Fraters, 1996). This was done to ensure appropriate coverage of the range of climatic conditions in EU arable agriculture.

Table 2.4 Climatic targets for selecting weather datasets for the nine FOCUS groundwater scenarios

Location	Code	Mean temperature (°C)	Target annual rainfall (mm)
Châteaudun	C	5-12.5	600
Hamburg	H	5-12.5	700
Jokioinen	J	<5	600
Kremsmünster	K	5-12.5	900
Okehampton	N	5-12.5	>1000
Piacenza	P	>12.5	750
Porto	O	>12.5	1150
Sevilla	S	>12.5	550
Thiva	T	>12.5	500

Weather data requirements of the selected leaching models

The required weather parameters for the selected leaching models (PRZM, PELMO, PEARL and MACRO) are given in Table 2.5. The data should be available on a daily basis. In order to come up with a reliable risk assessment procedure, long time series of these daily data should be available (26 years for application each year, 46 years for applications each two years, and 66 for applications each three years - these include 6 warm-up years).

Table 2.5 Weather data requirements for the 4 selected leaching models

Model	Weather parameter	Unit
MACRO & PEARL	Daily total precipitation	mm
	Daily potential evapotranspiration rate	mm
	Minimum daily temperature	° Celsius
	Maximum daily temperature	° Celsius
PELMO	Daily total precipitation	cm
	Daily potential evapotranspiration rate	mm
	Minimum daily temperature	° Celsius
	Maximum daily temperature	° Celsius
PRZM	Daily precipitation rate	cm
	Daily potential evapotranspiration rate	cm
	Average daily temperature	° Celsius
	Average daily wind speed	cm/s#

#Values should be representative for 10m above ground level

In order to ensure that natural variation in climatic conditions, in particular with regard to precipitation, is represented in the simulation, original weather data are preferable to applying a weather generator.

2.2.2 Establishing the weather files

Description of the primary data source: the MARS meteorological data base

The Space Applications Institute of the Joint Research Centre (JRC) at Ispra, Italy, hold long-term weather data, compiled as part of the Monitoring Agriculture by Remote Sensing (MARS) project (Vossen and Meyer-Roux, 1995). The data were derived using a method developed by the DLO-Staring Centre for Agricultural Research in the Netherlands (van der Voet *et al*., 1994). The MARS meteorological database contains daily meteorological data spatially interpolated on 50 x 50 kms grid cells. The original weather observations data set originate from 1500 meteorological stations across Europe, Maghreb countries and Turkey, and are based on daily data for the period 1971 to date (Terres, 1998). It was compiled from data purchased from various national meteorological services, either directly or via the Global Telecommunication System. Some of the data were obtained from the national meteorological services under special copyright and agreements for MARS internal use only, so that data at station level are not available, only interpolated daily meteorological data are available.

In the MARS database, the basis for the interpolation is the selection of the suitable combination of meteorological stations for the determination of the representative meteorological conditions for a grid cell. The selection procedure relies on the similarity of the station and the grid centre. This similarity is expressed as the results of a scoring algorithm that takes the following characteristics into account:

- Distance
- Difference in altitude
- Difference in distance to coast
- Climatic barrier separation

The following weather parameters are available:

- Date
- Minimum air temperature
- Maximum air temperature
- Precipitation
- Wind speed
- Deficit vapour pressure
- Calculated potential evaporation (Penman equation)
- Calculated global radiation following Angströms formula (sunshine hours based), Supit formula (cloudiness and temperature based) and Hargraves (temperature based).

The MARS dataset was found to be the most appropriate source for establishing the weather files for the FOCUS groundwater scenarios. Daily weather data for the selected scenarios for a period of 20 years were transferred to the working group, after negotiating the intellectual property rights and data use with the data provider.

Creating the FOCUS weather files

In handling the data from the MARS data base, the following issues were addressed:

No weather station available in the MARS data base for the selected scenario location. This is the case for the Châteaudun, Thiva, Jokioinen, Kremsmünster and Okehampton scenarios. In this case, data from nearby weather stations were considered. These are data obtained mainly from the Orleans weather station for the Châteaudun scenario, the Athens weather station for the Thiva scenario, the Tampere weather station for the Jokioinen scenario, the West München weather station for the Kremsmünster scenario, and the Exeter weather station for the Okehampton scenario.

Time series available in the MARS data base are incomplete. This was the case for the Thiva (only data for the Athens weather station from 1977-1994) and the Jokioinen scenario (missing data for the years 1992-1996). To complete a series of 20 years, data for missing years were replaced by the MARS data of another similar year which was identified using a second database. This second database contains long-term average climatic data for Europe and has been collated by the Climatic Research Unit (CRU) at the University of East Anglia, in the UK as part of the Climatic Impacts LINK Project. The data are held at a resolution of 0.5º longitude by 0.5º latitude and include long-term monthly averages of precipitation, temperature, wind speed, sunshine hours, cloud cover, vapour pressure, relative humidity and frost days based mainly on the period from 1961 to 1990 (Hulme *et al*., 1995a & 1995b). The database was derived from various sources and is based on daily data from between 3078 and 957 weather stations across Europe, depending on the specific variable. The year chosen to substitute for each missing year was defined by analysing the similarity between the total annual precipitation of the missing year and the other years, as reported in the weather data file of the CRU database. The year that matches the total annual precipitation of the missing year in the CRU file was selected to replace the missing year in the MARS data file.

The total annual rainfall of the MARS file do not match the original target. Given the procedure used to create the MARS database, actual meteorological data at the scenario site may deviate from the recorded data in the MARS data file (see Chapter 6). These deviations can be substantial for the precipitation data, which remain difficult to interpolate in time and space. As such,

generated data from the MARS records do not always correspond to the predefined targets. In order to comply with the original targets and data provided by other data sources, it was agreed to scale the daily precipitation data, such that the average precipitation of the FOCUS record was in line with the targets defined in Table 2.4. Therefore the precipitation data for the Okehampton and Kremsmünster scenarios were scaled up, while the precipitation for the Thiva and the Porto scenarios were scaled down.

An overview of the actions are given in the Table 2.6. The results of the processing was a complete 20 year time series of weather data, meeting the original targets.

Table 2.6 Overview of the handling of the MARS data files

Location	**Code**	**Station**	**Target annual rainfall (mm)**	**Rainfall from MARS (mm)**	**Data handling**
Châteaudun	C	Orleans	600	648	- Irrigation to be considered - Orleans station selected to be representative for Châteaudun
Hamburg	H	Hamburg	700	786	
Jokioinen	J	Tampere	600	638	- Tallinn (Estonia) and Finnish stations were selected to be representative for Jokioinen - Fill missing years
Kremsmünster	K	West-München	900	749	- West München (Germany) station selected to be representative for Kremsmünster (Austria) - Scale the precipitation to reach an annual target of 900 mm
Okehampton	N	Exeter	>1000	741	- Exeter station selected to be representative for Okehampton - Scale the precipitation to reach an annual target of 1038 mm
Piacenza	P	Piacenza	750	857	- Irrigation to be considered
Porto	O	Porto	1150	1402	- Scale the daily precipitation down to reach an annual target precipitation of 1150 mm
Sevilla	S	Sevilla	550	493	- Irrigation to be considered
Thiva	T	Athens	500	671	- Irrigation to be considered. - Athens station to be considered representative for Thiva station - Fill missing years. - Scale the precipitation to reach an annual target of 500 mm

From the 20 years time series, 66 weather files were constructed as follows:

- Renumbering of the data years. The years in the data files had to be renumbered so that the 40- and 60- year compiled files do not go past the year 1999, which is a problem for those programs that store years in 2-digit format. It was decided to start renumbering from 1901, which was thus formatted as "01" for the models.
- Extend the time series to include a 6 year warming up period. The last six years were copied and used as a "warming up" period. Calculation of outputs will not consider results for the "warming up" period.
- Extend the time series to 46 and 66 years. It was decide to repeat the 20 year weather sequence but with the years cycled round by one and two years to ensure that applications are made in each year of available weather data. When doing so, problems are encountered for 'leap' years. If a record for the 29-th of February is in a non leap year, then this record was skipped. If a record for the 29-th of February is not available for a leap year, the record for the 28-th of February was duplicated.
- The files were finally formatted to be compatible with the PRZM, PELMO, PEARL and MACRO shells.

2.2.3 Irrigation

A two-pronged approach was used to develop the irrigation schedules for the Piacenza, Thiva, Sevilla and Châteaudun scenario. In a first step, irrigation schedules were developed based on a modelling of the water balance at the sites, subjected to the boundary condition as predefined by the climatic, soil and crop scenario. Subsequently, the results were sent to local experts for evaluation. Correction of the irrigation schedules were considered if local experts recommended to do so. Some further details are described in Verlaine & Vanclooster 1999.

The irrigation scheduling model

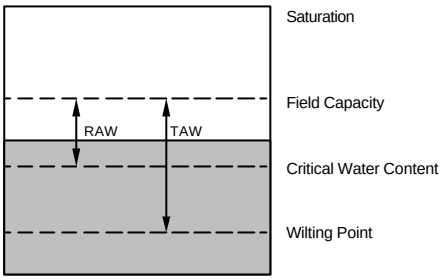
Irrigation scheduling is the action of planning the timing and depth of irrigation events. The primary objective is to apply the irrigation water at the right period and in the right amount. Untimely water deliveries and inappropriate water depths decrease the irrigation efficiency. Limited supply results in yield reduction due to water stress. Excess of water may result in deep percolation losses (which may leach nutrients and chemicals out of the root zone) and may also decrease the yield.

The irrigation scheduling software IRSIS (Irrigation Scheduling Information System) (Raes and al., 1988) developed by the Institute for Land and Water Management, Katholieke Universiteit Leuven has been selected in this study.

To generate irrigation schedules, information of the water content in the root zone is needed. This water content is simulated in IRSIS on a daily basis by means of a simplified water balance model. Such a model keeps track of all inputs of water through rainfall, irrigation and capillary rise and of all withdrawal of water through runoff, soil evaporation, crop transpiration and deep percolation. The water content of the root zone is affected by all these processes.

Figure 2.2 Schematic presentation of the water balance of the root zone

p = RAW/ TAW



The Total Available Water (TAW) in the model is the water content between field capacity and wilting point. The water content between field capacity and the critical water content is called the Readily Available Water (RAW). The fraction of TAW which is readily available is given by the p-factor which is a function of the climatic evapotranspiration demand, the soil, the specific crop and the particular growth stage. Field capacity and wilting point values are available directly from the scenario definitions. Values for critical water content were estimated in terms of matric potential from literature data specific to each crop, and these values were converted into moisture contents using the soil water retention data which formed part of the scenario definitions.

For the estimation of the crop water requirements, four data files need to be established: potential evapotranspiration, precipitation, crop parameters and soil properties. All data were derived from the available weather, soil and crop databases.

The climate, soil and crop data base

The climatic input data are the daily potential evapotranspiration (ET_0) rates and rainfall depths. Crop-specific potential evapotranspiration has been calculated by multiplying the ET_0 by a crop coefficient, kc (this is the ratio of the real crop evaporation rate to the reference evaporation rate from standard meteorological data; see Section 2.3.3) :

$ET_{crop} = kc * ET_0$

An effective rainfall rate is used in IRSIS. The effective rainfall is estimated from rainfall data as :

Effective rainfall = a * actual rainfall

with a = 0.8.

The actual rainfall rate has been adopted from the previously established files and are aggregated on a ten day basis.

Irrigation scenarios were generated for six crops - potatoes, maize, apples, alfalfa, tomatoes and sugar beet. For the purposes of irrigation these six datasets are then used for all irrigated crops. The crop data consists of information about :

- the length of the different growth stages and the variation of the crop coefficient (kc) throughout those stages,
- the variation of the rooting depth throughout the growing period,

- the variation of the p-factor throughout the growing period

The p-factor, the ratio between the readily and total available water (RAW/TAW), is in fact not only a function of the crop type and the growth stage, but depends also on the climatic evapotranspiration demand and the soil type. The considered crop data were compiled from the crop databases (see Chapter 2.3) and appropriate literature (Raes and al, 1988).

For normal field crops, the total growing period has been divided into four stages:
(1) initial stage :germination and early growth when the soil surface is not or is hardly covered by the crop (groundcover < 10%)
(2) crop development stage : from end of initial stage to attainment of effective full groundcover (groundcover 70-80%),
(3) mid-season stage : from attainment of effective full groundcover to time of start of maturing as indicated by discolouring of leaves or leaves falling off. This stage is normally reached well after the flowering stage of annual crops, and
(4) late season stage : from end of mid-season stage until full maturity or harvest

For alfalfa, the variation of kc over the cutting interval needs to be considered, that is from kc (low) just following harvesting, to kc (peak) just before harvesting. Alfalfa grown for seed production will have a kc value equal to kc (peak) during full cover until the middle of full bloom. For apples, values of kc were used on a monthly basis.

The irrigation scheduling options
Two options were initially considered :
Option 1 : depletion of 100 % of the RAW and irrigation until field capacity,
Option 2 : weekly irrigation and irrigation until field capacity is reached

For a crop having shallow rooting depths, (e.g. potato), Option 1 leads to a realistic schedule with acceptable irrigation depths (e.g.<40 mm). However, for crops having deep rooting depths, Option 1 leads to high irrigation amounts of up to 120 mm. In addition, such an approach does not consider off-site water availability and considers that water resources can be exploited for irrigation at any moment. These disadvantages can be avoided by applying water at a fixed time interval (7 days), i.e. Option 2, which corresponds to a sprinkler irrigation scenario. However in such an approach, critical water contents will not be reached.

Option 2 was finally chosen for the irrigation scenarios. A minor error was made when creating 46 and 66 year irrigation files, caused by the incorrect handling of leap years. This means that the irrigation after the 26^{th} year is sometimes a day earlier or later than intended. This error affects no other variable than irrigation, and does not occur in 26 year weather files.

Table 2.7 Irrigation results given as averages over a 26 year period

		Châteaudun	Piacenza	Sevilla	Thiva
Rain (mm)		621	849	478	656
Modified rain (mm)		621	849	478	492
ETp (mm)		745	769	1301	1028
Potatoes	Annually mean of depth (mm)	316	382	270	564
	Number of irrigations	18	20	16	20
Maize	Annually mean of depth (mm)	332	367	603	602
	Number of irrigations	18	17	20	19
Apples	Annually mean of depth (mm)	332	361	823	661
	Number of irrigations	20	18	24	26
Alfalfa	Annually mean of depth (mm)	313	371	866	618
	Number of irrigations	20	21	28	27
Tomatoes	Annually mean of depth (mm)	297	328	501	522
	Number of irrigations	14	14	14	15
Sugar beet	Annually mean of depth (mm)	359	396	463	669
	Number of irrigations	18	17	19	24

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.

2.2.4 References

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2.3 Soil and crop data

The principal criteria for the selection of scenarios (Chapter 2.1) state that they should represent realistic worst case conditions, in which the vulnerability is split evenly between the climate and the soil. The principal criteria do not attribute any vulnerability to other aspects of the scenarios; these other aspects should therefore reflect average conditions.

Whilst Chapter 2.1 gives the general approach for site selection, this chapter presents the parameterisation of the scenarios in detail. The soil profiles, their hydraulic properties and the crops are described in separate sections.

2.3.1 Soil profiles

After the definition of the scenarios with respect to temperature and precipitation, for each scenario a generalised soil profile was chosen that fulfilled the requirement in terms of vulnerability. Then workgroup members consulted local experts to assist them in finding the specific real soil profiles and their property details. Experts were asked to provide a description of the soil profile (at least down to a depth of 1 metre), the depth of the groundwater table and data on at least the following physical and chemical properties for each horizon:

- soil texture
- soil pH (pH-H20, pH-CaCl2 or pH-KCl)
- dry bulk density
- percentage organic carbon or percentage organic matter.

After checking the real profiles against the generalised target profiles, the real profiles were accepted and included in the scenario descriptions. Table 2.8 provides an overview of the selected soils.

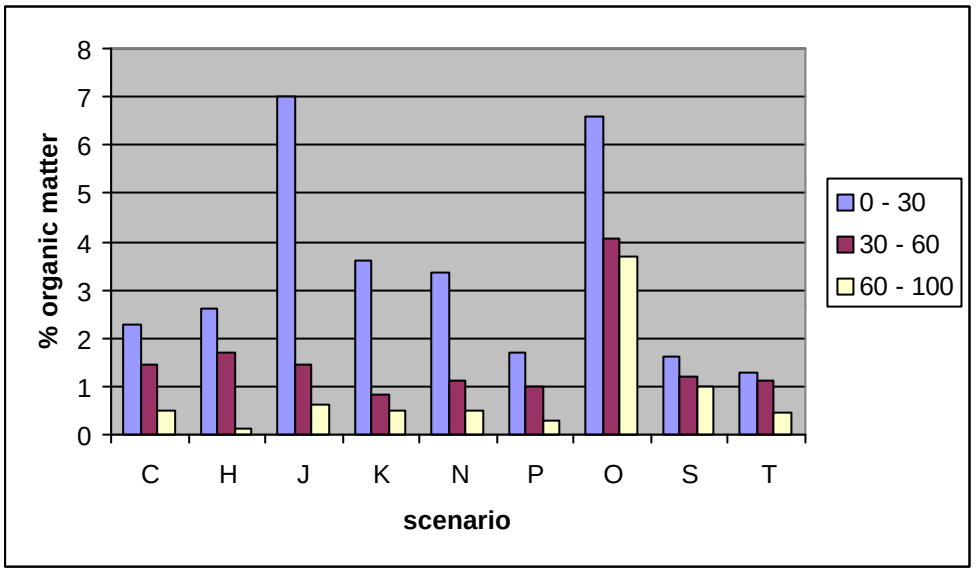
Table 2.8 Soil properties for the nine FOCUS groundwater scenarios.

Location	Code[1]	Properties of surface soil[2]		
		Organic matter (%)	Texture[3]	pH[5]
Châteaudun	C	2.4	silty clay loam	8.0
Hamburg	H	2.6	sandy loam	5.7
Jokioinen	J	7.0	loamy sand[4]	6.2
Kremsmünster	K	3.6	loam/silt loam	7.0
Okehampton	N	3.8	loam	5.8
Piacenza	P	1.7	loam	7.0
Porto	O	6.6	loam	4.9
Sevilla	S	1.6	silt loam	7.3
Thiva	T	1.3	loam	7.0

[1] code used in figures and tables for labelling the location
[2] in the plough layer
[3] USDA classification (USDA, 1975; FAO, 1977)
[4] the sand fraction may be further classified as fine
[5] measured in various media, see Appendix A

Figure 2.3 shows that the organic matter contents in the top 20 cm range between 1 and 4% for all scenarios except Jokioinen and Porto which are above 6%. The values for the deeper layers are lower: around 1 to 2 per cent for the 30 – 60 cm layer and around 0.5 % for the 60-100 cm layer, except for again the Porto soil profile which contains about 4 % organic matter in the deeper layers. The Hamburg soil profile has a very low organic matter content below a depth of 60 cm. When considering leaching to groundwater, the organic matter below the top 20 cm plays an important role (Boesten, 1991).

Figure 2.3 Organic matter content in the 0 - 30 cm, 30 – 60 cm and 60 – 100 cm layers of the nine FOCUS soil profiles. See Table 2.8 for explanation of the location codes.



For nearly all profiles some data handling was necessary (Table 2.9). If the original profile did not reach 1 m depth, the profile was extended to this depth by lengthening the lowest layer of the profile. For calculation reasons, some models need one or more additional soil layers below this depth. If not available in the original data, the lowest layer was extended to a depth well below 1 m. Only the depth-dependent degradation factor (see below) was set to zero below a depth of 1 m.

For some of the selected models there is a limitation in the number of horizons. For this reason it was decided to limit the number of horizons to a maximum of 6. Although it seems that Châteaudun has 7 horizons, there are in fact only 6: the C1 horizon has been split into two, just to cope with the depth-dependent degradation factor (see below). If the number of horizons had to be reduced, weighted averages were calculated for the physical parameters. For practical reasons it was decided to round the thickness of the horizons to the nearest 5 cm increment. In this procedure the physical and chemical data were not changed.

The scenario descriptions list both % organic matter and % organic carbon. If only one of the two was provided the other was calculated according to the formula:

$$\%\text{om} = 1.724 \cdot \%\text{oc}$$

where:

%om is the percentage organic matter (by weight)

%oc is the percentage organic carbon (by weight)

There is evidence that the transformation rate of substances decreases with depth (Boesten and Van der Linden, 1991). In general, this depth dependency will be a function of both the soil and the substance. The workgroup recognised this general tendency and decided to account for this decrease in activity. For this reason a depth-dependent degradation factor has been introduced. This relates the standardised transformation rate in the deeper layers to the rate in the top layer. The transformation rate coefficient of the top layer (plough layer) has to be multiplied by this factor to obtain the standardised rate for the deeper layer. Given the limited data available in literature, the workgroup decided to assume the same depth dependency for all soil profiles irrespective of substance properties. The factor is 0.5 for the layer just below the plough layer (generally c. 30 cm - 60 cm), 0.3 for the subsequent layer (generally 60 cm to 1 m) and 0.0 below 1 m depth (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). This depth-dependent degradation factor is added to the soil profile information. If the profile horizon boundaries deviated not more than 5 cm from the depths indicated above (i.e. 30 cm, 60 cm and 1 m), the depth factors were assigned to the appropriate layers. If the deviation was larger, the layer was artificially split into two separate layers, each layer with the appropriate depth factor. This is the default option for the scenarios. If more information is available for the substance considered, the user may adjust the depth dependency accordingly (see Section 5.4.2).

The average groundwater levels for four (Jokioinen, Kremsmünster, Porto and Piacenza) of the nine scenarios are close to 1.5 m depth. Two scenarios (Hamburg and Sevilla) have levels of about 2 m depth and the remaining three (Châteaudun, Okehampton and Thiva) have levels deeper than 5 m.

Table 2.9 Detailed information on physical and chemical soil parameter handling

Châteaudun	Several similar local profiles and their properties were available. These had differing horizon numbers and depths, and were interpreted to produce a single representative profile and associated properties.
Hamburg	Horizon thickness rounded to nearest 5 cm, profile extended below 1 m.
Jokioinen	Horizons rounded to nearest 5 cm
Kremsmünster	Lowest horizon extended beyond 1 m depth
Okehampton	No changes
Piacenza	No changes
Porto	Bottom horizon artificially split into three layers because of depth factor
Sevilla	Soil classification added, based on texture information
Thiva	No changes

2.3.2 Soil hydraulic parameters

All horizons for each site are described with van Genuchten parameters (van Genuchten, 1980). The equations have the following form:

$$q(h) = q_r + \frac{q_s - q_r}{\left(1 + |ah|^n\right)^{1-1/n}} = q_r + \frac{q_s - q_r}{\left(1 + |ah|^n\right)^m}$$

with:

θ(h)	moisture content dependent on the pressure head
θ_r	residual moisture content
θ_s	moisture content at saturation
α	reciprocal of the air entry value
h	pressure head
n	fitting parameter
m	fitting parameter (m = 1 – 1/n)

$$K(h) = K_s \frac{\left(\left(1 + |ah|^n\right)^{1-1/n} - |ah|^{n-1}\right)^2}{\left(1 + |ah|^n\right)^{(1-1/n)(l+2)}} = K_s \frac{\left(\left(1 + |ah|^n\right)^m - |ah|^{n-1}\right)^2}{\left(1 + |ah|^n\right)^{m(l+2)}}$$

with:

K	the hydraulic conductivity dependent on the water tension
K_s	the hydraulic conductivity at saturation
l	parameter for the pore size distribution

The parameters requiring estimations are thus θ_s, θ_r, K_s, α, n and *l*.
The general considerations for parameter selection have been the following:

- If a consistent and well-documented parameter set exists for a site, the preferred solution has been to use it for the simulations.
- For the sites where the data were incomplete or not consistent, van Genuchten parameters have been generated via the transfer functions developed in the HYPRES project (Wösten, 1998).
- For very sandy sites, HYPRES provides no or rather unrealistic predictions. For one of these sites, measured parameters exist, and this data has been copied to very sandy layers of other sites, where HYPRES was unable to provide reasonable estimates.

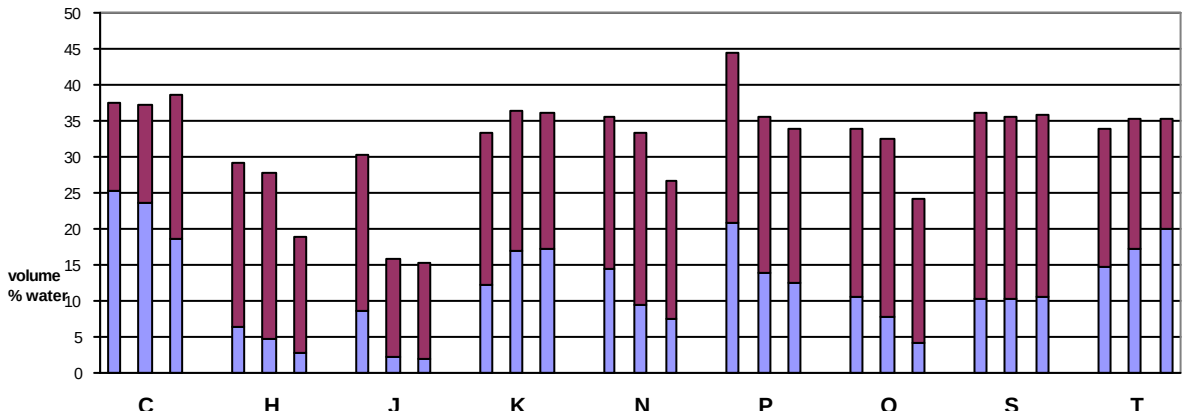
All parameter combinations have been used to generate plots in order to check whether they are realistic. The parameters are thus expected to be reasonable estimates of typical values for the selected soils. However, particularly the hydraulic conductivity (the saturated conductivity as well as the conductivity function) remains an uncertain parameter, due to the large variability found in nature. Table 2.10 summarises the sources of the data for each site.

Table 2.10 Source and derivation of soil hydraulic properties

Scenario	Data type	Comment	Data source
Châteaudun	Measured data	MACRO needs measured data for a proper calibration. Available water in the first metre is 152 mm for the measured data and 197 for the HYPRES data. The hydraulic conductivity measured and found by HYPRES are comparable (Horizon 1: 1.0 versus 1.3; Horizon 2: 2.0 versus 1.5 and Horizon 3: 2.0 versus 2.1 – units being 10^{-6} m/s).	Bruand *et al*. (1996), Coquet (1999) pers. communication
Hamburg	Measured data	Several data sets exist for this soil. HYPRES cannot deliver data for the 3 and 4th horizon, due to very low clay content. The HYPRES conductivities are 3-11 times smaller than the measured data.	Gottesbüren (pers.com.) and Kördel *et al*. (1989)
Jokioinen	HYPRES	No measured retention data are available. The HYPRES conductivities are slightly higher than the average measured conductivity on this soil type, but within a reasonable range.	
Kremsmünster	HYPRES	The HYPRES conductivities are rather low.	
Okehampton	HYPRES	The measured conductivities presented are 3-5 times above the HYPRES estimates	
Piacenza	HYPRES for 2 horizons; Hamburg data for the 3rd.	The last horizon does not contain any clay, similar to the deepest horizon in the Hamburg scenario. The HYPRES transfer functions cannot be used for soils without clay.	
Porto	HYPRES		
Sevilla	HYPRES	Bulk densities estimated from pedotransfer functions	
Thiva	HYPRES		

From the Van Genuchten parameters, the moisture contents at field capacity and at wilting point were calculated because these are needed for the capacity-flow models PELMO and PRZM. Figure 2.4 shows these volume fractions of water at field capacity (FC, 10kPa) and wilting point (WP, 1600kPa) respectively. Hamburg and Jokioinen have FC values that are lower than the other seven soils; Porto has a remarkably high field capacity compared to all other soils. The water content at wilting point is rather low for Hamburg. The plant available water is approximately 20 to 25 % in the plough layer, except in Châteaudun with only 12%.

Figure 2.4 Volume fraction of water in the layers 0 – 30 cm, 30 – 60 cm and 60 – 100 cm of the nine FOCUS groundwater scenarios. The total length of the column indicates the volume fraction of water at field capacity, the bottom part at wilting point. See Table 2.8 for explanation of the location codes.



The dispersion length of all soil profiles was set at 5 cm for all soil horizons. This parameter is only relevant for MACRO and PEARL because PELMO and PRZM simulate dispersion numerically. In general, the dispersion lengths of field soils range from 2 to 10 cm but the correlation with soil texture is too weak for estimating location-specific dispersion lengths (Vanderboght *et al*., 1999).

2.3.3 Crop data

Because the vulnerability of the scenarios is to be reflected in the soil properties and the climatic data rather than in the crop parameters, in general average or median values are chosen for the crop data. However, in all cases the compatibility of soil, climate and crop data was checked. When data were incompatible the crop data were modified and compatibility was forced. Finally, the consistency of the crop data between the different locations was checked; only a few data were modified because of this. The following sections describe the crop data in more detail.

The workgroup decided to gather only a limited amount of data, to meet the minimal requirements of the selected models. All models require information on crop management (at least sowing or planting date and harvest date) and on the growth stage of the crop (at least: emergence date and dates of maximum development of leaves and roots). The development of the crop is further characterised by the maximum leaf area index (LAI) or, alternatively, the maximum soil cover and the maximum effective rooting depth.

Parameter estimation procedures

The workgroup constructed a list of important crops or crop groups occurring in Europe. Five crops are considered to be relevant for all scenarios: apples, grass (or alfalfa), potatoes, sugar beets, winter cereals. Local experts were asked to indicate whether other crops on the list are significant in the region represented by the scenario conditions. The data on physiology and phenology of crops have been selected with the help of local experts or were extracted from published evaluations (e.g. Becker *et al*., 1999; Myrbeck, 1998; Resseler *et al*., 1997; Van de Zande *et al.*, 1999). It has to be noted, however, that in wide areas of agricultural practice generally valid data on cultivation management, phenology and physiology of crops must be given with reservations. When compiling data taken from *different* sources of literature, consistency with the natural course of plant growth in the desired scenario must be maintained, and artefacts are to be avoided (e.g. by compiling data from different studies where crops where subjected to significantly different growing conditions).

The FOCUS scenarios are virtual sites, representative for a broad region, not only for the immediate surroundings of the location. Therefore, it can happen that the crops and specific crop data proposed for a scenario are not exactly representative for the agricultural practice at the location of the soil associated with the respective region and scenario. Representative or average values have been selected if only ranges were provided, permitting a practice-oriented simulation of frequently cultivated crops for the regions of the FOCUS locations. A final check of crop data consistency for model input was applied.

Table 2.3 provides an overview of crops selected for the various scenario conditions. In most cases local experts were asked to provide specific crop data. Table 2.11 gives information on data modification after obtaining the primary information from the local experts.

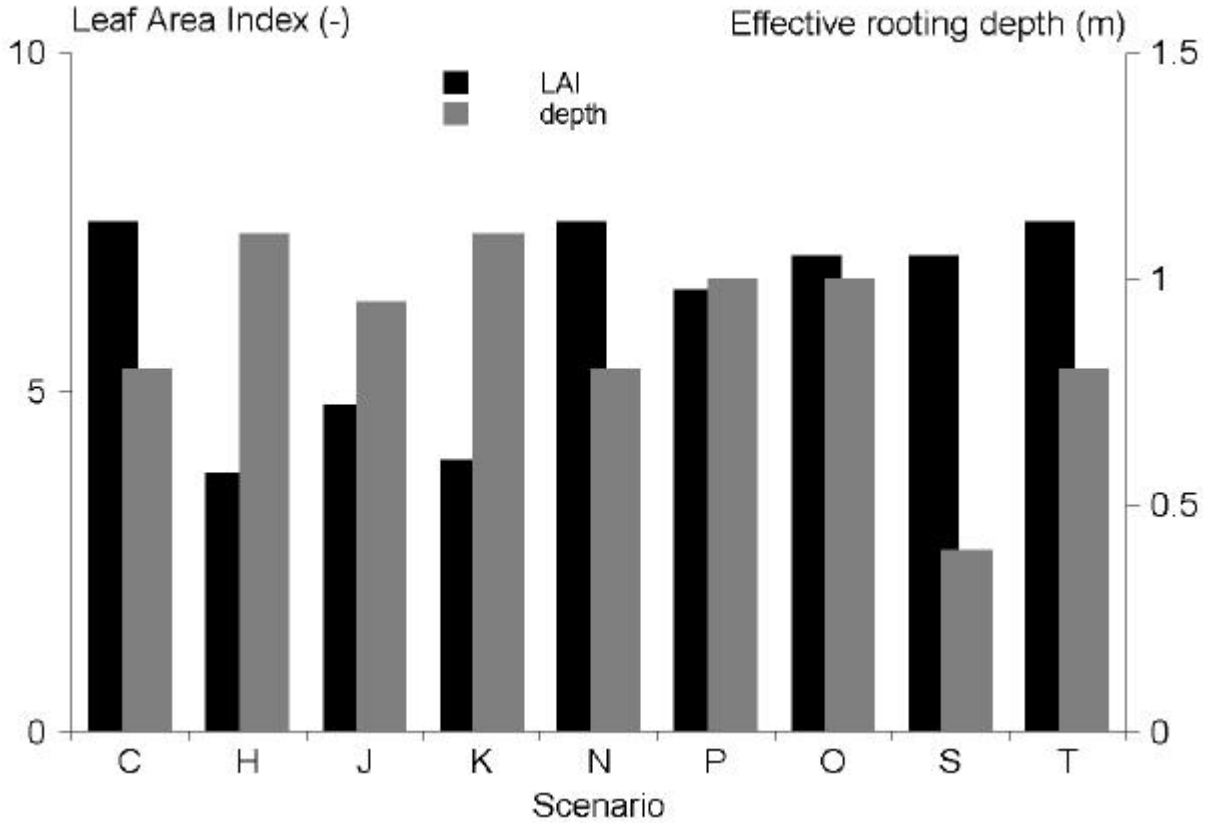
The effective rooting depth was taken to be 0.8 times the maximum rooting depth; the resulting figure was rounded to the nearest 10 cm or, alternatively, restricted to the maximum of a specific soil horizon. For all perennial crops (i.e. apple, citrus, vines, strawberries, bush berries and grass) a complete root system is assumed to be present throughout the simulation period, though leaves are lost each winter (except for citrus and grass). For all locations the grass/alfalfa crop has several defined harvest and emergence dates each year. These "harvests" represent the cutting of the crop, and its subsequent regrowth, and so they affect above ground biomass but not rooting depth.

Table 2.11 Crop data handling for each scenario.

Châteaudun	
apples, sugar beets, cereals, rape, maize	Rooting depth recalculated to effective rooting depth, if necessary adapted to the specific layering of the chosen soil.
grass, potatoes, cabbage, carrots, onions, peas, soybeans, tomatoes and vines	Deduced from other scenarios, taking into account soil restrictions and climatic conditions
Hamburg	
all crops	Recalculation of delivered data on rooting depth to effective rooting depth (maximum rooting depth x 0.8 = effective rooting depth). All recalculated data rounded to the nearest 10 cm, taking into account soil restrictions.
Jokioinen	
Carrots	data deduced from other scenarios
apples, peas, strawberries	LAI data deduced from other scenarios
all crops	Soil cover deduced from other scenarios
Kremsmünster	
all crops	Recalculation of delivered data on rooting depth to effective rooting depth. (maximum rooting depth x 0.8 = effective rooting depth) All recalculated data rounded to the nearest 10 cm, taking into account soil restrictions.
Okehampton	
sugar beet	Local expert deduced data from swede; sugar beet growing is possible under the scenario conditions, but sugar beet are rarely grown near the actual site.
Potatoes	LAI, root depth and soil cover deduced from other scenarios, taking into account soil restrictions
all crops	data on root depth brought in line with data from other scenarios, taking into account soil restrictions
Piacenza	
all crops	maximum soil cover deduced from other scenarios
Porto	
all crops	LAI deduced from other scenarios Root depths recalculated to effective root depths, taking into account soil restrictions (also rounded to nearest 10 cm)
Sevilla	
all crops	LAI deduced from other scenarios
Thiva	
all crops	LAI and soil cover deduced from other scenarios. Root depth deduced from other scenarios, taking into account soil restrictions.

As an example Figure 2.5 shows the maximum LAI and maximum effective rooting depth for winter wheat for the selected scenarios. The maximum LAI is less than 5 for Hamburg, Kremsmünster and Jokioinen and around 7 for the other scenarios. Possibly this is a result of the prevailing temperature. The maximum effective rooting depth seems to be influenced by soil restrictions rather than other factors.

Figure 2.5 Maximum leaf area index and maximum effective rooting depth for winter wheat for the nine FOCUS groundwater scenarios. See Table 2.8 for explanation of the location codes.



Crop kc factors

The amounts of water evaporating from the soil or transpired by plants depend on soil properties, climatic conditions and the development stage of the crops (Wallace, 1995). Although the relation between the real crop evaporation rate and a reference evaporation rate, which is calculated from standard meteorological data, is therefore not constant, this is assumed for the scenarios developed here. The constant, usually referred to as the kc-factor, is a calibration factor, taking into account soil surface and aerodynamic resistances. The procedure for standardising the kc-factors is described below.

The growing season of annual field and vegetable crops were divided into four growth stages:

- Stage 1: From sowing/planting date (Table Crop Scenarios Working Group, TCSWG) until emergence date (TCSWG);
- Stage 2: From emergence date (TCSWG) until full cover (TCSWG);
- Stage 3: From full cover (TCSWG) until maturity phase (the length of this stage is estimated from Doorenbos and Pruitt, as referred to in Raes *et al*., 1988);
- Stage 4: From maturity stage until harvest (TCSWG)

The growing season of perennial crops was also divided into four stages:

- Stage 1: From 1 January until appearance of foliage
- Stage 2: Crop development stage
- Stage 3: Mid season
- Stage 4: Late season

Crop kc factors for the four growing stages were derived from available literature as follows:

Field and vegetable crops

- stage 1 average kc factor from Table 18 from Doorenbos and Pruitt (1977);
- stage 2 average kc factor from Table 18 from Doorenbos and Pruitt (1977);
- stage 3 average kc factor from Doorenbos and Pruitt (1977), with selected relative humidity > 70 %, and mean wind speed between 5 and 8 m/sec;
- stage 3 average kc factor from Doorenbos and Pruitt (1977), with selected relative humidity > 70 %, and mean wind speed between 5 and 8 m/sec;

Perennial crops

- Apples: crop kc factors were derived from Table C6 of Raes *et al*. (1988). We assumed full grown trees with spacing providing 70 % ground cover, subjected to humid light to moderate windy conditions.
- Grass: crop kc factors were set equal to 1.
- Vines: we assume initial leaves early May and harvest mid-September. The ground-cover is 40-50 % at mid-season. The meteorological situation is humid, light to moderate windy.
- Citrus: crop coefficients were derived, from Table C5 of Raes *et al*. (1988) for full grown trees with 50 % ground cover. Weeds are controlled and soil is cultivated.
- Strawberries, bush berries: no appropriate literature was found. We therefore consider the kc=1.

Bare soil

The kc-factor of bare soil will strongly be influenced by the tillage practice (surface roughness), soil type, soil structure, etc. No coherent data source could be identified. Therefore, the kc of bare soil is set to 1.

Mean kc factors. A cropping period averaged kc factor, kc_{season} was calculated as follows:

$$kc_{season} = \sum_{1}^{4} w_i . kc_i$$

$$w_i = \frac{\Delta t_i}{\sum \Delta t_i}$$

with kc_i, the kc factor of crop stage i; w_i a crop stage dependent weighing factor; Δt_i, the average length of the crop stage, and $\Sigma\Delta t$, the length of the growing season.

A yearly averaged crop kc factor, kc_{year}, was calculated as follows:

$$kc_{year} = \sum_{1}^{4} w_i . kc_i + \left(1 - \sum_{1}^{4} w_i\right) . kc_{soil}$$

$$w_i = \frac{\Delta t_i}{365}$$

with kc_{soil}, the kc factor for bare soil.

Table 2.12 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 2.12 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 and LAI

The LAI or the soil cover determines to some extent the amount of substance intercepted by the crop. The number of data describing directly the interception of substances by crops at different growth stages of the crops is rather limited. Therefore also indirect data are used to estimate interception.

Becker *et al*. (1999) provide information on soil cover at different stages of growth for a number of crops. From this information they estimated the interception and, for the purpose of implementation in first tier assessments, they recommended simplified tables. Van de Zande *et al*. (1999) performed

a literature research on the soil deposition of substances depending on growth stage and spraying equipment (machine type, nozzle type, operating conditions like pressure, sprayed volume, etc.). Part of the data is direct deposition on the soil while the other part is calculated from the interception by the crop (assuming a perfect balance). Ganzelmeier (1997) compiled data on soil deposition in fruit, vines and hops cultivation. The agreement between the results of Becker *et al*., Ganzelmeier and Van de Zande *et al*. is remarkable. Becker *et al*. (1999)state that the number of available (measured) interception data is by far too small to present a comprehensive overview. Their opinion, however, is that the information on crop coverages (e.g. Becker *et al* used around 2000 field trials over four years in six Member States) is enough to estimate interception indirectly. The data of Van de Zande *et al*. (1999) support this opinion.

Tables 2.13 and 2.14 give interception data for distinguished growth stages of different crops. The interception data in general are derived from the results of Ganzelmeier (1997),, Becker *et al*.(1999) and Van de Zande *et al*. (1999). For crops not covered by these data sources, interception was estimated based on information on the LAI of crops as provided with the GLEAMS model. In deriving numbers from these references for use in the tables a generally conservative approach has been taken, e.g. using values for the earlier growth stages within a range of growth stages, and using values towards the lower end of the measured range. Tables 2.13 and 2.14 use the BBCH scale to indicate the growth stage where possible (BBCH, 1994).

Interception is limited to never exceed 90%, both for realism and also for compatibility with the simplified input guidance assumptions regarding substance applications and the fraction reaching the soil (see Chapter 5). For crops cultivated in beds an area-weighted average interception is assumed. Note that the interception data in Tables 2.13 and 2.14 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 2.13 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 2.14 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	10	20	40	25
Grass	90	90	90	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
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

The BBCH code is indicative.

2.3.4 References

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2.4 Substance parameters

Substance parameters in this context refers to the properties of active substances and metabolites of plant protection products. Although substance parameters might not be seen as a part of a scenario rather than generic data of the compound, recommendations are given in this FOCUS Report in order to

- facilitate checking model input
- reduce the uncertainty of the modeller
- give guidance on default values and parameter ranges and - if deviations are necessary - give appropriate justification
- give general guidance on parameter selection
- give specific guidance on substance-specific input parameters for different models

The parameters required for simulation of leaching to groundwater with the different models PRZM v.3.2, PELMO v.3.0, PEARL v.1.1 and MACRO v.4.2 were summarised.

Redundant information or related information or parameters that can be derived from each other (e.g. Henry's constant from water solubility and vapour pressure) are reduced to a minimum and checked for consistency. The parameters are categorised to be either substance specific or being in general constant for all substances in all FOCUS scenarios unless specific information has to be used.

For the parameters that are classified to be constant or for which specific information can not be expected within the EU review process, default values are given. It has to be stated clearly that the default values are recommendations that can be overruled by more specific data if a valid justification can be given.

Parameters from different models that contain the same or related information (e.g. sorption parameters like K_{OM} or K_{OC}) are grouped and all parameters are sorted into the categories physico-chemical parameters, degradation parameters of the active substance and metabolite(s), sorption parameters, metabolism, crop related substance parameters and management related substance parameters. See Table 2.15.

Information on model specific parameters and recommendations to generate the values for the input parameters from available environmental fate studies are given in Chapter 5.

To demonstrate and test the FOCUS scenarios the parameters for four examples 'dummy' substances are given in Chapter 4.

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Table 2.15 General List of Substance Parameters

No.	Parameters	Unit	Range	Constant for all substances at all scenarios - Yes/No	Remarks
	Physico chemical parameters				
1	molecular weight	[g/mol]	50 - 1000	N	
2	solubility in water	[mg/l]	10^{-3} - 10^{6}	N	
3	vapour pressure	[mPa]	10^{-8} - 2800	N	
4	pKa-value (if acid or base)	[-]	2 - 12	N	It needs to be thoroughly described which charge transfer between neutral and negative charged molecule is meant
5	reference pH-value at which Koc-value was determined	[-]	4 - 8	N	Details for selection and consequences in Chapter 5
6	dimensionless Henry-coefficient		10^{-2} - 10^{-10}	N	Conc. in gas phase / conc. in liquid phase Calculation given in Chapter 5
7	diffusion coefficient in water	[m^2/d]	10^{-5} - $3*10^{-4}$	N	See Chapter 5
8	gas diffusion coefficient	[m^2/d]	0.1 - 3	N	See Chapter 5
	Degradation parameters of the substance				
9	Half life in bulk top soil at reference conditions / under field conditions	[d]	0.5 - 365 d	N	Details for selection and consequences for moisture/temp. routines in Chapter 5
10	”reference temperature"	[°C]	20	Y	default value, deviations need justification
11	”reference soil moisture" (gravimetric;volumetric;pressure head)	[-]	40-50% mwhc; 0.1-33 kPa	N	FC for capacity models; 10kPa for Darcy flow models
12	factors for the adjustment of degradation rate in different depths	[-]	0 - 1.0	N	details for selection and consequences in Chapter 5

No.	Parameters	UNIT	Range	Constant for all substances at all scenarios - Yes/No	Remarks
	Parameter, relating degradation rate to soil temperature				
13	Q10-factor (increase of degradation rate with an increase of temperature of 10°C)	[-]	2.2 (default)	Y	default value, deviations need justification
14	g (=gamma) factor for relating degradation rate and soil temperature according to Boesten & van der Linden 1991)	[-]	0.079 (default)	Y	default value, deviations need justification
15	ARRHENIUS activation energy	[kJ/Mol]	54 (default)	Y	default value, deviations need justification
	Parameter, relating degradation rate to soil moisture				
16	B-value (exponent of degradation - moisture relationship according to Walker, 1974)	[-]	0.7 (default)	Y	default value, deviations need justification
	Sorption Parameters				
17	Koc-/Kom-value or Kf-values in different depth	[dm^3/kg]	1->100 000	N	Koc = 1.724 * Kom. Expressed at reference concentration of 1.0 mg/l
18	exponent of the FREUNDLICH-isotherm	[-]	0.7-1.0	N	0.9 is a recommended default value if data are missing
19	increase of the sorption coefficient with time or parameters describing non-equilibrium sorption	[-]		N	Refer to Chapter 5 for how to handle non-equilibrium sorption
	Metabolism				
20	Metabolism/metabolites with transformation fractions (parent -> metabolites)	[-]		N	almost all parameters (1-19) need to be given for each metabolite separately
	Crop related substance parameters				
21	TSCF = transpiration stream concentration factor	[-]	0.0 - 0.8	N	0.0 for non systemic; 0.5 for systemic compounds (default values), or use Briggs' equation (see Chapter 5)
	Management related substance parameters				
22	number of applications	[-]	depends	N	
23	dosages	[kg/ha]	depends	N	
24	dates of application	[-]	depends	N	
25	incorporation depth	[cm]	0-30	N	
26	factor(accounting for interception by crops)	[%]		N	default value for each crop and growth stage see Tables 2.13 & 2.14; deviations need justification

3. THE MODEL INPUT FILES

3.1 Summary of the MACRO parameterisation

MACRO 4.2 is a one-dimensional, non-steady state model of water flow and solute transport in a layered soil at the pedon/ field scale. The model describes a high-conductivity/low porosity macropore domain coupled to a low-conductivity/high porosity domain representing the soil matrix. Mass exchange between the domains is calculated with approximate, yet physically based, first order expressions. The model structure therefore enables quantitative evaluation of the impact of water flow and solute transport through macropores in structured soil. It is the only model evaluated in this report with this feature. However, types of preferential flow other than through macropores are not simulated.

MACRO includes the following processes:

-	Unsaturated water flow	Richards' equation in micropores, gravity flow in macropores
-	Root water uptake	Empirical sink term, water preferentially extracted from macropores
-	Seepage to drains and groundwater	Seepage potential theory. Sink term in vertical water flow equations. Drains are not simulated for the FOCUS groundwater scenarios.
-	Solute transport	Convection/dispersion equation in the micropores, mass flow only in the macropores
-	Mass exchange	Approximate first order rate equation for mass exchange of both solute and water
-	Sorption	Instantaneous equilibrium, Freundlich isotherm, sorption partitioned between micro- and macropores
-	Degradation	First-order kinetics, separate rate coefficients for four pools (solid and liquid, micro- and macropores).
-	Metabolism	One metabolite can be simulated at a time
	Canopy interception and washoff	The interception is calculated as a function of the cover percentage. Washoff is calculated as for PRZM. Both routines are turned off to follow FOCUS procedures.
	Plant uptake	Plant uptake is calculated as a function of the transpiration of the plant.

MACRO does not (or not fully) include the following processes

-	Volatilisation	A lumped dissipation rate including volatilisation, photolysis etc. may be given for the leaves, but this option is not active in the FOCUS scenarios. Volatilisation from the soil is not included.
-	Surface runoff	Surface runoff of water and solute is only included in the sense that if the surface layer is saturated, the excess water and solute is lost to the profile. But it cannot be used to model runoff processes as such.

The main issues encountered during parameterisation were

- the transformation of the van Genuchten parameters which were given for the profile to Brooks-Corey-parameters for the soil matrix. Both parameter sets were derived from measured data. Effectively the soil parameters used in the simulations are almost identical to what is used by the other models. The resulting parameters are listed in the MACRO appendix.
- the parameterisation of the specific macropore parameters (Ascale, ZN). The parameters received values based partly on the transfer functions available in MACRO DB which estimates the value of ASCALE based on a description of soil structure, and partly on a rough calibration of the model on measured data from lysimeters at Châteaudun. Macropores are few in the upper 25cm, significant between 25 and 60cm depth, and non-existent below 60cm.

In addition to the crop parameters specifically given for the FOCUS scenarios, a number of crop parameters had to be estimated. This concerns, among others, LAI at harvest, a root adaptability factor, maximum water interception by the crop, factors describing the change in leaf area development over time, critical soil air content for root water uptake, a factor describing the distribution of the roots in the root zone, critical tension for root water uptake, and a correction factor for evaporation from wet canopy. The parameter set for crops agreed upon is listed in the MACRO appendix.

The reduction of substance reaching the soil surface is parameterised as follows. The user should input the dose actually reaching the ground, excluding the amount intercepted by the crop. The fraction intercepted is determined from the interception tables as described in the guidelines in Chapter 2.3. Washoff is set to zero ensuring that only the amount of substance entering the soil directly continues in the leaching calculations.

Reference

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3.2 Summary of the PELMO parameterisation

PELMO is a one dimensional simulation model simulating the vertical movement of chemicals in soil by chromatographic leaching. The first version of PELMO was released in 1991 (Klein, 1991). PELMO is based on the US-EPA's PRZM 1 model (Carsel *et al*, 1984), but was improved with regard to the requirements of the German authorities. In version 2.01 of PELMO (released in 1995) the runoff routines were upgraded and routines for estimating the volatilisation of substances were added. PELMO 2.01 was validated within a joint project of the "Industrieverband Agrar" (IVA), the German Environmental Protection Agency and the "Fraunhofer-Institut für Umweltchemie und Ökotoxikologie" in Schmallenberg shared by the KfA Jülich and the SLFA Neustadt (Klein *et al*, 1997). In 1998 a complementary tool was added to PELMO 2.01 in order to enable the transformation of the applied a.i. to metabolites and to allow for further metabolism including the formation of CO_2 (PELMO 3.0; Jene, 1998). Recently, additional validation tests in lysimeters and field plots have been performed (Fent *et al*, 1998).

The PELMO version that was used for the implementation of the FOCUS-scenarios was developed in 1999 (PELMO 3.2). It was necessary to change the format of the scenario data files and the handling of leap years slightly because of the needs of the FOCUS-scenarios. Minor changes were also made in the routine that is estimating soil temperatures based on air temperatures to make sure that the results are correct also for soil depths below 1.0 m. Finally, the runoff routine in PELMO was calibrated based on field experiments by introducing a new parameter in the model ("fraction of soil water available for runoff").

Table 3.1 Summary of the processes in PELMO

Process	Approach
water movement	capacity-based water flow (tipping bucket approach) using a daily time step for all hydrological processes
substance movement	convection dispersion equation based on a daily time step
crop simulation	changing root zone during growing season, changing foliage (areal extent) during growing season, crop interception of water*, crop interception of substances*, foliar washoff*, foliar degradation*
degradation in soil	first order degradation rate, correction of rate constant with depth, soil moisture and soil temperatures
substance sorption to soil	Kd, Koc, Freundlich equation for sorption option for increase of sorption with time option for automated pH-dependence*
substance volatilisation (from soil)	simple model using Fick's and Henry's law
runoff	Soil Conservation Service curve number technique
drainage & preferential flow	not simulated
soil erosion*	Modified Universal Soil Loss Equation
soil temperature	An empirical model that uses air temperatures
plant uptake	simple model based on soil concentrations
substance applications	applications may be foliar sprays, applied to the soil surface, or incorporated into the soil; for soil incorporated applications a variety of soil distributions can be specified
metabolism	a sophisticated scheme with up to 8 metabolites (A -> B as well as A -> B -> C) may be simulated simultaneously with the parent

* = turned off for the FOCUS scenarios

References

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3.3 Summary of the PEARL parameterisation

PEARL (Pesticide Emission Assessment at Regional and Local scales) is a consensus model developed by two Dutch institutes (RIVM and Alterra Green World Research) in close co-operation (Leistra at al, 2000). It is based on PESTLA (PESTicide Leaching and Accumulation; version 1: Boesten & Van der Linden, 1991; version 3.4:Van den Berg and Boesten, 1999) and PESTRAS (PEsticide TRansport Assessment. Tiktak *et al*., 1994; Freijer *et al*., 1996), the latter being a modification of PESTLA version 1. PEARL is based on (i) the convection/dispersion equation including diffusion in the gas phase with a temperature dependent Henry coefficient, (ii) a two-site Freundlich sorption model (one equilibrium site and one kinetic site), (iii) a transformation rate that depends on water content, temperature and depth in soil, (iv) a passive plant uptake rate. The model includes formation and behaviour of transformation products and describes also lateral pesticide discharge to drains (but drainage is switched off for the FOCUS scenarios). PEARL does not simulate preferential flow. Volatilisation from the soil surface is calculated assuming a laminar air layer at the soil surface. PEARL uses an explicit finite difference scheme that excludes numerical dispersion (the dispersion length was set to 5 cm).

For the FOCUS scenarios, the default option is to ignore long-term sorption kinetics (i.e. zero sorption coefficient for the kinetic sorption site in PEARL). However, if long-term sorption data are available for a compound, these can be used to estimate the kinetic sorption parameters in PEARL (sorption coefficient and desorption rate constant).

PEARL does not simulate water flow and soil temperatures itself but uses the Soil Water Atmosphere Plant (SWAP) model version 2.0 for that purpose. In SWAP, flow of water is described with Richard's equation using a finite implicit difference scheme (Van Dam *et al*., 1997). SWAP can handle a wide variety of hydrological boundary conditions. Soil evaporation and plant transpiration can be calculated via multiplying a reference evapotranspiration rate with soil and crop factors. SWAP can simulate groundwater levels that fluctuate in response to the rainfall input. The groundwater level can also be introduced as a time table (option used for the Piacenza scenario). Figure 3.1 shows examples of yearly fluctuations in groundwater levels as calculated with SWAP for all relevant locations (excluding Châteaudun, Okehampton and Thiva because their groundwater levels are deeper than 5 m). For the FOCUS scenarios, crop growth is simulated with SWAP using a simple growth model that assumes a fixed length of the growing season. In this growth model, both the leaf area index and the rooting depth are a function of the development stage of the crop.

SWAP describes flow of heat with Fourier's Law with a finite implicit difference scheme. The thermal properties are a function of porosity and water content and are therefore a function of time and soil depth.

References

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Tiktak, A., A.M.A. van der Linden and F.A. Swartjes. 1994. PESTRAS: A one dimensional model for assessing leaching and accumulation of pesticides in soil. RIVM report 715501003, Bilthoven, the Netherlands.

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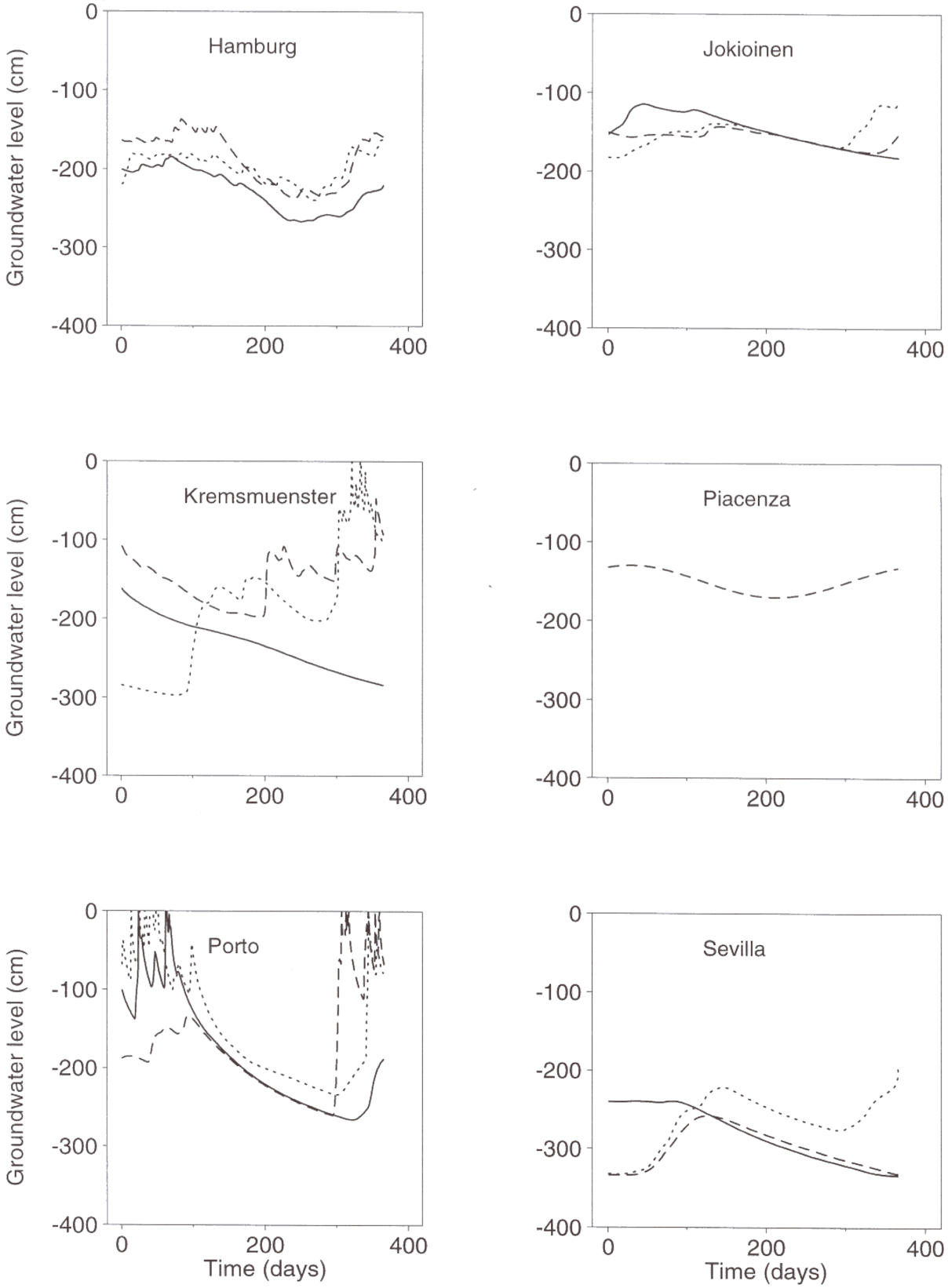
Van Dam, J.C., J. Huygen, J.G. Wesseling, R.A. Feddes, P. Kabat, P.E.V. van Walsum, P. Groenendijk and C.A. Van Diepen, 1997. Theory of SWAP version 2.0. Simulation of water flow, solute transport and plant growth in the Soil-Water-Atmosphere-Plant environment. Technical Document 45, DLO Winand Staring Centre, Wageningen, The Netherlands.

Figure 3.1 Examples of yearly fluctuations in groundwater level for FOCUS scenarios simulated with SWAP for PEARL. Heavily dashed lines are for average years, solid lines for dry years and lightly dashed lines for wet years. All simulations are for potatoes assuming no irrigation.



3.4 Summary of the PRZM parameterisation

PRZM is a one dimensional finite-difference model for prediction of the vertical movement of chemicals in soil by chromatographic leaching. The first official version (Carsel *et al*., 1984) was released in 1984 although beta versions were available from 1982. An upgraded version PRZM2 was issued as part of the RUSTIC package (Dean *et al*., 1989a & 1989b) and later as a stand-alone model. In the mid-1990's the runoff routines were upgraded as part of the work of the FIFRA Exposure Modeling Work Group and the FIFRA Environmental Model Validation Task Force to produce version 3.12. This version also included more flexibility with application techniques, the ability to make degradation a function of soil temperature, and output which is more user friendly. Version 3.12 is also the version that has been used by the FIFRA Environmental Model Validation Task Force in its program to compare model predictions with actual data from runoff and leaching field studies. For use in the FOCUS scenarios, version 3.2 was used, which in addition to the capabilities of version 3.12 has the option of using the Freundlich isotherm, the ability to make the degradation rate a function of soil moisture, the capability to consider increasing sorption with time and implementation of exact first order kinetics for metabolites. In version 3.2 major parts of the program code have been re-coded to achieve a truly Windows based 32bit PRZM3 code which is independent from any DOS limitations.

Table 3.2 Summary of the processes in PRZM 3.2 (FOCUS release)

Process	**Approach**
water movement	capacity-based water flow (tipping bucket approach) using a daily time step for all hydrological processes, option for Richard's equation below the root zone. *Preferential flow, capillary rise and drainage not considered
substance movement	convection dispersion equation based on a daily time step solved by an simplifying backward difference method which can produce artificially high numerical dispersion
crop simulation	changing root zone during growing season, changing foliage (both height and areal extent) during growing season, crop interception of water*, crop interception of substances*, foliar washoff*, foliar degradation*
degradation in soil	first order degradation rate with option for bi-phasic degradation, option for effects of soil temperature and moisture on degradation
substance sorption to soil	Kd, Koc, or normalised Freundlich equation for sorption; option for increasing sorption with time
substance volatilisation (from soil)	approach is a combination of results from previous research
runoff	Soil Conservation Service curve number technique
soil erosion*	Universal Soil Loss Equation
soil temperature	Approach is based on previous work by a number of researchers including Van Bavel and Hillel, Thibodeaux, Hanks, Gupta, and Wagenet and Hutson
plant uptake	simple model based on soil concentrations
substance applications	applications may be foliar sprays*, applied to the soil surface, or incorporated into the soil; for soil incorporated applications a variety of soil distributions can be specified
metabolism	up to two metabolites may be simulated simultaneously with the parent

*process not used in FOCUS scenarios

Development of Parameter Sets

The development of input parameter sets from the weather, soil, and crop information was generally straightforward. Details are provided in the appendix providing values of all of the input parameters. Dispersion was determined by the choice of the compartment sizes, which were 0.1 cm down to a depth of 10 cm and 5 cm below 10 cm. Crop specific runoff curve numbers were determined from the information in the PRZM 3.12 manual assuming a SCS hydraulic soil group of B for Hamburg and C for the rest of the locations.

References

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4. TEST RUNS USING THE FOCUS SCENARIO FILES

4.1 Definition of the 'Dummy' Substance Parameters

For four so called 'Dummy' Substances the complete parameter sets were established that are necessary for prediction of leaching to groundwater by the different models for all FOCUS scenarios.
The parameter sets are used to

- demonstrate the parameterisation process of the models
- perform test runs to check the models
- enable the inter-comparison of the scenarios (relative vulnerability)
- check the effect of different parameter combinations within the same scenario (intra-scenario check)

The dummy substances were established to demonstrate different sensitivity with respect to leaching of major agricultural regions in Europe. The individual substance parameter values chosen are in the range of values that can be found for registered plant protection products in Europe but are not intended to be attributable to individual compounds.

- Dummy substance A can be classified as a medium persistent low sorbing compound with a Kom of 60 dm^3/kg (Koc = 103) and a soil DT50 of 60 d which is non-volatile.

- Dummy substance B can be classified as a low persistent compound with a very low Kom of 10 dm^3/kg (Koc = 17) and a soil DT50 of 20 d which is somewhat volatile.

- Dummy substance C can be classified as low persistent compound with medium adsorption (Kom = 100 dm^3/kg, DT50 = 20 d) having a persistent and mobile transformation product with Kom = 30 dm^3/kg (Koc = 52) and DT50 = 100 d.

- Dummy substance D can be classified as a low persistent compound with a low Kom of 35 dm^3/kg (Koc = 60) and a soil DT50 of 20 d which is somewhat volatile. It is **exactly** the same as Dummy Substance B, except for this stronger soil adsorption.

The parameter values for the dummy substances are provided in Tables 4.1 - 4.3

Table 4.1 Substance A with Kom = 60 dm^3/kg, DT50 = 60 d, non-volatile

No.	Parameters	Unit	Value	Remarks
	Physico chemical parameters			
1	molecular weight	[g/mol]	300	
2	solubility in water	[mg/l]	90	
3	vapour pressure	[mPa]	$1 * 10^{-7}$	
4	pKa-value (if acid or base)	[-]	N/A	N/A = not applicable
5	reference pH-value at which Koc-value was determined	[-]	N/A	N/A = not applicable
6	dimensionless Henry-coefficient (can be calculated from solubility and vapour pressure)		N/A	N/A = not applicable
7	diffusion coefficient in Water	[m^2/d]	$4.3 * 10^{-5}$	
8	gas diffusion coefficient	[m^2/d]	0.43	
	Degradation parameters of the substance			
9	degradation rate or half life in bulk top soil at reference conditions	[1/d] or [d]	k = 0.012 HL = 60	
10	”reference temperature"	[°C]	20	
11	”reference soil moisture"	[-]	at 10kPa at field capacity;	
12	factors for the adjustment of degradation rate in different depths	[-]	standard	defined by scenarios

Table 4.1 continued

	Parameter, relating degradation rate to soil temperature	**Unit**	**Value**	**Remarks**
13	Q10-factor (increase of degradation rate with an increase of temperature of 10°C)	[-]	2.2	
14	g (=gamma) (factor for relating degradation rate and soil temperature according to Boesten & van der Linden, 1991)	[1/K]	0.079	
15	ARRHENIUS activation energy	[kJ/Mol]	54	
	Parameter, relating degradation rate to soil moisture			
16	B-value (exponent of degradation - moisture relationship according to WALKER)	[-]	0.7	
	Sorption Parameters			
17	Koc-/Kom-value or Kf-values in different depth	[dm^3/kg]	Koc = 103 Kom = 60	
18	exponent of the FREUNDLICH-Isotherm	[-]	0.9	
19	increase of the sorption coefficient with time or parameters describing non-equilibrium sorption	[-]	N/A	N/A = not applicable
	Metabolism			
20	metabolism scheme (if necessary) with transformation fractions (parent -> metabolites)	[-]	N/A	N/A = not applicable
	Crop related substance parameters			
21	TSCF = transpiration stream concentration factor	[-]	0.5	
	Management related substance parameters			
22	number of applications	[-]	1	in each year
23	dosages	[kg/ha]	1	in each year
24	dates of application	[-]	scenario specific	1 day before emergence
25	incorporation depth	[cm]	0	
26	factor (accounting for interception by crops)	[-]	0	no interception

Table 4.2 Substance B and D with DT50 = 20 d, somewhat volatile : Kom = 10 dm^3/kg for Substance B and 35 for Substance D, with all other properties equal.

No.	Parameters	Unit	Value	Remarks
	Physico chemical parameters			
1	molecular weight	[g/mol]	300	
2	solubility in water	[mg/l]	90	
3	vapour pressure	[mPa]	0.1	
4	pKa-value (if acid or base)	[-]	N/A	N/A = not applicable
5	reference pH-value at which Koc-value was determined	[-]	N/A	N/A = not applicable
6	dimensionless Henry-coefficient (can be calculated from solubility and vapour pressure)		N/A	N/A = not applicable
7	diffusion coefficient in Water	[m^2/d]	$4.3 * 10^{-5}$	
8	gas diffusion coefficient	[m^2/d]	0.43	
	Degradation parameters of the substance			
9	degradation rate or half life in bulk top soil at reference conditions	[1/d] or [d]	k = 0.0347 or HL = 20	
10	”reference temperature"	[°C]	20	
11	”reference soil moisture"	[-]	at 10kPa at field capacity;	
12	factors for the adjustment of degradation rate in different depths	[-]	standard	defined by scenarios

Table 4.2 continued

	Parameter, relating degradation rate to soil temperature	Unit	Value	Remarks
13	Q10-factor (increase of degradation rate with an increase of temperature of 10°C)	[-]	2.2	
14	g (=gamma) (factor for relating degradation rate and soil temperature according to Boesten & van der Linden, 1991)	[1/K]	0.079	
15	ARRHENIUS activation energy	[kJ/Mol]	54	
	Parameter, relating degradation rate to soil moisture			
16	B-value (exponent of degradation - moisture relationship according to WALKER)	[-]	0.7	
	Sorption Parameters			
17	Koc-/Kom-value or Kf-values in different depth	[dm^3/kg]	Koc = 17 & Kom = 10 for Substance B; Koc = 60 & Kom = 35 for Substance D	
18	exponent of the FREUNDLICH-Isotherm	[-]	0.9	
19	increase of the sorption coefficient with time or parameters describing non-equilibrium sorption	[-]	N/A	N/A = not applicable
	Metabolism			
20	metabolism scheme (if necessary) with transformation fractions (parent -> metabolites)	[-]	N/A	N/A = not applicable
	Crop related substance parameters			
21	TSCF = transpiration stream concentration factor	[-]	0.5	
	Management related substance parameters			
22	number of applications	[-]	1	application each year
23	dosages	[kg/ha]	1	application each year
24	dates of application	[-]	scenario specific	1 day before emergence
25	incorporation depth	[cm]	0	
26	factor (accounting for interception by crops)	[-]	0	no interception

Table 4.3 Substance C with Kom = 100 dm^3/kg, DT50 = 20 d, having a mobile transformation product with Kom = 30 L/kg, DT50 = 100 d

No.	Parameters	Unit	Value	Remarks
	Physico chemical parameters Parent			
1	molecular weight	[g/mol]	200	
2	solubility in water	[mg/l]	50	
3	vapour pressure	[mPa]	$1 * 10^{-7}$	
4	pKa-value (if acid or base)	[-]	N/A	N/A = not applicable
5	reference pH-value at which Koc-value was determined	[-]	N/A	N/A = not applicable
6	dimensionless Henry-coefficient (can be calculated from solubility and vapour pressure)		N/A	N/A = not applicable
7	diffusion coefficient in Water	[m^2/d]	$4.3 * 10^{-5}$	
8	gas diffusion coefficient	[m^2/d]	0.43	
	Physico chemical parameters Metabolite			
1.1	molecular weight	[g/mol]	150	
2.1	solubility in water	[mg/l]	90	
3.1	vapour pressure	[mPa]	$1*10^{-7}$	
4.1	pKa-value (if acid or base)	[-]	N/A	N/A = not applicable
5.1	reference pH-value at which Koc-value was determined	[-]	N/A	N/A = not applicable
6.1	dimensionless Henry-coefficient (can be calculated from solubility and vapour pressure)		N/A	N/A = not applicable
7.1	diffusion coefficient in Water	[m^2/d]	$4.3 * 10^{-5}$	
8.1	gas diffusion coefficient	[m^2/d]	0.43	

Table 4.3 continued

	Degradation parameters of the substance	**Unit**	**Value**	**Remarks**
9	degradation rate or half life in bulk top soil at reference conditions	[1/d] or [d]	k = 0.0347 or HL = 20	
10	”reference temperature"	[°C]	20	
11	”reference soil moisture"	[-]	at 10kPa at field capacity;	
12	factors for the adjustment of degradation rate in different depths	[-]	standard	defined by scenarios
	Degradation parameters of the metabolite			
9.1	degradation rate or half life in bulk top soil at reference conditions	[1/d] or [d]	k = 0.00693 or HL = 100	
10.1	”reference temperature"	[°C]	20	
11.1	”reference soil moisture"	[-]	at 10kPa at field capacity;	
12.1	factors for the adjustment of degradation rate in different depths	[-]	standard	defined by scenarios

Table 4.3 continued

	Parameter, relating degradation rate to soil temperature (same for Parent and Metabolite)	**Unit**	**Value**	**Remarks**
13	Q10-factor (increase of degradation rate with an increase of temperature of 10°C)	[-]	2.2	
14	g (=gamma) (factor for relating degradation rate and soil temperature according to Boesten & van der Linden, 1991)	[1/K]	0.079	
15	ARRHENIUS activation energy	[kJ/Mol]	54	
	Parameter, relating degradation rate to soil moisture (same for Parent and Metabolite)			
16	B-value (exponent of degradation - moisture relationship according to WALKER)	[-]	0.7	
	Sorption Parameters (Parent)			
17	Koc-/Kom-value	[dm^3/kg]	Koc = 172 Kom= 100	
18	exponent of the FREUNDLICH-Isotherm	[-]	0.9	
19	increase of the sorption coefficient with time or parameters describing non-equilibrium sorption	[-]	N/A	N/A = not applicable
	Sorption Parameters (Metabolite)			
17.1	Koc-/Kom-value or Kf-values in different depth	[dm^3/kg]	Koc = 52 Kom= 30	
18.1	exponent of the FREUNDLICH-Isotherm	[-]	0.9	
19.1	increase of the sorption coefficient with time or parameters describing non-equilibrium sorption	[-]	N/A	N/A = not applicable

Table 4.3 continued

	Metabolism	**Unit**	**Value**	**Remarks**
20	metabolism scheme (if necessary) with transformation fractions (parent -> metabolites)	[-]	P -> M -> Elimination + P-> Elimination	transformation fraction: P -> M = 0.71 relation molecular weight: M/P = 0.75 conversion factor = 0.75 * 0.71 = 0.53 [1]
	Crop related substance parameters (same for parent and metabolite)			
21	TSCF = transpiration stream concentration factor	[-]	0.5	
	Management related substance parameters			
22	number of applications	[-]	1	in each year
23	dosages (parent)	[kg/ha]	1	in each year
24	dates of application	[-]	scenario specific	1 day before emergence
25	incorporation depth	[cm]	0	
26	factor (accounting for interception by crops)	[-]	0	no interception

[1] P = Parent; M = Metabolite; transformation fraction is the portion of the parent that converts to the metabolite; the molecular weight of the metabolite in relation to the molecular weight of the parent is needed if the simulation model does not explicitly have the molecular weight as an input parameter; in this case transformation factor and the molecular weight relation are combined to provide the conversion factor which is an input parameter

4.2 Results of standard test runs

4.2.1 Introduction

The creation of nine scenarios intended to be representative of the range of climatic conditions in Europe and the implementation of these into input files for three (four) different models has involved a great deal of work. To provide confidence in the output obtained from these scenarios, especially if they are to be used for regulatory purposes, it was considered very important that some comparison of the output from the scenarios should be undertaken. The FOCUS group believe that there were three main reasons for this comparison work:
1. To provide an additional error check for the input files
2. To compare the variation in the results from the three (four) different models
3. To compare the variation in the results from the nine scenarios

Using the dummy substance parameters described in Chapter 4.1 a series of runs were undertaken simulating application to winter wheat on the day before emergence. In addition, further specific runs were undertaken for

- Substances A and C at Châteaudun to investigate the effect of biennial and triennial applications,
- Substance A on maize on the day before emergence at Châteaudun, Piacenza, Sevilla and Thiva to investigate the effect of irrigation and
- Substance A at Châteaudun, Piacenza, Sevilla and Thiva with PRZM only to investigate the effect of run-off.

The water and substance mass balances for all simulated years were initially investigated. Once these were regarded as satisfactory, subsequent comparison was directed at the intended regulatory endpoint, namely the 80th percentile annual average concentration at 1m depth (representative of an overall 90th percentile vulnerability).

4.2.2 Results

Error checks
During the course of the exercise a number of errors were identified from consideration of the comparative results from the water and substance mass balances. These originated both from input error and from bugs introduced into the model code and model shell during the development process. All known errors have now been corrected.

Variation in model output
Certain processes are treated differently in different models and therefore certain differences found in the water mass balances were unsurprising. Run-off is only simulated to occur in PEARL when the infiltration capacity of the soil profile is exceeded. For the FOCUS scenarios, run-off of water was very much lower in PEARL (when winter wheat is simulated it only occurs at Kremsmünster, Porto and Sevilla). Additionally, when there is low water stress and the evapotranspiration predicted is similar for all models (the majority of scenarios), the predicted recharge is also higher in PEARL

since the water balance is re-adjusted (i.e. that which is run-off in PRZM and PELMO is percolate in PEARL). Figures 4.1, 4.2 and 4.3 illustrate this point by showing the predicted run-off, evapotranspiration and percolate for winter cereals at Okehampton. It is evident that the difference in run-off volume is principally reflected in the difference in percolation volume, whilst the predicted evapotranspiration is very similar for all models.

In contrast, when there is a high water stress (primarily Sevilla and Thiva) the increased evapotranspiration predicted by PEARL in winter cereals is greater than or equal to the run-off predicted by PELMO and PRZM. Hence the overall percolation predicted from PEARL is equal to or less than that from PRZM and PELMO. This is illustrated for Sevilla in Figures 4.4, 4.5 and 4.6.

Figure 4.1 Simulated water run-off from winter cereals at Okehampton over 20 years

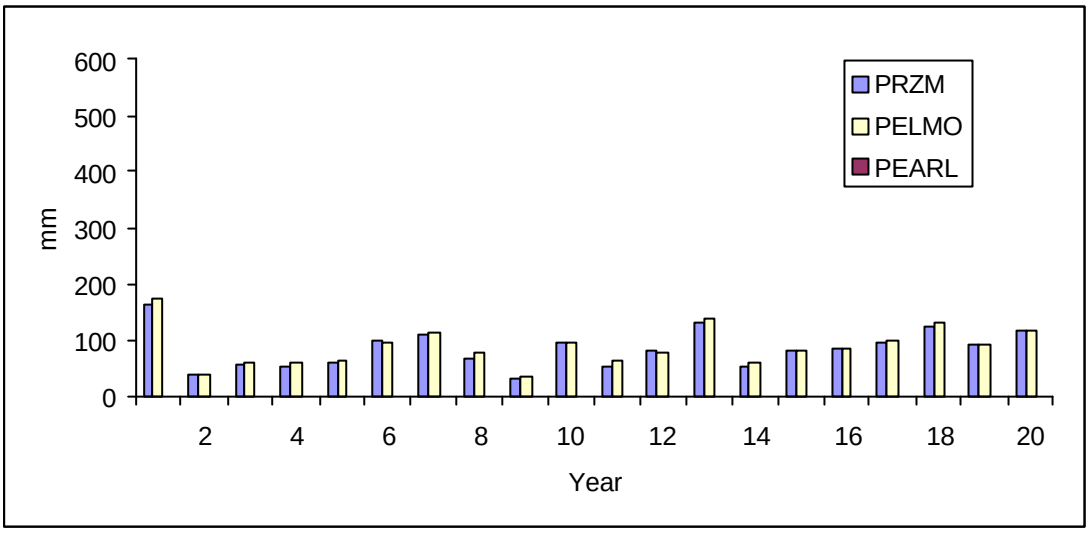


Figure 4.2 Simulated evapotranspiration from winter cereals at Okehampton over 20 years

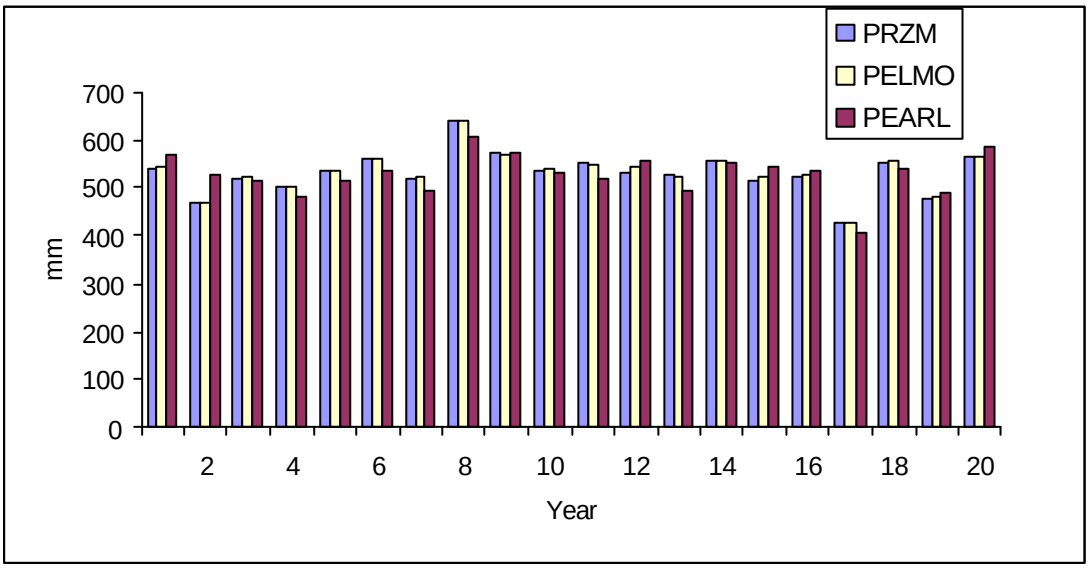


Figure 4.3 Simulated percolation from winter cereals at Okehampton over 20 years

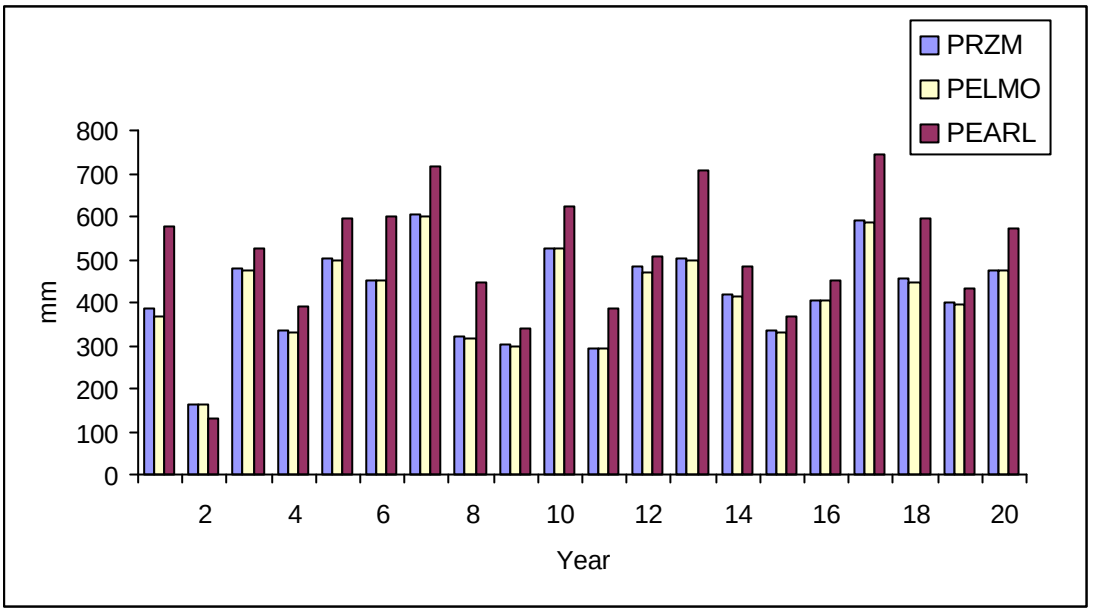


Figure 4.4 Simulated water run-off from winter cereals at Sevilla over 20 years

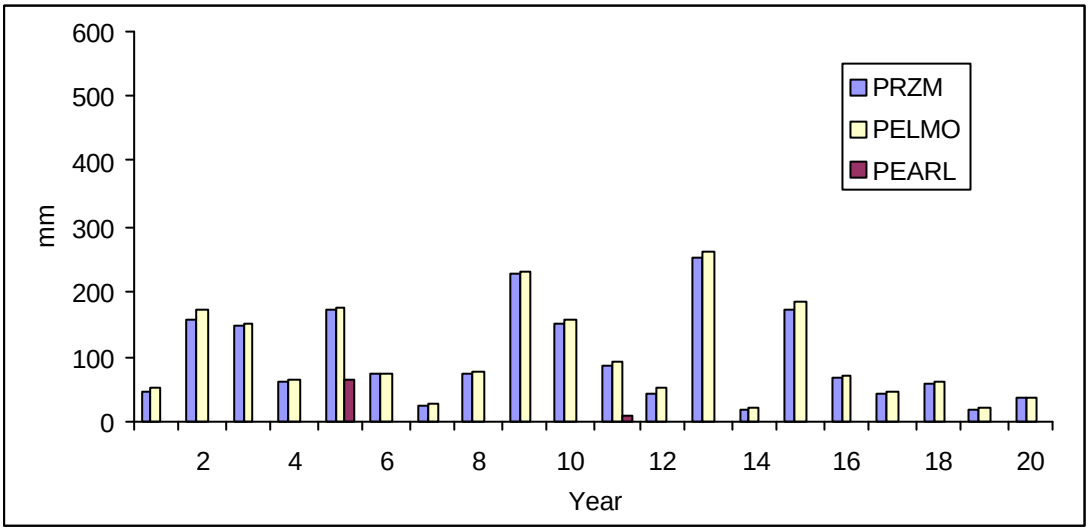


Figure 4.5 Simulated evapotranspiration from winter cereals at Sevilla over 20 years

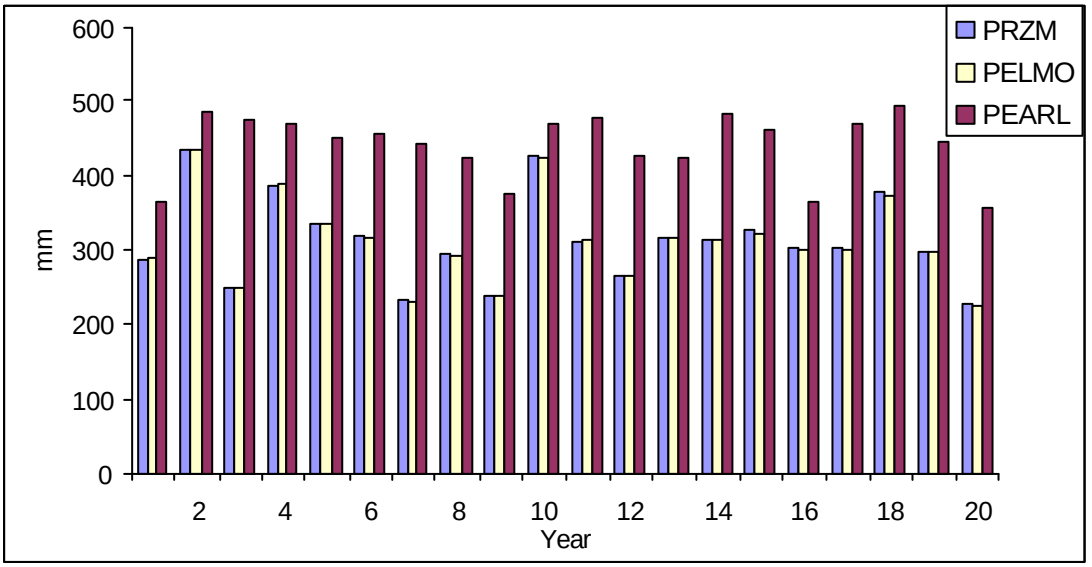
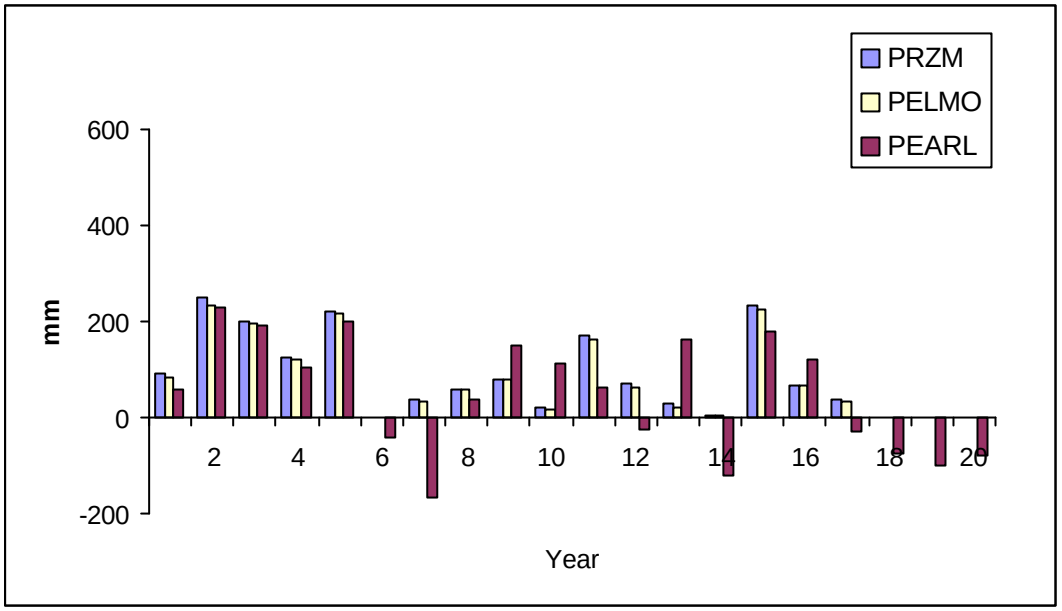


Figure 4.6 Simulated percolation from winter cereals at Sevilla over 20 years

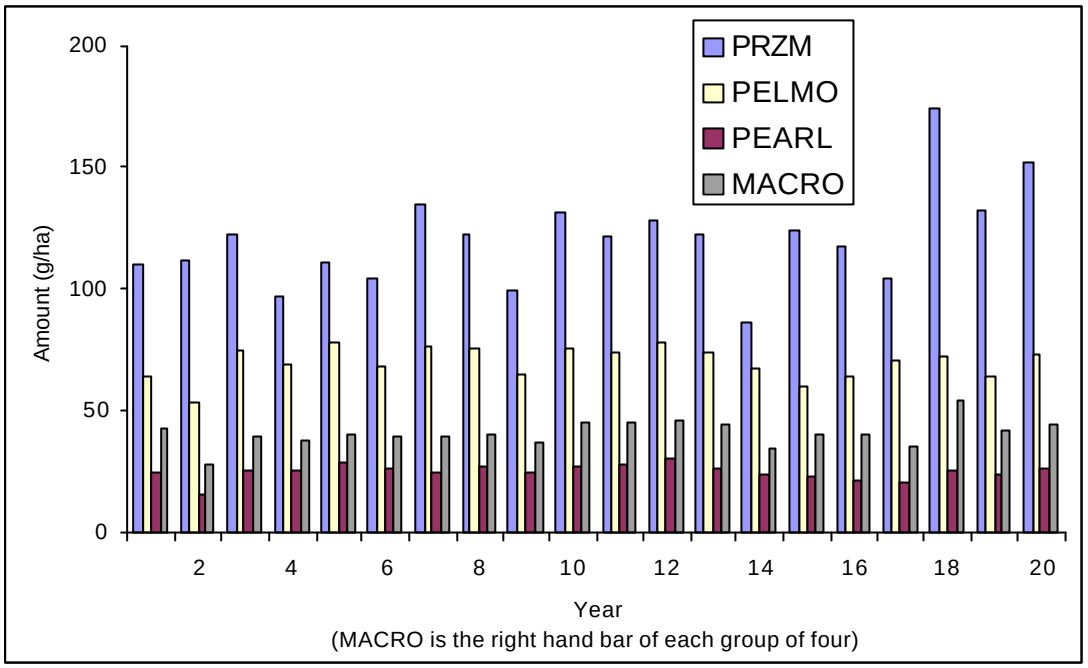


The differences between the substance mass balances are generally insignificant since the latest versions of the chromatographic flow models (PEARL 1.1, PRZM 3.2 and PELMO 3.2) now have many similar routines.

The most significant difference between models was in the amount of crop uptake (see Figure 4.7). The models consistently showed uptake in the order PRZM>PELMO>MACRO>PEARL as illustrated for Substance A in winter cereals at Châteaudun. However, the overall proportion of the application rate (1000 g/Ha) that these variations represent is relatively small. The reason that PRZM simulates the highest uptake can be explained by the fact that removal of water is simulated as a triangular profile within the root zone. Therefore the greatest amount of water is being removed from the zones with the highest substance concentration implying that this will lead to the greatest plant uptake of substance.

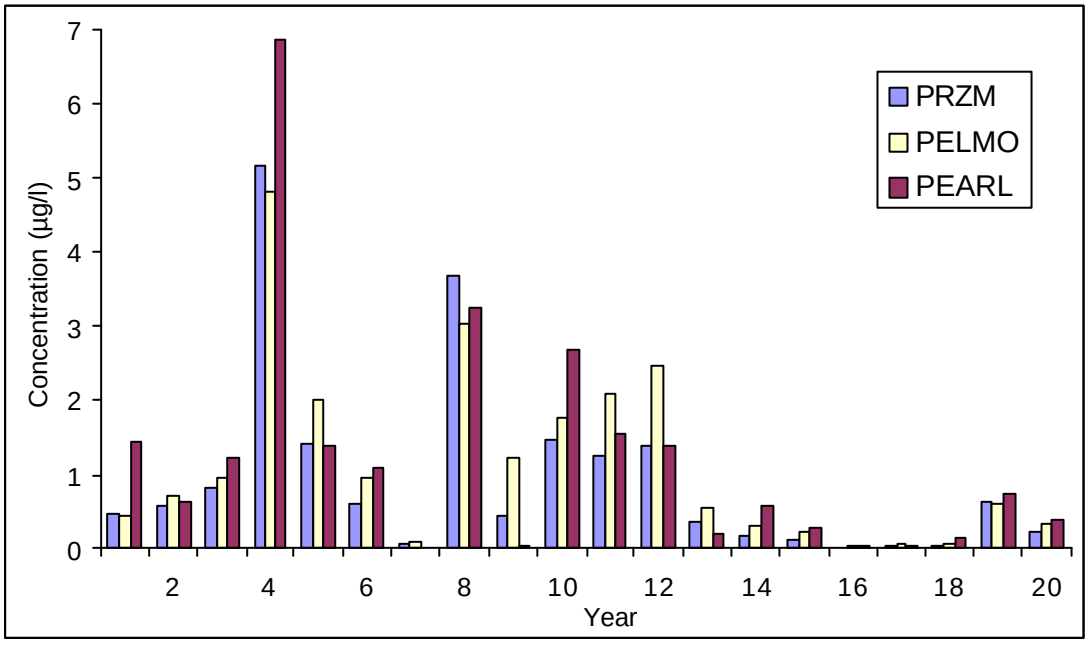
In addition, at Jokioinen only, PRZM simulates lower storage of substance than PELMO and PEARL and this may be related to slight differences in the routines for degradation at low temperatures.

Figure 4.7 Crop uptake of Substance A in winter cereals at Châteaudun over 26 years



Despite these significant variations some of the individual processes in the chromatographic flow models, the annual average concentrations at 1 m depth (the intended output) showed considerably less differences. Figure 4.8 shows an example of this from Substance D at Piacenza

Figure 4.8 The predicted annual concentrations of Substance D at 1 m depth following application to winter cereals at Piacenza over 26 years



Following examination of all parts of the mass balances, the intended regulatory output (i.e. the 80th percentile year) was examined and the results are shown in Table 4.4. On some occasions, models identified the exact same year as being the 80th percentile, namely; 38% for PRZM and PELMO, 16% for PELMO and PEARL, 13% for PRZM and PEARL.

The 80th percentile concentrations predicted showed a high degree of similarity, particularly at higher concentrations. On the 25 occasions when concentrations >1µg/l were predicted in all three of the chromatographic flow models the difference between these three models was always less than a factor of four, and in 23 of the cases was less than a factor of two. On the 13 occasions where values were 0.001-1 µg/l, the variation between the chromatographic flow models was a little higher and was approximately within an order of magnitude. In these cases (which were largely from substances A and B) PEARL gave the highest results. Any predicted concentrations <0.001 µg/l were considered to be zero and on 7 occasions all three models predicted 0 µg/l.

For the five substances simulated at Châteaudun the effect of macropore flow (as judged using the MACRO model) was to increase the predicted 80th percentile concentration by an average factor of 3 compared to the chromatographic flow model giving the highest output (PEARL). This difference appeared to be smaller when high concentrations were predicted by chromatographic models and higher when lower concentrations were predicted.

Table 4.4 80th percentile years and 80th percentile substance concentrations at 1 m depth for four substances on winter cereals

			Year				Substance Conc. (µg/L)			
			PRZM	PELMO	PEARL	MACRO	PRZM	PELMO	PEARL	MACRO
Pest A	Châteaudun	C	6	8	9	6	1.2	1.3	2.3	4.3
Pest A	Hamburg	H	20	20	1		7.5	6.0	7.5	
Pest A	Jokioinen	J	13	8	8		0.44	1.4	2.0	
Pest A	Kremsmünster	K	7	7	9		2.5	3.1	4.5	
Pest A	Okehampton	N	1	18	18		8.9	6.2	9.1	
Pest A	Piacenza	P	4	12	8		9.1	11	11	
Pest A	Porto	O	9	9	7		0.017	0.034	0.15	
Pest A	Sevilla	S	7	7	11		0.000	0.001	0.006	
Pest A	Thiva	T	12	11	3		0.11	0.50	2.3	

			Year				Substance Conc. (µg/L)			
			PRZM	PELMO	PEARL	MACRO	PRZM	PELMO	PEARL	MACRO
Pest B	Châteaudun	C	7	7	3	7	5.0	4.8	8.4	14
Pest B	Hamburg	H	14	14	6		41	32	32	
Pest B	Jokioinen	J	4	9	8		14	20	23	
Pest B	Kremsmünster	K	5	5	8		9.8	12	14	
Pest B	Okehampton	N	9	6	4		31	30	29	
Pest B	Piacenza	P	10	8	8		34	32	23	
Pest B	Porto	O	4	4	4		5.2	6.7	6.3	
Pest B	Sevilla	S	4	4	2		1.1	1.9	3.5	
Pest B	Thiva	T	2	7	1		2.7	3.9	5.3	

			Year				Substance Conc. (µg/L)			
			PRZM	PELMO	PEARL	MACRO	PRZM	PELMO	PEARL	MACRO
Pest C	Châteaudun	C	6	8	6	6	0.000	0.000	0.000	0.006
Pest C	Hamburg	H	1	7	1		0.000	0.000	0.000	
Pest C	Jokioinen	J	5	8	10		0.000	0.000	0.000	
Pest C	Kremsmünster	K	8	8	8		0.000	0.000	0.000	
Pest C	Okehampton	N	20	8	19		0.000	0.000	0.001	
Pest C	Piacenza	P	11	12	8		0.000	0.002	0.013	
Pest C	Porto	O	8	8	8		0.000	0.000	0.000	
Pest C	Sevilla	S	16	16	20		0.000	0.000	0.000	
Pest C	Thiva	T	14	6	12		0.000	0.000	0.000	

			Year				Substance Conc. (µg/L)			
			PRZM	PELMO	PEARL	MACRO	PRZM	PELMO	PEARL	MACRO
Met C	Châteaudun	C	9	9	11	8	18	18	24	22
Met C	Hamburg	H	20	6	5		32	30	31	
Met C	Jokioinen	J	6	20	6		19	22	24	
Met C	Kremsmünster	K	14	12	4		20	22	24	
Met C	Okehampton	N	14	14	17		33	29	30	
Met C	Piacenza	P	8	4	18		23	29	27	
Met C	Porto	O	7	12	14		3.8	4.4	5.2	
Met C	Sevilla	S	7	7	11		0.57	1.1	5.2	
Met C	Thiva	T	6	13	3		7.7	14	21	

			Year				Substance Conc. (µg/L)			
			PRZM	PELMO	PEARL	MACRO	PRZM	PELMO	PEARL	MACRO
Pest D	Châteaudun	C	9	9	5	14	0.016	0.014	0.14	0.97
Pest D	Hamburg	H	10	7	10		1.2	1.1	1.1	
Pest D	Jokioinen	J	11	8	5		0.005	0.076	0.19	
Pest D	Kremsmünster	K	7	13	3		0.066	0.15	0.51	
Pest D	Okehampton	N	1	6	6		1.7	1.1	1.9	
Pest D	Piacenza	P	5	11	11		1.4	2.1	1.6	
Pest D	Porto	O	7	7	13		0.001	0.001	0.008	
Pest D	Sevilla	S	16	16	5		0.000	0.000	0.010	
Pest D	Thiva	T	8	8	6		0.004	0.017	0.14	

These results can also be considered in terms of the variation between the selected scenarios, irrespective of the model used. Figures 4.9, 4.10, 4.11, 4.12 and 4.13 present the information from Table 4.4 as a comparison of the results from each substance, for all scenarios.

Figure 4.9 80th percentile concentrations for Substance A applied to winter cereals

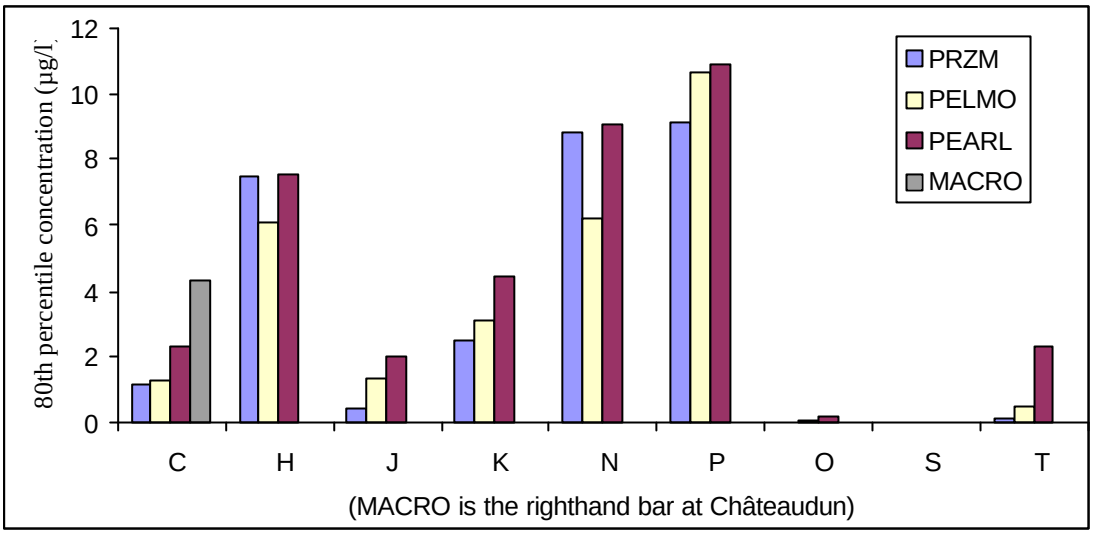


Figure 4.10 80th percentile concentrations for Substance B applied to winter cereals

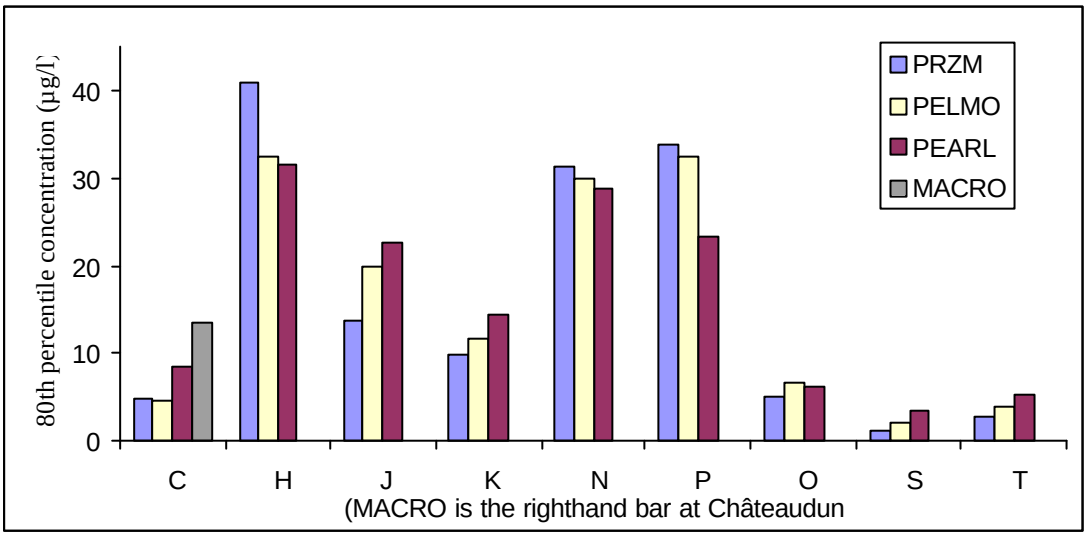


Figure 4.11 80th percentile concentrations for Substance C applied to winter cereals

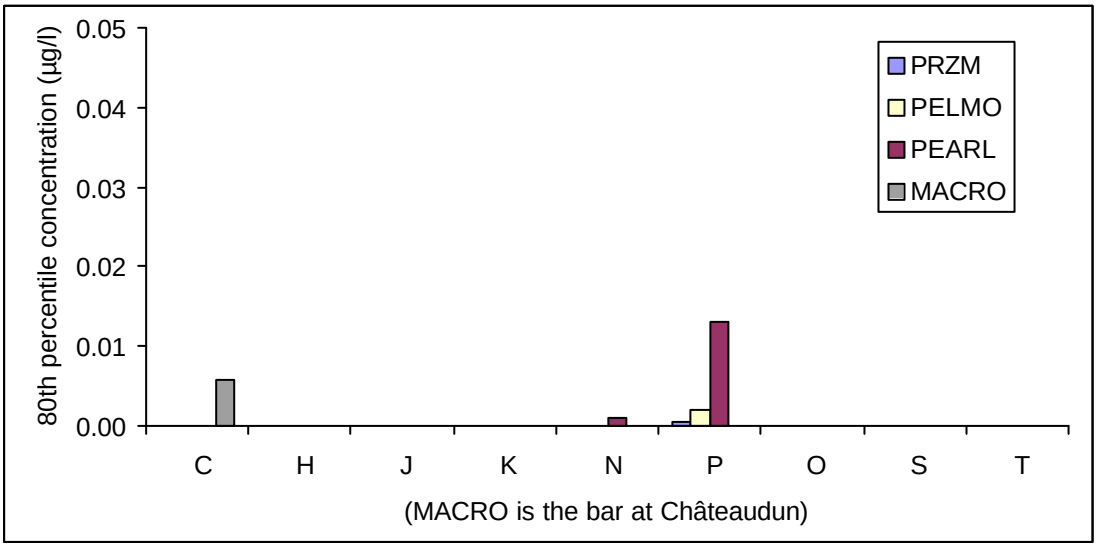


Figure 4.12 80th percentile concentrations for Metabolite C applied to winter cereals

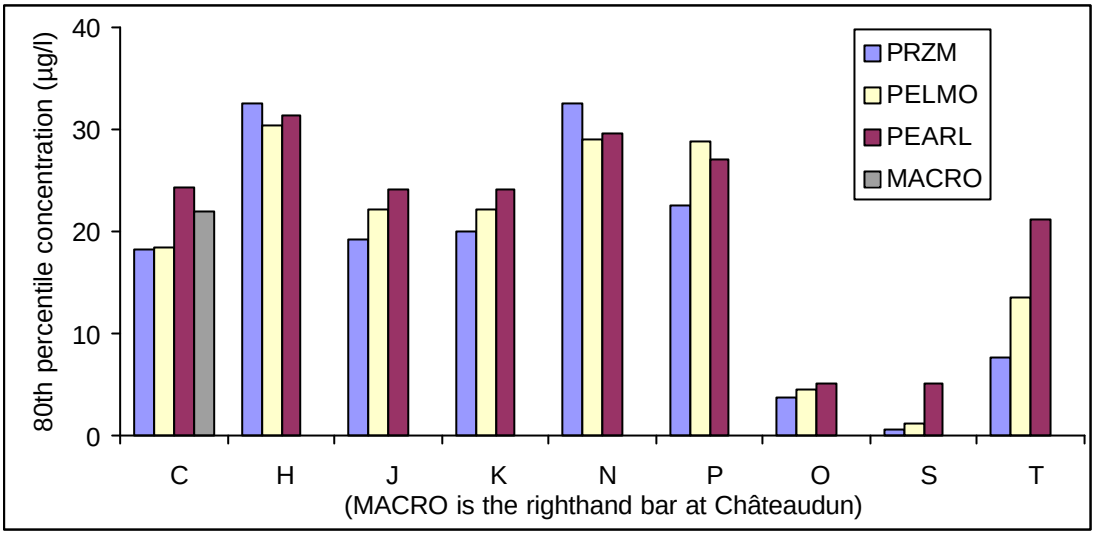
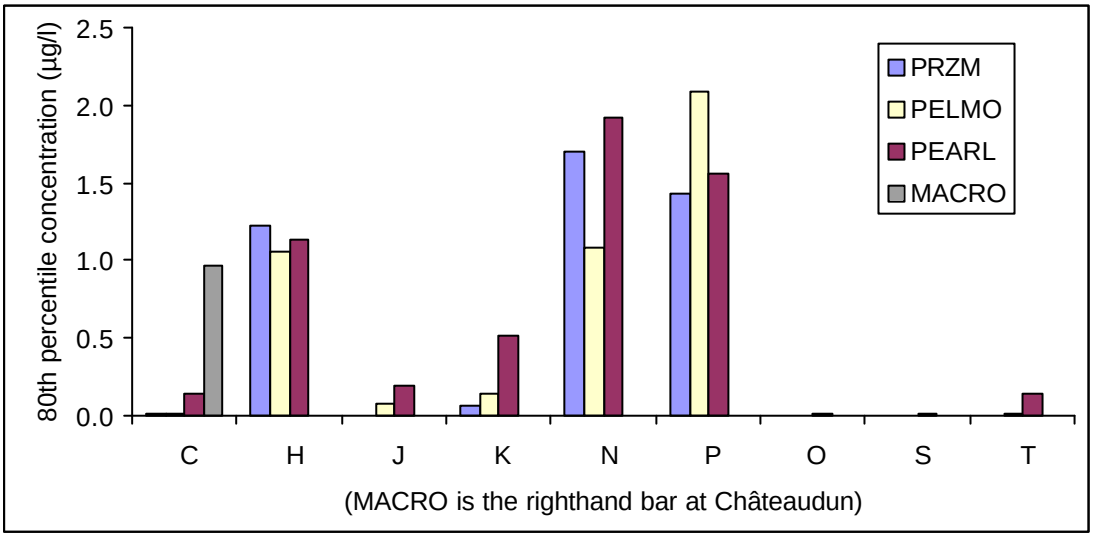


Figure 4.13 80th percentile concentrations for Substance D applied to winter cereals



Based on the results shown in Figures 4.9-4.13 there appears to be a trend that Hamburg, Okehampton and Piacenza provide the highest results for the chromatographic flow models whilst Porto and Sevilla provide the lowest results. For these example substances the range of 80th percentile concentrations for the nine scenarios was approximately two orders of magnitude for substances with leaching in the range 0.01-10 µg/l (Substances A and D) and one order of magnitude for those in the lower (0.01- <0.001 µg/l) leaching range (Substance C) and the upper (10-100µg/l) leaching range (Substance B and Metabolite C)

The four dummy substances used had a range of properties that provided a range of susceptibility to leaching. Nevertheless they are a very small sample size considering the range of real plant protection products in commercial use and in development. In addition, the model runs were only compared for one crop and one application timing and hence the general significance of all of these results, and their likely applicability to other situations, should be treated with care.

The effect on the 80th percentile concentration of; (i) annual application of substance, (ii) application one year in two (biennial) and (iii) application one year in three (triennial) was assessed for Substances A and C with winter cereals at Châteaudun. The results are presented in Table 4.5 and Figures 4.14 and 4.15.

Table 4.5 80th percentile years and substance concentrations for annual, biennial and triennial applications

		Year				Substance Conc. (µg/L)			
		PRZM	PELMO	PEARL	MACRO	PRZM	PELMO	PEARL	MACRO
Pest A	annual	6	8	9	6	1.2	1.3	2.3	4.3
Pest A	biennial	5	5	12	13	0.37	0.36	0.87	2.0
Pest A	triennial	16	16	16	15	0.23	0.24	0.61	1.2
Pest C	annual	6	8	6	6	0.000	0.000	0.000	0.006
Pest C	biennial	5		5	13	0.000	0.000	0.000	0.002
Pest C	triennial	10		16	15	0.000	0.000	0.000	0.001
Met C	annual	9	9	11	8	18	18	24	22
Met C	biennial	4	14	17	3	8.4	8.7	11	10
Met C	triennial	10	10	3	5	5.7	6.1	7.1	6.8

Figure 4.14 80th percentile concentrations, Substance A, winter cereals, at Châteaudun

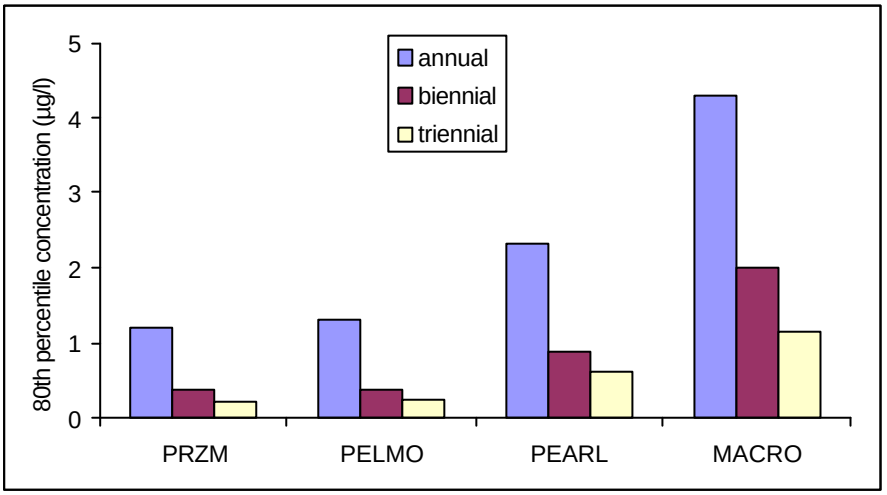
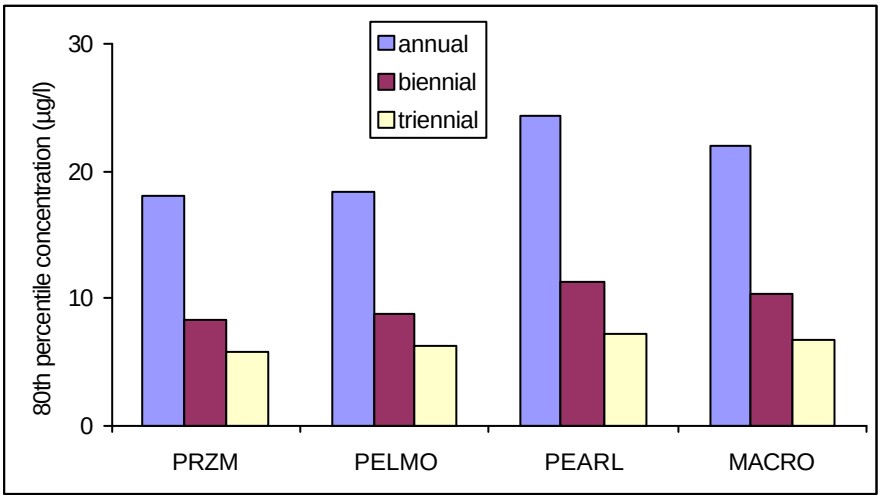


Figure 4.15 80th percentile concentrations, Metabolite C, winter cereals, at Châteaudun



These results show that approximate pro rata decreases in the 80th percentile concentration occur under the test conditions for a single application averaged over two years and three years respectively. This does not seem to be effected by the fact that the 80th percentile period changes.

The effect of irrigation water and substance outputs was investigated for a single crop (maize) with one of the dummy substances (Substance A) at the four sites where irrigation is used for some crops (i.e. Châteaudun, Piacenza, Sevilla and Thiva). To investigate this feature of the FOCUS scenarios it was also necessary to undertake simulations for a non-irrigated crop. However, these simulations are not part of the FOCUS scenarios and the results presented are only to help elucidate the effect of irrigation. The aim of this work was to find the effect of the additional irrigation water on the relative composition of the water balance and to determine the extent of the effect on the 80th percentile substance concentration.

In the Thiva and Sevilla (see Figure 4.16) scenarios the additional irrigation had virtually no effect on the amount of percolate predicted by PRZM and PELMO. The additional water is removed from the profile by a combination of increased surface run-off and increased evapotranspiration. In contrast, the PEARL model predicts a marked increase in percolation since no run-off is predicted at Thiva and only very small amounts (av. 26 mm/yr) at Sevilla. The increased evapotranspiration on the other hand, is similar to that of PRZM and PELMO (i.e. closer to the potential evapotranspiration which is the upper limit for all models). Therefore, in practice the majority of the additional water that becomes run-off in PRZM and PELMO becomes percolate in PEARL. This was confirmed in a further check in which the run-off routines were switched off in PRZM (eliminating run-off water from both rainfall and irrigation) and the amount of percolate predicted in the irrigated run became much closer to that in PEARL.

In the Châteaudun (see Figure 4.17) and Piacenza scenarios the effect of irrigation is to increase the amount of percolate predicted by PRZM and PELMO, but to a lesser extent than for PEARL. The reason for this is that the irrigation scheduling was done with a capacity-based model, which mirrored the soil moisture contents in PRZM and PELMO more closely than those in the Richard's equation-based model PEARL. In these scenarios the absolute amounts of run-off predicted by PRZM and PELMO are relatively low and since the predicted evapotranspiration in the non-irrigated scenario is already appreciable, then a proportion of the additional irrigation water is lost as percolate. When the run-off routine is switched off in PRZM there is no effect on the predicted evapotranspiration (suggesting that the maximum amount has already been reached) and hence the additional percolate water predicted for PRZM (from eliminating run-off from both rainfall and irrigation) brings the amount closer to that for PEARL. MACRO gives similar results to PEARL at Châteaudun .

Figure 4.16 Average annual percolation volumes predicted at Sevilla in the absence and presence of irrigation

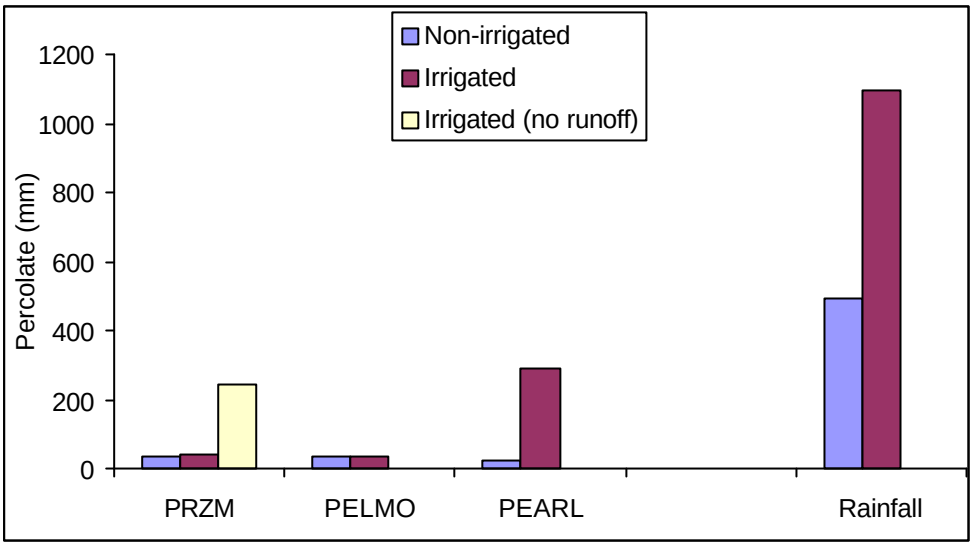
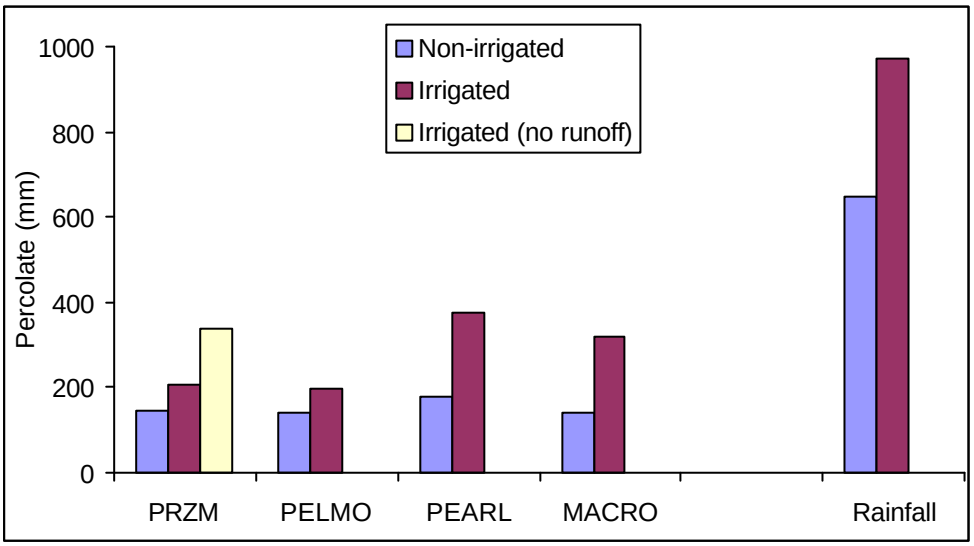


Figure 4.17 Average annual percolation volumes predicted at Châteaudun in the absence and presence of irrigation



In PRZM and PELMO the main effect of irrigation on the substance mass balance was to increase the amount of plant uptake and decrease the amount of degradation and storage. This effect was most noticeable at Sevilla and Châteaudun. A similar trend seemed to occur in PEARL and MACRO, although the variation between irrigated and non-irrigated runs was much smaller.

The year of the 80th percentile concentrations showed little agreement between the irrigated and non-irrigated scenarios (or the irrigated scenarios with and without run-off in the case of PRZM). The concentrations in the irrigated scenario were within a factor of 6 of those in the non-irrigated scenario for all of the models with this crop/substance combination (except for PEARL in Sevilla). However, in all cases (irrigated or non-irrigated) the 80th percentile concentration was higher in PEARL than in PELMO or PRZM. The effect of switching off run-off in the irrigated scenarios in PRZM led to a significant increase in the predicted 80th percentile concentration at Thiva (in excess of a factor of 500; see Figure 4.18) and Sevilla (see Figure 4.19) but not at Piacenza (see Figure 4.20) or Châteaudun (see Figure 4.21).

Figure 4.18 80th percentile concentrations predicted at Thiva in the absence and presence of irrigation

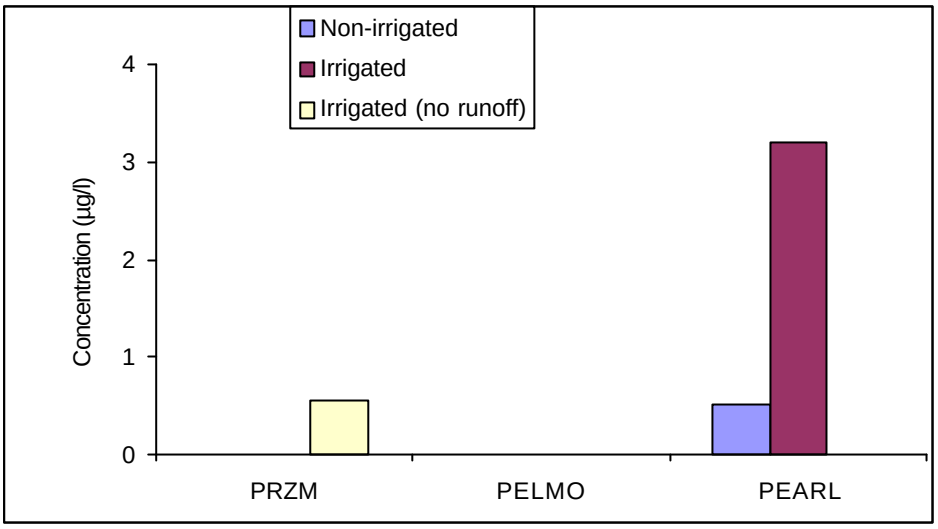


Figure 4.19 80th percentile concentrations predicted at Sevilla in the absence and presence of irrigation

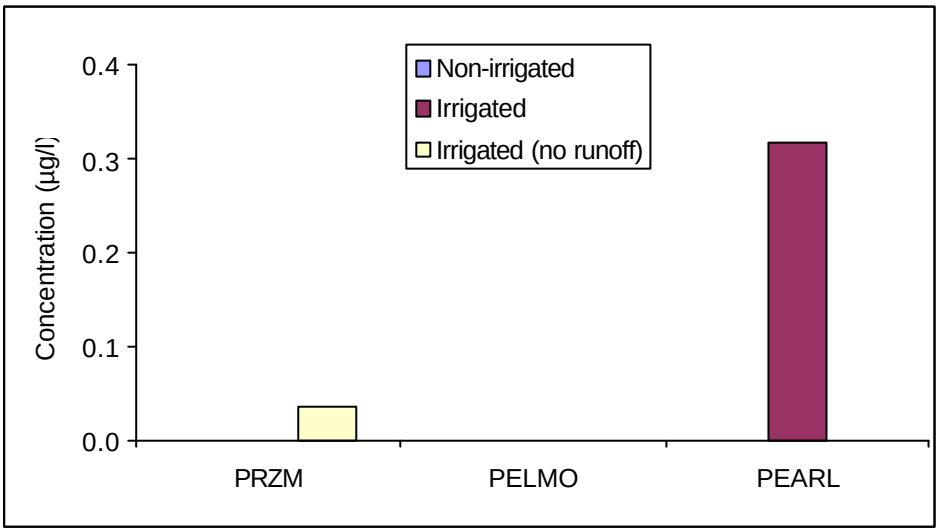


Figure 4.20 80th percentile concentrations predicted at Piacenza in the absence and presence of irrigation

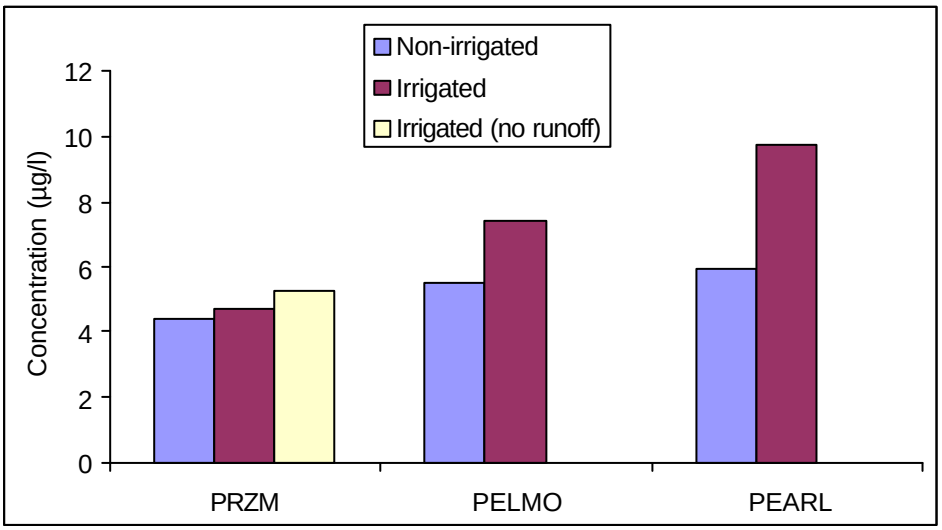
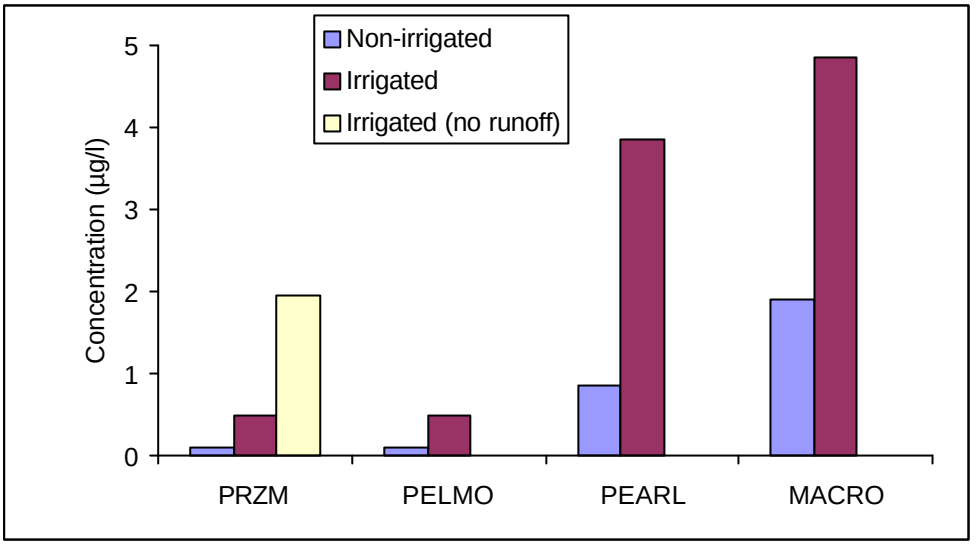


Figure 4.21 80th percentile concentrations predicted at Châteaudun in the absence and presence of irrigation



Based on these limited results it would appear that the presence or absence of irrigation causes less effect on the 80th percentile concentration (the intended regulatory output) than the differences between the selected scenarios (i.e. Thiva, Sevilla, Piacenza, Châteaudun). However, switching off the run-off routines in PRZM (and presumably PELMO) results in the 80th percentile concentrations being higher and rather more similar to PEARL (which predicts the presence of run-off in very few cases).

5. PESTICIDE INPUT PARAMETER GUIDANCE

5.1 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).

5.2 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).

5.3 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.

5.4 Guidance on substance-specific input parameters

5.4.1 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/m^3) but in PELMO the units are Pa m^3 mol^{-1} (equivalent to J/mole). The conversion factor from K_{aw} (dimensionless) to H (Pa m^3 mol^{-1}) is as follows H = K_{aw} *R* T, where R is the universal gas constant (8.314 Pa m^3 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} m^2/day (Jury, 1983; PEARL units) which is equivalent to 5.0 x 10^{-10} m^2/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 m^2/day (Jury, 1983; PEARL units) which is equivalent to 4300 cm^2/day (PRZM units) and 0.050 cm^2/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)

5.4.2 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 5.1 & 5.2 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 5.1 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 5.1 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 5.1. 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 5.2
% 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 5.2	Use default gravimetric value at field capacity for texture type given in Table 5.2
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 5.2. Calculate % gravimetric at given % of 1/3 Bar	Use default gravimetric value at field capacity for texture type given in Table 5.2
% MWHC (Maximum water holding capacity; assumed 1kPa, i.e. pF1)			Use default gravimetric value for texture type at MWHC given in Table 5.2. Calculate % gravimetric at given % of MWHC	Use default gravimetric value at field capacity for texture type given in Table 5.2

Table 5.2 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 5.1 & 5.2

(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 5.3.

Table 5.3. 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 5.1 & 5.2 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).

5.4.3 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.

5.4.4 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.

5.4.5 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 2.3 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.

5.5 References

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6. Uncertainty issues in relation to the use of the FOCUS leaching scenarios

6.1 Introduction

In the following sections, the main uncertainties related to the simulation of the leaching of substances with the FOCUS groundwater scenarios are discussed. This chapter also assesses the relevance of the various sources of uncertainty associated with modelling these scenarios. Some of these uncertainties are common to all modelling and thus not limited to the proposed scenarios. Possible alternatives and strategies chosen to reduce these uncertainties are discussed.

Despite the uncertainties considered in this chapter, the workgroup concludes that the final scenarios and modelling strategies recommended by the group are suitable for assessing the leaching potential of substances at Tier 1 in the EU review process given the state of the art.

The four main types of uncertainty described in this chapter are:

- The uncertainty related to the correctness of the process descriptions within the leaching models. Mathematical models necessarily need to simplify the complex processes found in nature for their simulations. As the various models sometimes contain different process descriptions, the way in which processes are conceived in the models will also influence model output.
- The uncertainty related to the choice of scenarios for weather, soil and crop. Leaching to groundwater is influenced by many factors and, in order to be pragmatic, only a limited number of factors were taken into consideration when selecting the scenarios.
- The uncertainty related to the estimation of input for the scenarios. The input for the scenarios was generated by combining
    - the information obtained from locally measured data,
    - data available in regional geographical information systems such as the MARS data base for weather parameters and the HYPRES data base for soil parameters,
    - up-to-date literature sources,
    - expert knowledge, and
    - generic parameter strategies such as pedotransfer rules for the deriving soil hydraulic properties.

  By combining all this information results may be obtained, which could deviate from the results inferred from other input resources, i.e. local measurements.
- The uncertainty related to the calculation and interpretation of output. The simulation results of the models with the established scenarios can be post-processed in different ways in order to calculate target quantities for assessing leaching. The final procedures have been established through a process of discussion and selection of a reasonable convention. Choices of other alternatives could have resulted in slightly different procedures with corresponding differences in output.

6.2 Uncertainties related to model choice and model parameterisation

The substance in soil is subject to a number of processes, be it transport processes in the soil water and vapour phase, biotic and abiotic mediated transformation and degradation processes, or exchange processes. Theoretical and empirical descriptions for these processes exist, and are implemented in the different model codes. However, the various considered model codes do not always implement the same processes and do not use identical process descriptions. For example: PRZM/ PELMO describe the water flow in the soil in a rather simple manner (tipping bucket), but they include descriptions of surface runoff and volatilisation. PEARL, on the other hand describes the flow by Richards's equation, and contains rather detailed process descriptions, but contains no description of surface runoff for substances. MACRO contains the most advanced flow description as it includes preferential flow, but surface runoff and volatilisation are not represented.

If a compound is subject to processes, which are not considered in the model structure, then this will contribute to the modelling error. Three easily understandable examples are

- The erroneous simulation due to a wrong model concept. For instance, process implemented in the model assumes that the substance degrades according to first order kinetics, but the degradation of the substance does not follow these kinetics.
- The ignorance of a process relevant for the behaviour of the substance. For instance, a volatile chemical is simulated with a model not accounting for volatilisation.
- The erroneous simulation due to a biased model concept. For instance leaching in a (strongly) structured soil is simulated with a model that accounts only for chromatographic leaching.

Model validation studies attempt to quantify the model and modelling error. A reasonable method for selecting a model for one particular scenario would be to select the model, which results in the smallest modelling error. In the FOCUS framework, four models were selected. These selected models have been subject to a range of validation studies in the past (e.g.; Beusen *et al*, 1997; Boekhold *et al*., 1993; Boesten, 1994; Boesten and Gottesbüren, 1999; Bosch and Boesten, 1995, Carsel *et al*., 1985; Carsel, 1986; Fent *et al*., 1998; Jarvis et. al., 1994; Jene *et al*. 1996; Klein 1994; Klein *et al*. 1997; Klein *et al* 2000; Mangels & Jones, 1998; Mueller, 1994; Nicholls, 1994; Parrish, *et al*., 1992; Thorsen *et al*. 1998, Vanclooster *et al*., 2000). Both the validity of the concepts, represented in the selected modelling codes, and the way how parameters and input were estimated by the model user were considered as a part of the validation assessment.

Leaching models continue to be improved, but a leaching model validated for all conditions does not exist. Three models have been parameterised for the FOCUS scenarios (four for Châteaudun). These models have differing strengths and weaknesses , which allows the possibility that a model may be chosen which is the most appropriate for the particular substance and scenarios being considered.

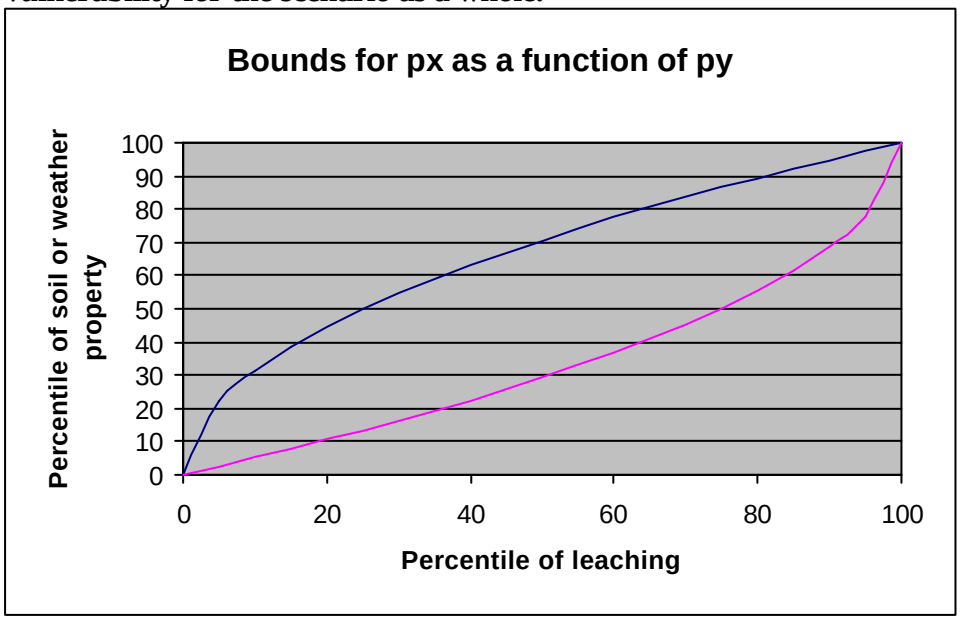
Some studies have highlighted the issue of the high degree of influence of the subjective input estimation of the model user on the modelling output (Brown *et al*., 1996; Jarvis *et al*., 2000; Boesten, 2000). In order to minimise the uncertainty induced by the model users, an input parameter guidance document has been provided (Chapter 5).

6.3 Uncertainties related to the choice of scenarios

The realistic worst case was identified by the concept that scenarios should correspond to 90th percentile vulnerability situations. This is, in reality, a function of all system properties (weather, soil, groundwater, crop, substance application and chemical properties). A correct theoretical approach would imply development of a few hundred scenarios at the EU-level, which should all be run for the specified substance. A 90th percentile vulnerable scenario could then be identified from the resulting frequency distribution. However, the development of hundreds of scenarios was beyond the scope of the working group and databases for soil properties and crop parameters were not available to the working group.

It was assumed that the final scenarios should have a probability, pY, of 90 % and that the vulnerability should be divided equally on weather and soil (both equal to pX). Figure 6.1 illustrates how these percentages were defined and the uncertainty related to this approach. It is not possible to calculate the value of pX exactly, but minimum and maximum values may be established. If the weather and the soil are independent events, we can infer from conditional probability theory that the minimum value of pY, is described by neither the soil nor the weather condition being vulnerable, pXsoil*pXweather (lower boundary) . The maximum value of pY is described by the situation where both the soil and the weather conditions are considered vulnerable, pY = 1-(1-pXsoil)*(1-pXweather) (upper boundary). The probability of one factor being vulnerable, and the other not, makes up the area between the curves.

Figure 6.1 Illustration of the procedure used for defining the desired percentile vulnerability of weather and soil conditions, to result in an overall 90th percentile vulnerability for the scenario as a whole.



From these considerations an 80th percentile was chosen for the weather data. Due to lack of available databases on soil properties at the European scale, the selection of the appropriate soils

had to be performed mainly by expert judgement, and based on an assumption of chromatographic flow (see Chapter 2.1).

6.3.1 Specific issues related to preferential flow

Preferential flow can be an important transport mechanism for water and solutes into soils and subsoils. For sites with significant preferential flow, the site-specific properties rather than compound-specific properties are the major factors affecting transport into the soil, at least within the upper metre. Even small mass fluxes may result in large concentrations if preferential flow is occurring. Yet, preferential flow will only seldom represent a complete shortcut from the surface to the groundwater. In soils with preferential flow, substances may be transported past layers of high organic matter and fast degradation and therefore the attenuation and degradation may be reduced. On the other hand, substance in the soil matrix may be delayed if "clean water" is channelled through the preferential flow paths rather than through the matrix. Organic matter may be transported and accumulated in the preferential flow regions and may retain and degrade chemicals transported therein (Pivetz and Steenhuis, 1995). The importance of the preferential flow process will be greatest if the groundwater is relatively shallow, and the interval between substance application and rainfall is small.

Two typical examples may be considered.

- In cracking clay soils macroporous flow will occur under dry conditions, when the cracks are open. Water and chemicals will be transported through the cracks, especially when rainfall intensity exceeds the infiltration capacity of a thin surface layer.
- In non-cracking soils earthworm holes are often the dominating pathways for water and chemical transport through the soils.

Many heavy soils are drained if used for agricultural purposes. If soils are influenced by a high water table, the flow direction of the water in the upper metre is often not dominated by vertical percolation – instead water runs off horizontally, via runoff, through drains or via shallow groundwater to streams. Under such circumstances, the concentration estimates in a depth of one metre are unlikely to be realistic for the water eventually percolating to deeper layers. The concentration of the substance in the percolating water will probably be lower.

The assumption of chromatographic flow as only transport mechanism may therefore be a limitation in some of the scenarios. Preferential flow occurs in many soil types, including soils which are not particularly fine textured as recent research shows. The dependency of this process on structure, tillage practices and other factors not included in the generalised databases makes it impossible to include it as a selection criterion. It is also impossible to parameterise a macropore flow model without measured or empirical soil parameters for hydraulic conductivity. However, such data were available for the Châteaudun site.

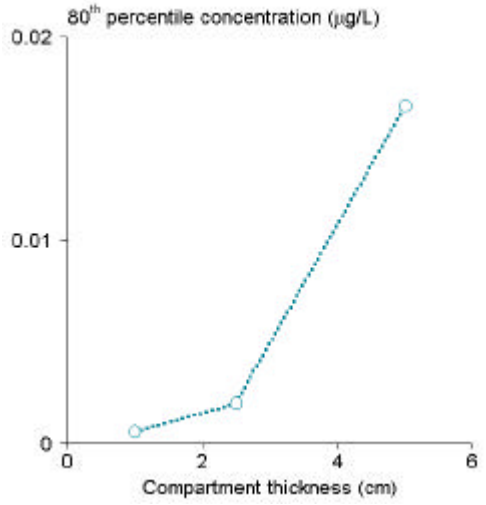
6.3.2 Specific issues related to hydrodynamic dispersion

The dispersion length of all soil profiles was set at 5 cm for all soil horizons. In general, the dispersion lengths of field soils range from 2 to 10 cm and varies in terms of soil type and soil water

flux (Beven *et al*., 1993). However, given the fact that at present no standardised reference technique exist to quantify the dispersion , no scenario specific values could be adopted. The dispersion estimate is therefore subjected to uncertainty, and will have an impact on the calculated substance concentrations, especially at the leading edge of the breakthrough curve (Jury and Gruber, 1989).

In the PRZM and PELMO models the dispersion is controlled by the thickness of the compartments. The effective dispersivity, considered by these models, will therefore be different from those adopted in mechanistic models such as PEARL and MACRO. Calculations were made with PRZM 3.2 to illustrate the effect of the compartment thickness at low leaching levels. Figure 6.2 shows that the compartment thickness has a very large effect: the 80th percentile concentration for 1-cm compartments is about 30 times lower than that for 5-cm compartments.

Figure 6.2 The 80th percentile of the substance concentration leaching below 1 m depth as a function of the compartment thickness. PRZM calculations for the Porto location and Substance A applied to winter wheat at sowing at 1 kg/ha. Compartment thickness was 1 mm in the top 10 cm. The horizontal axis shows the compartment thickness below 10 cm depth.



6.4 Uncertainties related to input

6.4.1 Weather

As explained in a Chapter 2.2, different data sources were used to establish the weather scenarios. The FOCUS scenarios are virtual scenarios, and so no real site will exactly match them in terms of weather or other conditions. Future weather is also not predictable, leading to some inevitable uncertainty. Notwithstanding this, it is appropriate to consider some uncertainties associated with the weather data, and that is the purpose of this section.

The MARS database was used as a primary data source. This database comprises long-term weather parameters representative for each 50 km by 50-km grid in Europe. This database was

generated from archives of meteorological data as available from national meteorological institutes. The archives contain data from different weather stations. Different measuring devices and measuring protocols will therefore affect the value of the weather parameter, as reported in the meteorological archives, and affect the outcome of the MARS data base generation procedure.

Further, in order to cover the European region for sufficiently long time intervals, data from the meteorological archives were compiled, and interpolated in time and space. Time interpolation was needed if missing data were reported in the original archives, while spatial interpolation was needed to cover each grid point of Europe. Each interpolation is based on a hypothetical model, linking the data as observed at different locations in time and space. Interpolation is therefore subject to the uncertainty of the model that characterises the spatial and temporal structure of the weather data. While the models of the spat-temporal structure may be well established for parameters such as temperature and daily evaporation rates, these models remain poor for the precipitation data. It is well known that rainfall intensity may vary extremely within small time and space intervals, which complicates the interpolation of rainfall from sparse data sources.

An illustration is given in the Table 6.1 showing the rainfall data as observed measured at the weather station in Jokioinen, and the values as inferred from the MARS data base. Considerable deviation can be observed for extreme rainfall events within some particular years, as for instance in 1991. The reason for this is that part of the MARS-data for Jokioinen stems from Estonia on the other side of the Gulf of Finland. However, when looking to the parameters of the daily rainfall probability density functions, only small differences occur. It was, however, easy to pick out for which years the data were provided by one station and for which years the source was different, indicating a difference in pattern.

Ample corrections on rainfall data were therefore considered when developing the FOCUS weather scenarios. In order to comply with the original weather targets, other data sources and observations from local experts were considered (see Chapter 2.2). Again, combining data from different sources will introduce uncertainty in the FOCUS weather data set. In conclusion, further evaluation and improvements of the data generation techniques should be envisaged in future (see section Strategies to further reduce the uncertainty on strategies to reduce the uncertainty).

Furthermore, no evaluation has been made of whether or how the selected weather data differs from other weather data within the agricultural zone represented by the scenario.

Table 6.1 Statistical descriptors for the daily precipitation rates of the MARS data and the Finnish Meteorological Institute (FMI) data for Jokioinen. (Part of the MARS-data for Jokioinen stems from Estonia on the other side of the Gulf of Finland Sea.)

	MARS 1975-1991	**FMI 1975-1991**	**MARS 1991**	**FMI 1991**
Number of observations	6209	6209	365	365
Median	0.0	0.1	0.0	0.1
75th percentile	2	2	2	2
95th percentile	8	8	11	8
99th percentile	18	18	29	16
Maximum	119	79	104	28
Mean	2	2	3	2
Standard deviation	4.6	3.8	8.2	3.4
Skewness	10.1	5.4	8.6	3.5

6.4.2 Irrigation

Four irrigation scenarios were generated with an irrigation scheduling software, using the previously defined soil, weather and crop data, as described in Chapter 2.2. The theoretical scenarios were corrected based on expert judgement. However, ample options need to be fixed in order to come up with a limited set of irrigation scenarios. These options were related to the adopted irrigation practice and farmers criteria used to schedule irrigation. Again, agricultural practice with respect to irrigation is extremely variable from site to site and is difficult to resume in only 4 scenarios. Users should be aware that the adopted irrigation scenarios might have large differences to particular local situations.

A comparison of the effect of irrigation on percolation of water and leaching for the four irrigated scenarios is shown in Chapter 4.2. The irrigation has been added as additional rainfall to the weather files. This means that the models consider irrigation water as subject to runoff, which is normally not the case since irrigation is applied at a lower intensity than assumed for an equivalent rainfall event. Since PRZM and PELMO predict higher run-off losses than PEARL, this additional run-off contributes more to the uncertainty of the predictions with these two models (see Chapter 4.2).

6.4.3 Soils

When a particular soil was selected for a scenario, it had to be parameterised. Measurements of the soil profile development, the soil texture, the soil organic matter, and the pH was available for all scenario soils. Measurements of the soil bulk densities were available for all horizons, except for the Sevilla soil and the deeper horizons of the Châteaudun soil.

For two scenarios (Châteaudun and Hamburg), soil hydraulic parameters have been fitted from observed retention and hydraulic conductivity data. These hydraulic parameters were appropriate

for the simulation of observed water balances at the sites. However, as soil hydraulic properties vary considerably within short distances, concern may still exist about the reliability of these local scale parameters to represent effective field scale water transport.

For the remaining soil horizons, the HYPRES database was used for defining the hydraulic parameters. Hydraulic data can be generated from appropriate pedotransfer rules. These, however, remain subject to uncertainty, especially for the soil hydraulic parameters related to soil structure such as the saturated hydraulic conductivity, the air entry value of the moisture retention curve and the tortuosity factor of the hydraulic conductivity curve (see Espino *et al*., 1995).

As bulk density is an independent variable for the HYPRES pedotransfer rules, it was necessary to estimate this parameter for the Sevilla soil. Use was made of the bulk density pedotransfer function of Rawls (1983). The standard error of estimate for this pedotransfer function was found by Rawls (1983) to be 0.17 g/cm^3, which will of course also influence the quality of the HYPRES estimate of the rest of the parameters.

To illustrate the effect of such variation, soil parameters were estimated based on the Sevilla soil data and an estimated bulk density $\pm$ 0.17 g/cm^3. Key data are given in Table 6.2.

Table 6.2 Average values of percolation, evapotranspiration, runoff and leaching over 20 years for Substance B at Sevilla (winter wheat), calculated with PEARL on the basis of three different sets of hydraulic parameters generated with the HYPRES pedotransfer functions by varying the bulk density.

	High bulk density	Low bulk density	Average bulk density used for the scenario
Percolation below 1 m (mm/yr)	64	28	48
Total Evaporation (mm/yr)	422	462	441
Runoff (mm/yr)	7	3	4
Change in storage (mm/yr)	0	0	0
Substance leached (µg/(m^2.yr))	174	38	91
Average concentration (µg/l)	2.7	1.4	1.9
80th percentile concentration (µg/l)	3.9	2.3	3.4

It is obvious that the water balance is severely affected: percolation and surface runoff differ by a factor greater than two. The amount of substance leached in this case differs by a factor greater than four. The substance concentrations in the 80th percentile year differ by a factor of 1.8.

The HYPRES estimates of the saturated water content and the n value appears to be of better quality than the estimation of α, λ and K_s (see soils Chapter 2.3). For the three last values, the R^2 of a ln-transformation of the parameters (see Wösten *et al*. 1998 for the exact transformations) is $\leq$ 20 %, indicating that the predictions are very uncertain. α influences the shape of the retention curve, and thus all the model simulations. The influence of the saturated hydraulic conductivity and the value of λ is relevant only for MACRO and PEARL, and influences mainly the hydraulic conductivity at low moisture contents. This again influences the simulation of capillary raise and evaporation.

The retention curves generated with the HYPRES pedotransfer rules were compared with retention curves from the Staring reeks (Wösten *et al*, 1994). In some cases the estimates were very similar.

In most cases the shape of the retention curve close to saturation was less steep using the HYPRES pedotransfer rules. Additionally, the amount of plant available water was generally lower than the values obtained from the Staring reeks. An additional note needs to be made for the sub-soil of the Piacenza site. Due to the fact that the HYPRES database is not able to handle horizons with no or very little clay, the parameters for the lowest horizon in Piacenza was simply substituted from the Hamburg soil. This must be considered as a very rough approximation, which appears, however, acceptable.

6.4.4 Crops

The FOCUS scenarios are virtual sites. Therefore, it may occur that the crop data proposed for the scenario are not exactly representative for the agricultural practice at the location of the soil associated with the respective region and scenario. It has been tried, however, to select the best possible representative or average values in order to set up a representative standard cropping scenario for the regions of the FOCUS locations.

The data on physiology and phenology of crops have been selected with the help of local experts or were extracted from published evaluations (e.g. Becker *et al*. 1999; Myrbeck, 1998; Resseler *et al*. 1997; Van de Zande *et al*. 1999). The parameters of relevance are mainly sowing and harvesting dates and the date of maximum leaf area development, as well as corresponding values for LAI and rooting depth. The data base for the soil cover of major crops is based on a very large number of measurements and therefore very reliable. On the other hand, estimates of the rooting depth, which depends heavily on subsoil properties and which can vary considerably, are based only on a few measurements.

The LAI values influence the evaporation calculated by the models. The main sensitivity is between a value of 0 and about 2.5 (Houcine, 1999, Kristensen and Jensen, 1975). For higher values, the sensitivity is low. The fact that cropping data are constant for all years means that the sensitive period may be slightly out of phase with the correct situation. The rooting depth does influence the evaporation of all models, and this factor may be of significance. The crop cover at spraying is estimated independently of LAI by the user, so the uncertainty on this factor is independent of the other estimates, but can be inconsistent with the LAI development.

6.4.5 Substance parameters

A very significant effect on the prognosis of leaching can arise from the choice of substance sub-routines and the corresponding parameterisation of the substance. The simulated leaching behaviour of a substance is very sensitive to these two factors. The issue of selection of the correct process descriptions is already discussed in Section 6.2 and is very pertinent for substance processes. Uncertainties related to the substance parameters may be attributed to:

- selection of default values for parameters for which specific information is unlikely to be obtained
- rules applied regarding the choice of degradation and sorption parameters.

Most important for leaching are degradation and sorption properties of the substance in soil and therefore discussed more in detail, though other parameters may also be relevant.

Degradation

The degradation of a substance can be determined in the laboratory and in field experiments. The use of data from these two types of experiment will contribute to uncertainty in a different way.

Degradation experiments in the laboratory are conducted under controlled and standardised conditions, in which modes of degradation such as biotic degradation, abiotic hydrolysis and photolysis can be distinguished, and the effects of temperature and moisture can be isolated. This makes laboratory results relatively easy to use as modelling inputs. However there is uncertainty associated with extrapolating photolysis and abiotic hydrolysis rates from the laboratory to in use conditions, as lab vs. field comparisons for these processes have in general not been done. This uncertainty could result in an over or underprediction of true field degradation. The very high concentrations used in laboratory experiments, and the potential loss of biological activity over time (especially >100 days) can also result in uncertainty in the specification of degradation for modelling, and these factors will tend to result in an underprediction of true field degradation.

Beulke *et al*. (1999, submitted) and Wagenet and Rao (1990) give a detailed review on other factors leading to a tendency for laboratory data to overestimate substance persistence in the field . The first authors conclude that in 44% of the 178 studies evaluated the persistence was overestimated for more than 25%, whereas underestimation (> 25%) occurred in only 16% of the studies. Other examples where overestimating of persistence and leaching can occur when using lab data are given by Ma *et al* (2000) and Bromilow *et al* (1999).

There are also uncertainties introduced by the use of field data. In the field it is difficult to distinguish the various possible modes of degradation, as well as other types of dissipation such as volatilisation, leaching and runoff. The fact that data from field studies clearly relate directly to real examples of field behaviour of a substance reduces uncertainty. However, environmental conditions in field studies cannot be standardised, and the average behaviour may differ from the average behaviour in all conditions in which the substance may be used in practice, which introduces some uncertainty.

Sorption

The sorption of substances is mostly characterised by determination of the Freundlich isotherm with the parameters k_f (sorption coefficient to soil) and 1/n (exponent of the isotherm) from batch experiments with soil/water slurries. The sorption can be related to soil organic matter content which then gives the K_{oc}-values, which attributes the retention in the soil profile totally to the presence of organic carbon. This relationship, however, ignores the possible interaction with other soil components like clay and ferro-oxides, which can be significant for certain types of molecules.

The Freundlich exponent 1/n ranges usually between 0.7 and 1.0 (Allen & Walker, 1987). Calculated leaching is very sensitive to this exponent: changing the exponent from e.g. 0.9 to 0.8 may lead to a tenfold decrease in calculated leaching for KOC values above 50 L/kg and percentages leached below 1% (Boesten, 1991).

The occurrence of long-term increase of adsorption, which is a well-recognised process further reducing leaching is also ignored by standard modelling procedures (unless specific data are available) and underestimates adsorption. On the other hand, substance residues that are increasingly adsorbed and thus less available to leaching processes will also be less bioavailable to degrading micro-organisms and will have a higher residence time in soil (after desorption, however,

biodegradation starts again). Overprediction of the actual sorption by the Koc value will occur if freshly applied substances and intensive rainfall meet.

A range of error for substance sorption estimates from lab measurements to field application was given by Green and Karickhoff (1990) for the modelling context: The authors concluded from their studies likely error factors from +2X (overprediction for freshly applied substances) to –10X to –1000X (underprediction for sorption of aged residues and in subsoils).

6.4.6 The use of mean values in worse case scenarios

The FOCUS approach for the assessment of the leaching potential of substances to groundwater is to set up 90th percentile worse case scenarios for simulation model runs (see Chapter 2.1). As many other test scenarios the FOCUS scenarios for main agricultural regions consists of several subscenarios: Weather (precipitation and irrigation), soil, crop and substance (degradation, sorption). The subscenarios (e.g. weather) can be split up further (in precipitation and irrigation) as indicated above. As outlined in the respective chapters, the 90th percentile vulnerability of the scenario is achieved by evenly creating an 80th percentile vulnerability or worse case situation for the soil and the weather subscenarios leading with a high probability to a 90th overall percentile target for the whole leaching scenario. More favourable situations in one subscenario (e.g. weather) can be theoretically balanced by less favourable situations elsewhere (e.g. substance sorption). If the target value for the overall worse case is a 90th percentile and determined by the settings of the vulnerability in the soil and weather scenarios the use of further subscenarios with a significant different percentile than the 50th percentile (median) would probably change the overall targeted value significantly. If further subscenarios are parameterised by a 90th percentile worse case, for example, this would lead to a situation that represents clearly more than a 95 or 99th percentile worse case, at least if the parameters are independent. The addition of several worse case subscenarios may therefore sometimes lead to a very unrealistic overall scenario that hardly can be found in nature.

Soil Properties

Due to the variability of nature, a set of measurements of any parameter, even within an otherwise homogeneous field or plot, will produce a number of different values. For hydraulic conductivity, single values may vary with a factor of 10^3. This leaves the modeller with the problem of choosing a value to use in modelling. Some scientific efforts have been put into determining ways of estimating “effective parameters” for field scale simulations. An "effective parameter" in this sense means the parameter value which best represents the average conditions for the given parameter within a given area, e.g. a field. For soil hydraulic parameters, the common approach for estimating effective parameters is to use the arithmetic mean for water retention and geometric mean for hydraulic conductivity (e.g. Jensen and Refsgaard, 1991; Sonnenborg *et al*., 1994).

The results from literature on whether effective parameters can be used to simulate average field scale behaviour are ambiguous. Based on numerical analyses of infiltration, Bresler and Dagan (1983) and Smith and Diekkrüger (1996), among others, concluded that effective soil hydraulic parameters are not adequate for modelling water flow in spatially variable fields. Jensen and Refsgaard (1991), Jensen and Mantoglou (1992) and Sonnenborg *et al*. (1994), comparing field observations of water content and suction vs. simulated data, found that effective soil hydraulic parameters provided a practical approach for estimating the field-averaged water balance. This approach has recently been shown also to be valid in connection with nitrate simulations (Djurhuus

et al., 1999). It is expected that the soil parameters generated by HYPRES, and used in the FOCUS leaching scenarios, produce values which may be assumed to be "effective parameter values".

Substance properties
The variability of substance degradation (DT50) in various soils has been estimated to have a coefficient of variation of around 100 % (e.g. Wagenet and Rao 1990); sorption (K_{oc} value) seem to vary about half of that. The use of appropriate mean values (arithmetic or geometric means/medians) for these relatively variable input values can reduce the uncertainty of model predictions, compared to the use of a single value from one experimental year or soil.

Repeated use of the same substance over 20 years is already a worst case assumption. To also assume worst-case substance properties for each of these 20 applications would be truly extreme.

Note that although the recommendation in Chapter 5 is to use an average Kom or Koc value, the Kd value used in the simulation for a given scenario is not a mean, since it depends on the soil %om, which is defined as a part of the set of realistic worst case soil properties, and is in general low. An average Koc value multiplied by a low %oc results in a low soil adsorption coefficient.

6.5 Uncertainties related to the interpretation of output

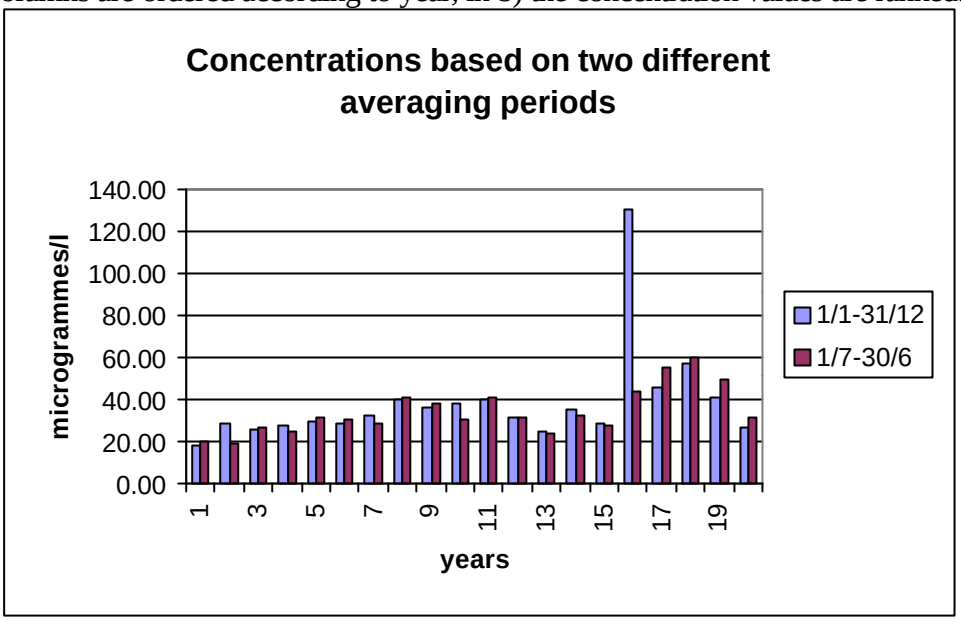
The models generate large amounts of data, which have to be interpreted. The method of interpretation chosen and the method of calculation of the annual concentration are described in Chapter 2.1. In short, the average annual concentration in one-meter depth is calculated over a calendar year. This rather precise definition is a pragmatic one. Other methods of interpretation could have been selected and would have resulted in different values for the concentration to be evaluated against the target value. In the following, some of the implications of different choices are given.

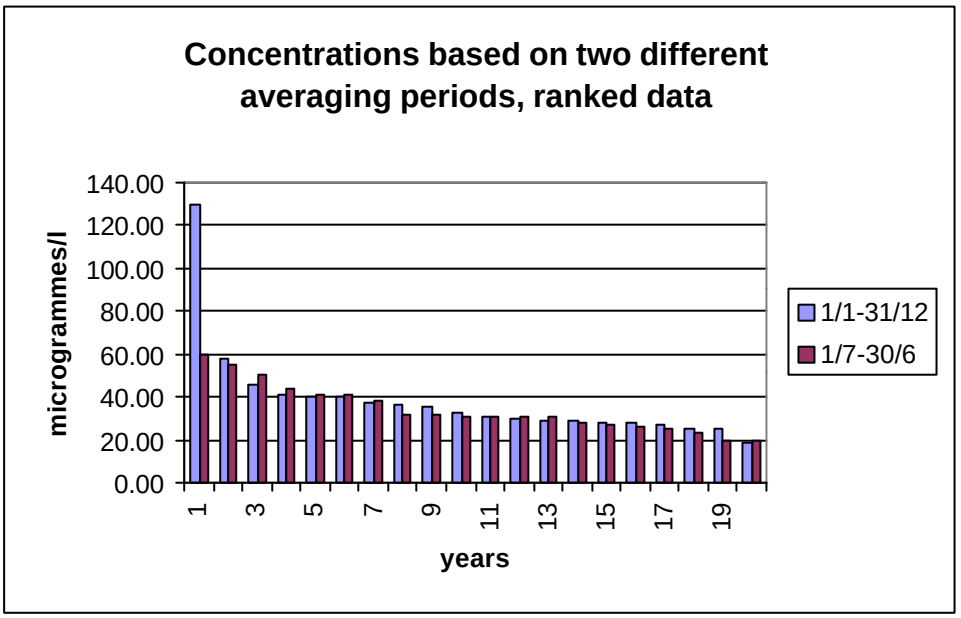
6.5.1 Hydrological year versus calendar year

In many studies, the averaging period is a hydrological year, which is different from a calendar year. The exact timing of a hydrological year differs from place to place in Europe, but in general the divide is placed in a dry period during spring or summer. In a hydrological year, the percolation peaks during winter are merged into one evaluation period, while in a calendar year, the peaks in November-December falls in one period, and the peaks in January February falls in another period. If the leaching in all years is approximately the same, the division point between the years is of no importance. If the leaching differs between years, the calculated concentrations will differ as a function of the averaging period. Figure 6.3 shows an example of the effects of averaging over a hydrological years versus averaging over a calendar years for a time series of leaching.

Figure 6.3 Example of the effect of different averaging periods on concentrations for an arbitrary substance. Columns to the left refer to averages produced over a calendar year, while

columns to the right are concentration averages produced over the period from 1st. July to 30th June. In a) the columns are ordered according to year, in b) the concentration values are ranked.





In the example, the result of one simulation is averaged based on a year running from 1st Jan to 31st. Dec, and on 1st July to 30th of June. In Figure 6.3a, the data are listed in the order in which they are obtained, and in some cases, there are significant differences between the adjacent columns. In Figure 6.3b, the values are ranked, and the difference between the two records is rather small. It is also not systematic. Although one peak is much diminished if the averaging period is changed, it was concluded this uncertainty would in general be very small and not lead to systematic errors in predictions.

6.5.2 1 year average versus 3 year average

The averaging periods of one, two and three years were chosen on the basis of convenience, but do pose a problem regarding consistency. The advantage is that 20 substance applications results in 20 output concentrations, which can be evaluated according to one rule. The disadvantage is that

substances applied with a different frequency in practice will be evaluated according to different criteria.

The following example may show some light on this: For a fast leacher in a sandy soil, the leaching related to one event might take place within one year. When using an averaging period of 2 to 3 years, the load leached in one year is diluted with clean water of the next two years in the calculation. Assuming approximately the same amount of percolating water every year, the concentration of a three year average will be about one third of the concentration in the peak year, calculated as a one year average. An example of this is given in Figure 6.4.

The different averaging periods affect the results. An example is shown in Fig 6.5, where yearly applications were made over 60 years (rather than over 20 years) and three years averages were made. For the annual values of the first 20 years, the 80th percentile value is 0,17 ug/l, while for the three-year averages over 60 years, the 80th percentile value is 0.1
ug/l. So cases could occur, where a substance, which failed the test if applied every year for 20 years would pass if applied every year for 60 years, due to the averaging. It should be noted that the FOCUS group is not recommending a 60 years simulation with yearly applications and three-year averages. The example was purely made to illustrate the effect of the different averaging periods.

Figure 6.4 Example of leaching after application every three years, calculated as annual averages and averages over three years

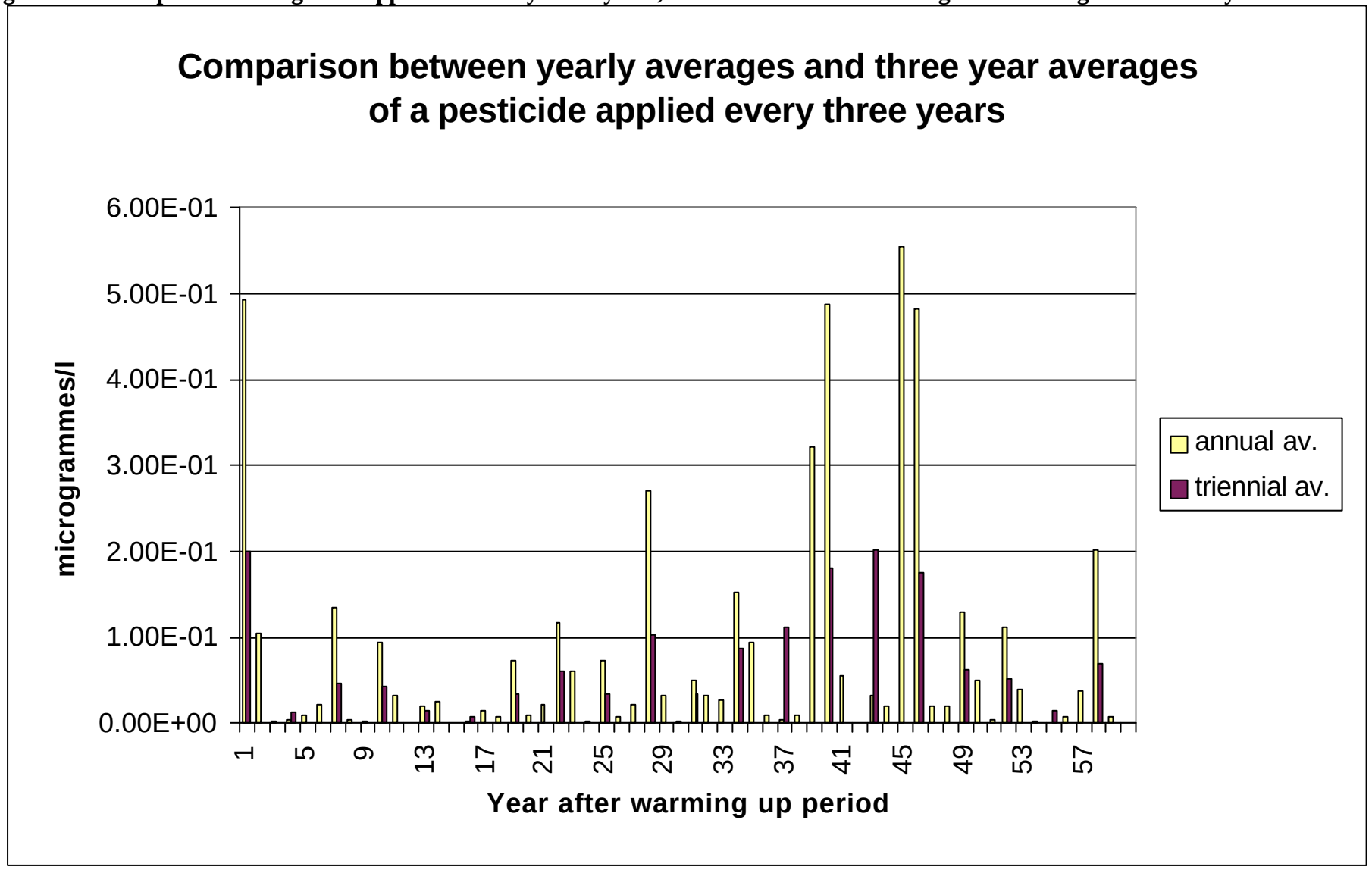
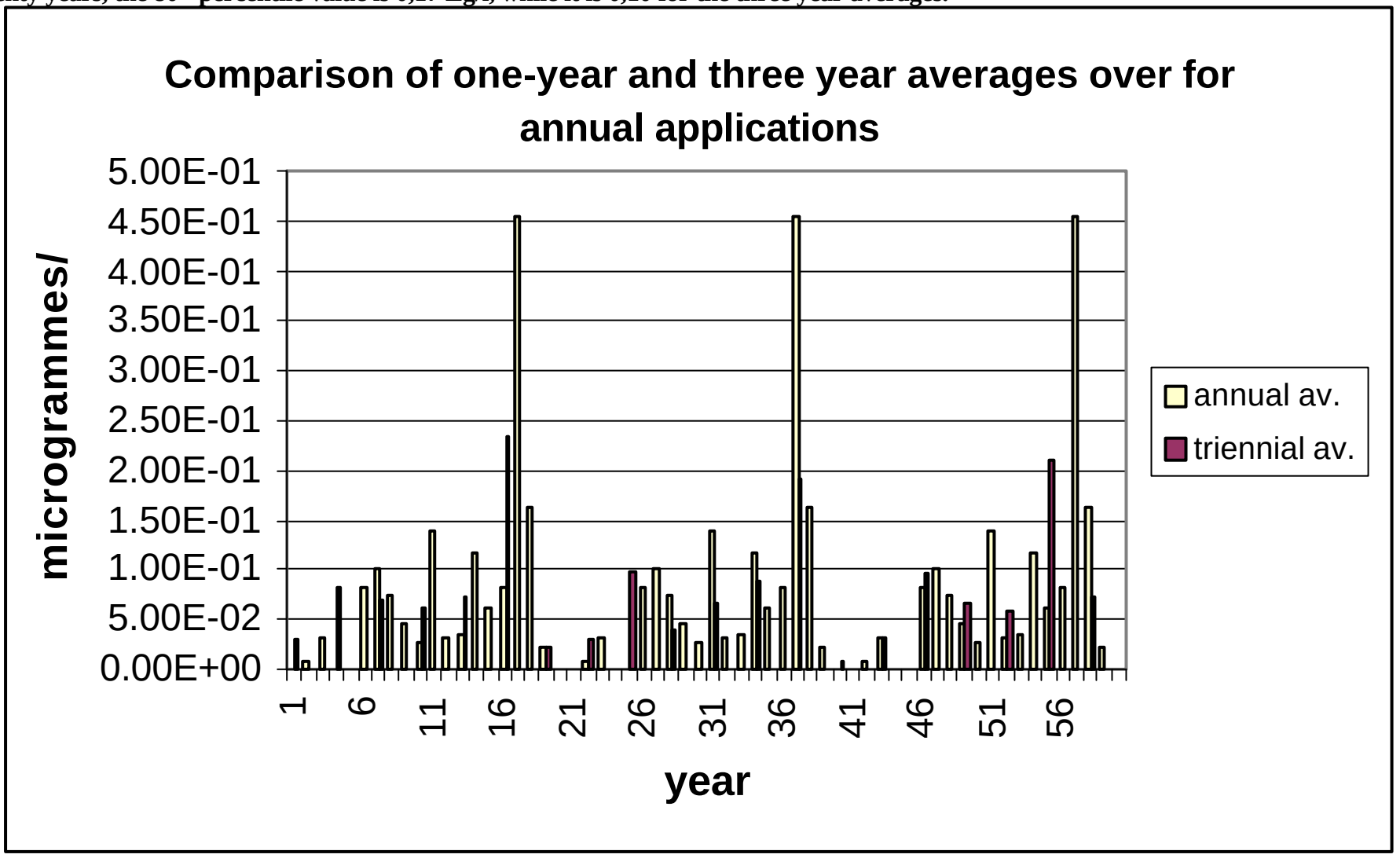


Figure 6.5 A 20 years leaching series is repeated three times and annual averages are compared with three-years averages. Result: Over twenty years, the 80th percentile value is 0,17 µg/l, while it is 0,10 for the three year averages.



6.5.3 Leaching when percolation is @ 0

Particularly for the models using Richards's equation as flow description, capillary rise may result in "strange" substance concentrations. If the net percolation is negative or zero, the substance concentration will be set to zero. If it is approximately zero, but positive, the substance load is divided with a small number, sometimes resulting in arbitrarily high concentrations. In practice, these concentrations are somewhat arbitrary, as a high concentration in hardly any water is not likely to affect the groundwater. As an example, the highest value shown in Figure 6.3 (approx. 130 µg/l) is obtained in a year with only 5 mm of percolation. A low recharge rate is usually also associated with a low mass flux to groundwater and, hence, also a low potential for contamination.

6.5.4 80 % criteria in dry climates

In a dry climate like Sevilla, the percolation is only positive in some years. This means that the number of leaching events will be less than 20. This distorts the statistics somewhat. As an example, if only eight leaching events take place over 20 years, the fourth highest will still be the determining concentration. However, the threat to the groundwater will depend on the amount leached, and that is only made up of eight events. Figure 6.6 and Table 6.3 show that while the fourth highest concentration is below 0.1 µg/l, the average concentration may be above 0.1 µg/l. This may, in fact, happen in all scenarios, but the likelihood is highest in the dry climates. However, as mentioned in the last section, these concentrations are somewhat arbitrary if percolation is near zero.

Figure 6.6 An example of a case where the average concentration in the water leached over 20 years exceeds 0.1 µg/l, while the 4th highest value is below the target quantity.

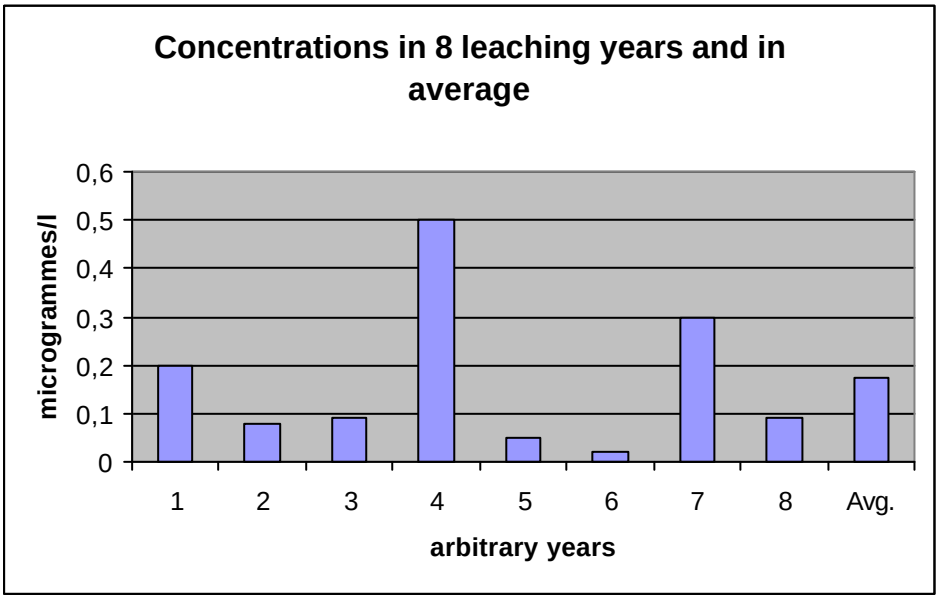


Table 6.3 Percolation, concentrations and loads used for calculating Figure 6.6

Percolation l/m2		Concentration µg/l	Total load µg/m^2
150		0.20	30.00
120		0.08	9.60
100		0.09	9.00
80		0.50	40.00
50		0.05	2.50
40		0.02	0.80
20		0.30	6.00
10		0.09	0.90
Sum:	570	Av. Conc: 0.17	Sum: 98.80

6.5.5 Calculation of mean annual concentrations

The mean annual concentration moving past a specified depth is the integral of the solute flux over the year (total amount of 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 is set to zero. 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, e.g. 1 m, the upward movement can result in an artificial overestimation of the predicted solute concentration in the case of these models.

6.6 Strategies to further reduce the uncertainty

The scenarios and modelling strategies recommended by the group are suitable for assessing the leaching potential of active substances at Tier 1 of the EU review procedure given the state of the art. However, as in all things, there is the potential for improvement. Certain steps to further reduce uncertainty have already been taken. Firstly, independent quality checks of the scenario files and model shells were performed, and identified problems were removed. Secondly, 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. Finally, a FOCUS version control group is being formed to eliminate mistakes and revise the scenarios as appropriate.

In addition to these steps, three further areas where improvements are possible have been identified:

- Review of the appropriateness of the scenario selection procedures
- Data set improvement: Soil profile analysis, and real weather data;
- Comparison of model results for virtual scenarios with reality, i.e. improving the validation status of the modelling for the different scenarios.

6.6.1 Scenario selection

Once suitable datasets are available, the scenario-sites and combinations between weather and soil could be critically reviewed in order to investigate what leaching risk they actually represent. A more detailed evaluation of vulnerability would require simulation of a (large) number of sites within each climatic region, with a few model substances, but this amount of work has not been feasible within the FOCUS framework. From such an evaluation, an "80% vulnerable soil" or soil/weather combination could be chosen on a more scientific basis. However, due to the fact that soil vulnerability depends on many factors, including the substance, this could result in a different number of scenarios to the present nine, and they might be different in character to the present scenarios. In practice, it may not be possible to validate the exact scenarios as they exist at the moment, as they are virtual scenarios which do not exactly represent any specific location which could be located.

6.6.2 Parameter estimation

The uncertainties linked to the use of soil and weather databases could be avoided by use of real values established for the scenario sites selected, however this might not increase their representativeness.

6.6.3 Model validation and parameter estimation

Model validation studies envisage quantifying the error that is made when predicting leaching with different leaching models. Complete validation of a computer model is, in principle, an impossible task (Oreskes *et al*, 1994; Refsgaard & Storm, 1996), as it has to be substantiated that it can be parameterised for a number of different sites with acceptable results. As a new site is always a bit different from an earlier test site it is never PROVEN that the computer model will perform adequately in the new situation. However, with many positive tests, the probability of success in a new site, with similar properties, increases. As substances have different properties and are subject to different reactions, it is also not proven that a model, which has been validated for one substance, will simulate a different substance correctly as well. The uncertainty related to the description of substance processes will be substance-dependent. It is not possible to remove this uncertainty factor, even if the model simulation of flow and conservative matter is perfect. Only through a number of simulations of substances with similar properties can this uncertainty be reduced. All the computer models included in the FOCUS work have been through validation exercises, and such work continues. However, the exercises documented so far represent a very limited number of cases (not least soil types), and results of such exercises are rather variable (see references in Section 1.2).

However, the issue is somewhat less complicated for a given scenario implemented for a given computer model. It is less complicated and time consuming to substantiate that this combination of model and scenario performs adequately.

The model parameters and model input considered in the finally selected scenarios could, in principle, be calibrated and validated against real data in order to comply with the local site conditions and in particularly the measured leaching fluxes (of water, conservative solute, and perhaps one or two substances). Stepwise validation protocols such as presented by Anderson and Woessner (1992), Styczen (1995), Thorsen (1998) and Vanclooster *et al*., 1999 could be adopted

to reduce the uncertainty associated with the parameters, model inputs algorithms and code, thus adding credibility to the simulation results. This may also provide some guidance for future model users regarding which model performs best in which scenario.

6.7 References

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